Second-order eikonal exchange amplitudes

T. T. Gien

Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada A1B 3X7 (Received 28 June 1985; revised manuscript received 31 March 1986)

The analytic expressions of the second-order eikonal exchange amplitudes are derived for electron-hydrogen scattering in both post and prior forms. In the case of the Glauber exchange amplitude, these expressions are shown to be reducible to closed forms. The results are applied to the calculation of elastic e-H(1s) scattering. Useful conclusions are drawn.

I. INTRODUCTION

In a recent paper¹ Franco and Halpern showed that the technique used earlier^{2,3} for approximating the Born exchange amplitude is not suitable for the eikonal-exchange amplitude and introduced a new method of approximation to be used in this case. The justification for the need to consider an approximation for the eikonal exchange amplitudes, even though this amplitude for electronhydrogen collision had been obtained^{4,5} in terms of the two-dimensional integral, was already expounded in the introductory part of another paper by Franco and Halpern.⁶ Besides providing much better approximate values for the amplitude in both the phase and the modulus, the new method of approximation yields, in particular, an exchange amplitude without an unwanted indeterminate phase contained in the previous technique.⁷⁻¹⁰ Essentially, the new method of approximation suggested an approximate expansion of the eikonal exchange amplitude around the position of one of the electrons instead of relying on the Bonham-Ochkur type of expansion^{2,3} for the factor $e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}/|\mathbf{r}_1-\mathbf{r}_2|$ of the amplitude as the previous technique did. Subsequently,¹¹ we pointed out that the contribution from the so-called electron-nucleus scattering term to the exchange amplitude is quite significant and thereby cannot be excluded in the approximation. In their subsequent work,^{6,12} Franco and Halpern included the first-order contribution of the expansion to the approximate amplitude and succeeded in dramatically improving the accuracy of their analytic approximations. They showed, in particular, that the contribution from the electron-nucleus scattering term only starts to become significant from this first-order correction and that their first-order eikonal exchange amplitude can provide both the modulus and the phase in remarkably good agreement with those of the exact eikonal exchange amplitude over a wide range of energies and scattering angles.

In view of the amazing success of the method, it is very tempting to include the next-order correction to the approximate amplitude. In this work, we shall, therefore, obtain the second-order eikonal exchange amplitude in the Franco-Halpern approximation. In Sec. II we derive the analytic expressions for both post and prior forms. We show that in the case of the Glauber exchange amplitude, these terms can be put in closed forms which can therefore be computed quite easily and fast. In Sec. III we specialize our general results to elastic scattering from the ground state of hydrogen. Finally, the results of numerical calculation of elastic scattering in the Glauber approximation are presented with discussion in Sec. IV. It may be worth mentioning that although the eikonal exchange amplitude is just one of the many forms used in the literature to approximate the exchange amplitude, it should, for the sake of consistency, be employed preferably in the eikonal and eikonal-related calculations where the direct eikonal scattering amplitude has been known to work remarkably well for e^{\pm} -atom scattering at intermediate energies.

II. SECOND-ORDER CORRECTIONS TO THE EIKONAL EXCHANGE AMPLITUDE

The post and prior forms of the eikonal exchange amplitude are, respectively,^{1,6}

$$g_{fi}^{+}(\mathbf{k}_{i},\mathbf{k}_{f}) = -\frac{1}{2\pi} \int d\mathbf{r}_{1} d\mathbf{r}_{2} e^{-i\mathbf{k}_{f}\cdot\mathbf{r}_{2}} \phi_{f}^{*}(\mathbf{r}_{1})$$

$$\times \left[\frac{1}{r_{12}} - \frac{1}{r_{2}}\right] e^{i\mathbf{k}_{i}\cdot\mathbf{r}_{1}}$$

$$\times \phi_{i}(\mathbf{r}_{2}) \left[\frac{\mathbf{r}_{12} - \mathbf{r}_{12}\cdot\hat{\mathbf{z}}}{r_{1} - \mathbf{r}_{1}\cdot\hat{\mathbf{z}}}\right]^{i\eta_{i}} \qquad (1a)$$

and

$$g_{fi}^{-}(\mathbf{k}_{i},\mathbf{k}_{f}) = -\frac{1}{2\pi} \int d\mathbf{r}_{1} d\mathbf{r}_{2} e^{-i\mathbf{k}_{f}\cdot\mathbf{r}_{2}} \phi_{f}^{*}(\mathbf{r}_{1})$$

$$\times \left[\frac{1}{r_{12}} - \frac{1}{r_{1}}\right] e^{i\mathbf{k}_{i}\cdot\mathbf{r}_{1}}$$

$$\times \phi_{i}(\mathbf{r}_{2}) \left[\frac{r_{12} - \mathbf{r}_{12}\cdot\hat{\mathbf{z}}}{r_{2} + \mathbf{r}_{2}\cdot\hat{\mathbf{z}}}\right]^{i\eta_{f}}, \quad (1b)$$

where $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ and $\eta_{i,f} = 1/k_{i,f}$. These amplitudes may be separated into two terms, the electron-electron (corresponding to $1/r_{12}$) and the electron-nucleus (corre-

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sponding to $1/r_2$ or $1/r_1$) scattering term.

Following the same procedure of approximation as described in Franco and Halpern's papers^{1,6} we change the variables of integration from $(\mathbf{r}_1, \mathbf{r}_2)$ to either $(\mathbf{r}_{12}, \mathbf{r}_2)$ or $(\mathbf{r}_1, \mathbf{r}_{12})$ and then expand the integrands in Eq. (1a) and (1b) around $\mathbf{r}_{12}=\mathbf{0}$ to obtain the second-order correction for the approximate eikonal exchange amplitudes. For post exchange the first case was referred to by Franco and Halpern⁶ as case *I* of the approximation while the second was referred to as case *F*. With the initial- and final-state wave functions ϕ_i and ϕ_f given in the forms

$$\phi_{i} = D_{i}(\mu, \tau)(e^{i\tau \cdot \mathbf{r} - \mu r}) \mid_{\tau=0},$$

$$\phi_{f} = D_{f}(\beta, \lambda)(e^{i\lambda \cdot \mathbf{r} - \beta r}) \mid_{\lambda=0}$$
(2)

where $D_i(\mu, \tau)$ and $D_f(\beta, \lambda)$ are the appropriate differential operators, we obtain, after some very tedious derivations, the following expressions for the second-order correction to the electron-electron scattering term of the post and prior eikonal exchange amplitudes in case I (the upper sign is for post and the lower sign is for prior exchange),

$$g_{fi}^{\pm(2)} = \frac{1}{4\pi} D_{if} \left[[(\mathbf{q} \cdot \nabla_{k_{\pm}})(\mathbf{q} \cdot \mathbf{f}_{\pm}) + 2(\mathbf{q} \cdot \nabla_{k_{\pm}})(\lambda_{\pm} \cdot \mathbf{f}_{\pm}) + (\lambda_{\pm} \cdot \nabla_{k_{\pm}})(\lambda_{\pm} \cdot \mathbf{f}_{\pm})] \frac{d}{d\beta} M(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, i\eta_{\pm}) \right] \\ - 2\gamma_{\pm} (\mathbf{q} \cdot \nabla_{k_{\pm}} + \lambda_{\pm} \cdot \nabla_{q}) [\mathbf{f}_{\pm} \cdot \nabla_{q} M(\mathbf{q} + \tau + \lambda, \beta + \mu, \pm \hat{\mathbf{z}}, i\eta_{\pm})] \\ + \gamma_{\pm} \frac{d^{2}}{d\delta^{2}} M(k_{\pm}, \delta, \hat{\mathbf{z}}, -i\eta_{\pm}) |_{\delta=0} M(\mathbf{q} + \tau + \lambda, \beta + \mu, \pm \hat{\mathbf{z}}, i\eta_{\pm}) \\ - \gamma_{\pm}^{2} i K(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, \mathbf{f}_{\pm}, i\eta_{\pm}) - \gamma_{\pm} i L(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, \mathbf{f}_{\pm}, i\eta_{\pm}) \right|_{\tau=\lambda=0},$$
(3a) ere

where

$$\mathbf{f}_{\pm} = \nabla_{k_{\pm}} M(\mathbf{k}_{\pm}, \mathbf{0}, \mathbf{\hat{z}}, -i\eta_{\pm}) . \tag{3b}$$

In Eq. (3) we use the same notations used by Franco and Halpern,⁶ namely,

$$\lambda_{+} \equiv \tau , \ \mathbf{k}_{+} \equiv \mathbf{k}_{i} , \ \gamma_{+} \equiv \mu , \ \eta_{+} \equiv \eta_{i} ,$$

$$\lambda_{-} \equiv \lambda , \ \mathbf{k}_{-} \equiv \mathbf{k}_{f} , \ \gamma_{-} \equiv \beta , \ \eta_{-} \equiv \eta_{f} ,$$

$$D_{if} \equiv D_{i}(\mu, \tau) D_{f}(\beta, \lambda) .$$
(4)

 $M(\mathbf{A},d,\hat{\mathbf{z}},i\eta), K(\mathbf{A},d,\hat{\mathbf{z}},\mathbf{f},i\eta)$, and $L(\mathbf{A},d,\hat{\mathbf{z}},\mathbf{f},i\eta)$ are shown to be expressed in the following forms:

$$M(\mathbf{A},d,\hat{\mathbf{z}},i\eta) = 4\pi\Gamma(1-i\eta)(\mathbf{A}^{2}+d^{2})^{i\eta-1}(2d-2i\mathbf{A}\cdot\hat{\mathbf{z}})^{-i\eta},$$

$$K(\mathbf{A},d,\hat{\mathbf{z}},\mathbf{f},i\eta) = 4\pi\Gamma(1-i\eta)2^{-i\eta}\{-2i(i\eta-1)(\nabla_{k}\cdot\mathbf{f})u(\mathbf{A},d,i\eta-2,i\eta)$$

$$+2i\eta(i\eta-1)[\hat{\mathbf{z}}\cdot\nabla_{k}(\mathbf{f}\cdot\mathbf{A}) + \mathbf{A}\cdot\nabla_{k}(\mathbf{f}\cdot\hat{\mathbf{z}})]u(\mathbf{A},d,i\eta-2,i\eta+1)$$

$$-4i(i\eta-1)(i\eta-2)[\mathbf{A}\cdot\nabla_{k}(\mathbf{f}\cdot\mathbf{A})]u(\mathbf{A},d,i\eta-3,i\eta)$$

$$-\eta(i\eta+1)[\hat{\mathbf{z}}\cdot\nabla_{k}(\mathbf{f}\cdot\hat{\mathbf{z}})]u(\mathbf{A},d,i\eta-1,i\eta+2)\}$$
(5b)

and

$$L(\mathbf{A}, d, \mathbf{\hat{z}}, \mathbf{f}, i\eta) = 4\pi \Gamma(1 - i\eta) 2^{-i\eta} \{-2i(i\eta - 1)(\nabla_{k} \cdot \mathbf{f})v(\mathbf{A}, d, i\eta - 2, i\eta) + 2i\eta(i\eta - 1)[\mathbf{\hat{z}} \cdot \nabla_{k}(\mathbf{f} \cdot \mathbf{A}) + \mathbf{A} \cdot \nabla_{k}(\mathbf{f} \cdot \mathbf{\hat{z}})]v(\mathbf{A}, d, i\eta - 2, i\eta + 1) - 4i(i\eta - 1)(i\eta - 2)\mathbf{A} \cdot \nabla_{k}(\mathbf{f} \cdot \mathbf{A})v(\mathbf{A}, d, i\eta - 3, i\eta) - \eta(i\eta + 1)\mathbf{\hat{z}} \cdot \nabla_{k}(\mathbf{f} \cdot \mathbf{\hat{z}})v(\mathbf{A}, d, i\eta - 1, i\eta + 2)\},$$
(5c)

where the functions $u(\mathbf{A}, d, a, b)$ and $v(\mathbf{A}, d, a, b)$ are defined as

$$u(\mathbf{A}, d, a, b) \equiv \int_0^\infty d\theta [\mathbf{A}^2 + (d+\theta)^2]^a (d+\theta - i \mathbf{A} \cdot \hat{\mathbf{z}})^{-b} , \qquad (6a)$$

$$v(\mathbf{A}, d, a, b) \equiv \int_0^\infty \int_0^\infty d\theta \int_0^\infty d\phi [\mathbf{A}^2 + (d + \theta + \phi)^2]^a (d + \theta + \phi - i\mathbf{A}\cdot\hat{\mathbf{z}})^{-b} .$$
(6b)

For the conventional Glauber amplitude where the direction of the momentum transfer is chosen to be perpendicular to the \hat{z} direction $(\mathbf{q}\cdot\hat{\mathbf{z}}=0)$, we succeed in putting both these functions in closed forms. $u(\mathbf{q},d,a,b)$ is expressed in terms of a hypergeometric function as

$$u(\mathbf{q},d,a,b) = \frac{d^{2a+1-b}}{b-1-2a} {}_{2}F_{1}\left[-a,\frac{b-1}{2}-a;\frac{b+1}{2}-a;-\frac{q^{2}}{d^{2}}\right],$$
(7)

while the method of reduction of v(q,d,a,b) to a closed form and its closed-form expression are shown in the Appendix. On the other hand, the second-order correction for the electron-nucleus scattering is found to be

$$h_{fi}^{\pm(2)} = \pm \frac{1}{2\pi} D_{if} \{ (\mathbf{q} + \lambda_{\pm}) \cdot l_{\pm} M(\mathbf{q} + \tau + \lambda, \beta + \mu, \pm \hat{\mathbf{z}}, i\eta_{\pm}) + iH(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, l_{\pm}, i\eta_{\pm}) + i\gamma_{\pm} G(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, l_{\pm}, i\eta_{\pm}) \} |_{\lambda = \tau = 0}, \qquad (8)$$

where

$$I_{\pm} = \nabla_{k_{\pm}} \frac{d}{d\delta} M(\mathbf{k}_{\pm}, \delta, \hat{\mathbf{z}}, -i\eta_{\pm}) |_{\delta=0},$$

$$G(\mathbf{A}, d, \hat{\mathbf{z}}, \mathbf{l}, i\eta) = 4\pi \Gamma(1 - i\eta) 2^{-i\eta} [-2i(i\eta - 1)(\mathbf{l} \cdot \mathbf{A})u(\mathbf{A}, d, i\eta - 2, i\eta) + i\eta(\mathbf{l} \cdot \hat{\mathbf{z}})u(\mathbf{A}, d, i\eta - 1, i\eta + 1)]$$
(9)

and

$$H(\mathbf{A}, d, \hat{\mathbf{z}}, \mathbf{l}, i\eta) = 4\pi\Gamma(1 - i\eta)2^{-i\eta} [-2i(i\eta - 1)(\mathbf{l} \cdot \mathbf{A})v(\mathbf{A}, d, i\eta - 2, i\eta) + i\eta(\mathbf{l} \cdot \hat{\mathbf{z}})v(\mathbf{A}, d, i\eta - 1, i\eta + 1)].$$
(10)

In case F we obtained the following expressions for the second-order corrections to the electron-electron and electronnucleus scattering terms, respectively:

$$\overline{g}_{fi}^{\pm(2)} = \frac{1}{4\pi} D_{if} \left[(\lambda_{\pm} \cdot \nabla_{k_{\mp}}) (\lambda_{\pm} \cdot \mathbf{f}'_{\pm}) \frac{d}{d\beta} M(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \mathbf{\hat{z}}, i\eta_{\pm}) - 2\gamma_{\pm} (\lambda_{\pm} \cdot \nabla_{q}) [\mathbf{f}'_{\pm} \cdot \nabla_{q} M(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \mathbf{\hat{z}}, i\eta_{\pm})] \right] \\ + \gamma_{\pm} \frac{d^{2}}{d\delta^{2}} M(\mathbf{k}_{\mp}, \delta, -i\eta_{\pm}) |_{\delta=0} M(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \mathbf{\hat{z}}, i\eta_{\pm}) - i\gamma_{\pm}^{2} K(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \mathbf{\hat{z}}, \mathbf{f}'_{\pm}, i\eta_{\pm}) \\ - i\gamma_{\pm} L(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \mathbf{\hat{z}}, \mathbf{f}'_{\pm}, i\eta_{\pm}) \right] \Big|_{\tau=\lambda=0}$$

$$(11)$$

and

$$\overline{h}_{fi}^{\pm(2)} = \pm \frac{1}{2\pi} D_{if} [(\lambda_{\pm} \cdot l'_{\pm}) M(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, i\eta_{\pm}) + i\gamma_{\pm} G(\mathbf{q} + \lambda + \tau, \beta + \mu, \pm \hat{\mathbf{z}}, l'_{\pm}, i\eta_{\pm})$$

$$+iH(\mathbf{q}+\boldsymbol{\lambda}+\boldsymbol{\tau},\boldsymbol{\beta}+\boldsymbol{\mu},\pm\hat{\mathbf{z}},\boldsymbol{l}'_{\pm},i\eta_{\pm})]|_{\boldsymbol{\lambda}=\boldsymbol{\tau}=\mathbf{0}},$$

where

$$\mathbf{f}_{\pm}' = \nabla_{k_{\pm}} M(\mathbf{k}_{\pm}, 0, \hat{\mathbf{z}}, -i\eta_{\pm}) , \qquad (13a)$$

$$l'_{\pm} = \nabla_{k_{\mp}} \frac{d}{d\delta} M(\mathbf{k}_{\mp}, \delta, \hat{\mathbf{z}}, -i\eta_{\pm}) \mid_{\delta=0} .$$
 (13b)

It is worth mentioning that with a similar procedure of approximation, one can also obtain equivalent forms for $g_{fi}^{\pm(2)}$, $h_{fi}^{\pm(2)}$, $\overline{g}_{fi}^{\pm(2)}$, and $\overline{h}_{fi}^{\pm(2)}$ which are expressed in terms of the functions K and G only if in the process of reduction, one performs an integration by parts for the relevant expressions only once. In the case of eikonal exchange amplitude, the latter forms are somewhat easier to calculate as the functions K and G are expressed in terms of some one-dimensional integrals only. It should also be stressed that the formulas obtained above for the second-order correction terms are quite general and valid for both the eikonal and Glauber exchange amplitudes as well as for arbitrary initial and final states of the hydrogen atom. It is also easy to verify that there is no post and prior discrepancy in the second-order Glauber ($q \perp \hat{z}$) and eikonal exchange amplitudes provided that we choose the \hat{z} direction as that of \mathbf{k}_i for post exchange and as that of \mathbf{k}_f

for prior exchange in the case of eikonal exchange amplitude.

III. ELASTIC SCATTERING

In this section we apply the general results obtained above to derive the second-order Glauber exchange amplitude $(q \perp \hat{z})$ for elastic scattering by a hydrogen atom in its ground state. In this case

$$\beta = \mu = 1 , \quad \eta_i = \eta_f = \eta , \quad k_i = k_f = k ,$$

$$\tau = \lambda = 0 , \quad D_{if} = \frac{1}{\pi} .$$
 (14)

Consequently, we have

$$\mathbf{q} \cdot \mathbf{k}_{i} = -\mathbf{q} \cdot \mathbf{k}_{f} = \frac{q^{2}}{2} , \quad q = 2k \sin \frac{\theta}{2}$$
$$\mathbf{k}_{f} \cdot \hat{\mathbf{k}}_{i} = \hat{\mathbf{k}}_{i} \cdot \hat{\mathbf{k}}_{f} = k \cos \frac{\theta}{2} , \quad \mathbf{q} \cdot \hat{\mathbf{z}} = 0$$
$$\mathbf{k}_{i} \cdot \hat{\mathbf{z}} = \mathbf{k}_{f} \cdot \hat{\mathbf{z}} = k \cos \frac{\theta}{2} .$$
(15)

Both case I and case F of the approximation are considered. The second-order term of the electron-electron scattering in case I is found to be

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<u>34</u>

(12)

$$g_{fi}^{G(2)} = \overline{g}_{fi}^{G(2)} + \frac{4\pi\eta}{\sinh(\pi\eta)} e^{(\pi/2)\eta} (k^2)^{-i\eta-2} \left[k \cos\frac{\theta}{2} \right]^{i\eta-1} q^2 (i\eta+1) \\ \times \left[(q^2+4)^{i\eta-1} 2^{-i\eta} \left[-i\frac{q^2}{2k^2} (i\eta+2)\cos\frac{\theta}{2} + i\cos\frac{\theta}{2} + \frac{2}{k} (i\eta+2)\cos^2\frac{\theta}{2} - \frac{i}{k^2} \right] \\ - 8\eta (i\eta-1) \left[-2(i\eta+2)\cos^2\frac{\theta}{2} + i\eta \right] \left[u(\mathbf{q},2,i\eta-2,i\eta+1) + v(\mathbf{q},2,i\eta-2,i\eta+1) \right] \right],$$
(16)

where $\overline{g}_{fi}^{G(2)}$ is the second-order electron-electron scattering term in case F,

$$\overline{g} \, \overline{f}_{l}^{Q(2)} = \frac{4\pi\eta}{\sinh(\pi\eta)} e^{(\pi/2)\eta} (k^{2})^{-i\eta-2} \left[k \cos\frac{\theta}{2} \right]^{1/2} \\ \times \left[-2^{-i\eta} (q^{2}+4)^{i\eta-1} k^{2} \left[2(i\eta+1)\cos^{2}\frac{\theta}{2} + i\eta(i\eta-1) \right] \\ -2k^{2}(i\eta-1) \left[2(i\eta+1)\cos^{2}\frac{\theta}{2} + i\eta(i\eta-1) \right] \left[u(q,2,i\eta-2,i\eta) + v(q,2,i\eta-2,i\eta) \right] \\ -4(1+\eta^{2})q^{2}\cos\frac{\theta}{2} \left[-2(i\eta+2)\cos^{2}\frac{\theta}{2} + i\eta \right] \left[u(q,2,i\eta-2,i\eta+1) + v(q,2,i\eta-2,i\eta+1) \right] \\ +8(1+\eta^{2})(i\eta-2)q^{2}k^{2}\cos^{2}\frac{\theta}{2} \left[(i\eta+2)\frac{q^{2}}{2k^{2}} - 1 \right] \left[u(q,2,i\eta-3,i\eta) + v(q,2,i\eta-3,i\eta) \right] \\ +ik(i\eta+1) \left[i\eta(i\eta-1) - 2(i\eta+1)(2i\eta+1)\cos^{2}\frac{\theta}{2} + 4(i\eta+1)(i\eta+2)\cos^{4}\frac{\theta}{2} \right] \\ \times \left[u(q,2,i\eta-1,i\eta+1) + v(q,2,i\eta-1,i\eta+2) \right] \right].$$
(17)

The second-order electron-nucleus scattering term in case I is

$$h_{fi}^{G(2)} = \bar{h}_{fi}^{G(2)} + \frac{8\pi\eta}{\sinh(\pi\eta)} e^{(\pi/2)\eta} (k^2)^{-i\eta-2} \left[k \cos\frac{\theta}{2} \right]^{i\eta-2} \cos\frac{\theta}{2} (i\eta+1)q^2 \\ \times \left\{ 4(i\eta-1) [u(\mathbf{q},2,i\eta-2,i\eta) + v(\mathbf{q},2,i\eta-2,i\eta)] + (q^2+4)^{i\eta-1}2^{-i\eta} \right\},$$
(18)

where $\overline{h}_{fi}^{G(2)}$ is the corresponding term in case F and is given by

$$\overline{h}_{fi}^{G(2)} = \frac{8\pi\eta}{\sinh(\pi\eta)} e^{(\pi/2)\eta} (k^2)^{-i\eta-2} \left[k \cos\frac{\theta}{2} \right]^{i\eta-2} \\ \times \left[-2(i\eta-1)(i\eta+1)\cos\frac{\theta}{2}q^2 [u(\mathbf{q},2,i\eta-2,i\eta)+v(\mathbf{q},2,i\eta-2,i\eta)] + \left[i\eta-1-2(i\eta+1)\cos^2\frac{\theta}{2} \right] [u(\mathbf{q},2,i\eta-1,i\eta+1)+v(\mathbf{q},2,i\eta-1,i\eta+1)] \right].$$
(19)

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In comparison to the first-order terms,⁶ these expressions are also relatively simple. The calculation of these closed-form second-order amplitudes can, therefore, be done quite easily and fast.

IV. NUMERICAL RESULTS AND DISCUSSION

For the zeroth- and first-order Glauber exchange amplitude we use the results of Franco and Halpern.⁶ Equations (16), (17), (18), and (19) are employed to evaluate the second-order electron-electron and electron-nucleus scattering terms. To verify the correctness of the closed forms derived for the functions u and v, we have tentatively calculated these functions with the use of both their closed and integral forms and have found that the two results of calculation agree with each other within the numerical error of a relative order of 10^{-6} .

In Figs. 1-4 we display the results of our calculations

for the phases and the moduli of the zeroth-, first-, and second-order Glauber exchange amplitudes at small and large scattering angles. Except at 100 eV, we present only the results of case I for small angles since the values for cases F and I are very close. For large angles and at energies about 200 eV and above, we display the values of the moduli of the second-order exchange amplitudes in case Ionly since the values of cases I and F are also very close to each other. The phases of the amplitude at large scattering angles are, however, presented for both cases Iand F.

We find that at energies of 200 eV and above, the inclusion of the second-order correction terms shows a clear improvement in the agreement of the approximate amplitude with its exact one at large scattering angles $(30^\circ-60^\circ)$ for both the modulus and the phase. The agreement of the second-order Glauber exchange amplitude with its exact one is excellent at scattering angles of 30° and smaller.

Glauber. (d) Same as in (c) for moduli at large scattering angles $(20^\circ - 60^\circ)$.

In general, the second-order values of case I agree better with the exact ones than those of case F. At lower energies, the second-order approximation tends to overestimate the exact values of the modulus a bit at small scattering angles while the first-order one tends to underestimate them a bit [see Fig. 2(c)].

At scattering energies of 100 eV and below, the second-order exchange amplitude worsens the agreement with the exact amplitude somewhat at scattering angles of $0^{\circ}-30^{\circ}$. However, in comparison to the zeroth-order approximation amplitude, the agreement of the second-order amplitude with the exact one is still very much improved. In fact, the values of the modulus of the second-order amplitude at 100 eV are of the order of 80-90% of those of the exact amplitude in this range of scattering angles. The difference between the phases also does not exceed 3° . It should be warned that the differences falsely appear to be great with the scale of the graph used in Figs. 1(a) and

(b)

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AMP. PHASE - TT

-0. 10 15 20 25 30 40 50 60 SCATTERING ANGLE (deg) SCATTERING ANGLE (deg) (d) 0.4 0.20 (c) AMP. MODULUS (a. u.) 0 (a. u.) MODULUS 0.100 0.25 UN 0.20 0.05 0.02 0.15L SCATTERING ANGLE (deg) 20 20 30 50 40 SCATTERING ANGLE (deg) FIG. 1. (a) Elastic e-H(1s) scattering. Comparison of phases of zeroth-, first- and second-order analytic approximations to Glauber exchange amplitude with those of the exact Glauber amplitude as function of scattering angles $(0^{\circ}-25^{\circ})$ at 100 eV. zeroth order; --, first order, case $I; \cdots$, second order, case $I; \cdots$, first order, case $F; \cdots$, second order, case F; -exact Glauber. (b) Same as in (a) at large scattering angles (20°-60°) and at 100 eV. (c) Comparison of moduli of zeroth-, first-, and second-order analytic approximations (case I) to Glauber exchange amplitude with those of the exact numerical Glauber amplitude as function of scattering angles $(0^{\circ}-25^{\circ})$ at 100 eV. ——, zeroth order; – –, first order; · · · , second order; —, exact

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(a)



1(c). Considering the fact that there is some difference in the values among the zeroth-, first- and second-order approximations, and that the zeroth- and second-order approximations tends to overestimate the values of the modulus of the exact amplitude at small scattering angles while the first-order one tends to underestimate them, we believe that the series expansion used in the method of approximation seems to converge more slowly at low energy, but there also seems to be a tendency for the terms of consecutive order to cancel each other. The slow convergence of the series expansion at low energy is also seen to reflect in the more significant difference between the first-order values of the phase in cases I and F [Figs. 1(a) and 1(b)]. Although the phases of the second-order exchange amplitude do not agree with the exact ones as well as those of the first order at small angles and low energies, the second-order values in cases I and F tend to be more consistent with each other in both ranges of scattering angles, large and small [see Figs. 1(a), 1(b) and 1(d)]. Therefore we conjecture that in order to improve the approximate eikonal exchange amplitude at low energy significantly,

one would need to choose the right place to stop the series expansion of the amplitude and the next more suitable stop would probably be at the third-order one. However, handling the third-order exchange amplitude may be too tedious a job and it may therefore no longer be worth the effort to carry out the approximation further. At energies of 200 eV and above, the second-order exchange amplitude definitely provides an improvement over the firstorder one for both the phase and the modulus of the amplitude in a wider range of angles. Thus, the second-order eikonal exchange amplitude may safely be used in place of the first-order one for a wider range of scattering angles and at energies of 200 eV and above.

Equations (16) and (17) show that the second-order electron-electron scattering term in both cases I and F falls off as k^{-4} at large k. Since these second-order terms also depend on $q^2\cos^{-2}(\theta/2)$ in the form of a factor, it is therefore expected that their contribution to the second-order eikonal exchange amplitude increases significantly at large scattering angles. This is exactly the same situation one encounters in the first-order eikonal exchange

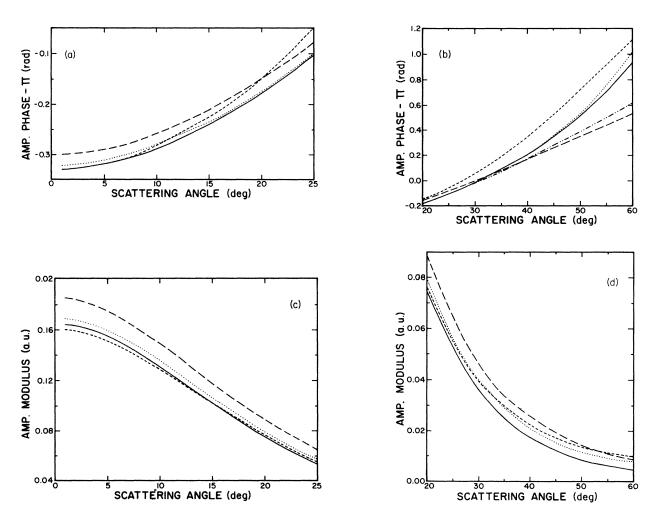


FIG. 2. (a) Same as in Fig. 1(a) at 200 eV. (b) Same as in Fig. 1(b) at 200 eV. The first-order values in case F are very close (at this scale of the graph) to those of the zeroth order and are thereby not displayed. (c) Same as in Fig. 1(c) at 200 eV. (d) Same as in Fig. 1(d) at 200 eV (case I).

amplitude determination. Therefore, both the first- and second-order eikonal exchange amplitudes may, as expected, not work too well at large scattering angles. However, if one sticks to the small scattering angle area for which the Glauber approximation is essentially designed, the Franco-Halpern approximation seems to work remarkably well, and in general the range of angles where the approximation is accurate could be extended significantly when the second-order amplitude is used in place of the firstorder one. It is also possible to see that the difference between the second-order electron-electron scattering terms in cases I and F falls off as k^{-5} . Again, since some of the terms of the difference depend linearly on q^2 or on $\cos^{-2}(\theta/2)$, this difference increases at large scattering angles and decreases at small scattering angles. Consequently, the approximate values in cases I and F are almost identical at small scattering angles and only differ significantly from each other at larger angles.

Through Eqs. (18) and (19) one can see that the second-order electron-nucleus scattering term of both cases I and F falls off as k^{-6} . It should be stressed that although the order of falling off in k^{-1} of this term is higher than that of the electron-electron scattering counterpart, the contribution from this term to the second-

order eikonal exchange amplitude at lower intermediate energies is in no way less significant. This is because at a reasonably low energy, say 50 eV, the value of k^{-1} in a.u. is about 0.52 and with that value of k^{-1} , the reduction of a term of one or two orders higher in k^{-1} can easily be made up either by a coefficient of great value of the term or by the summation of a great number of these terms. Thus, at lower energies, the leading degree of falling off in k^{-1} of a term should not be used as an absolute mean to distinguish the size of that term in the scattering amplitude. A term of higher order of falling off in k^{-1} will be small in value only when the scattering energy is sufficiently high. Even at these high energies, since many of these terms of higher order of falling off in k^{-1} also depend linearly on q^2 or on $\cos^{-2}(\theta/2)$, the relative magnitudes of these terms should depend as well on whether they are compared at small or large scattering angles.

In Tables I and II we display the real and imaginary parts of the second-order electron-electron and electronnucleus scattering terms in case I at 100 and 1600 eV respectively, while in Table III the real and imaginary parts of the zeroth-, first-, and second-order terms of the Glauber exchange amplitude in case I at 100 eV are shown. We see that the magnitudes of the second-order

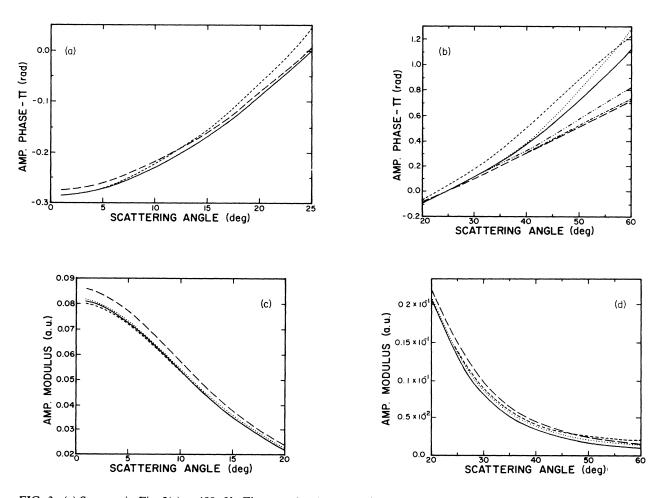


FIG. 3. (a) Same as in Fig. 2(a) at 400 eV. The second-order curve almost coincides with the exact one and is thereby not shown. (b) Same as in Fig. 1(b) at 400 eV. (c) Same as in Fig. 2(c) at 400 eV. (d) Same as in Fig. 2(d) at 400 eV.

TABLE I. The real and imaginary parts of the electron-electron and electron-nucleus scattering terms in the second-order Glauber exchange amplitude at 100 eV (case I). The numbers in the square

brackets are powers of 10. Angles Real part of Imaginary part Real part of Imaginary part (deg) e-e term of e-e term e-N term of e-N term 1 -0.296[-1] 0.906[-2] -0.2783[-1]-0.12545[-1] 2 -0.294[-1] 0.911[-2]-0.2780[-1] -0.12538[-1]3 -0.291[-1] 0.919[-2]-0.2776[-1]-0.12526[-1] 5 -0.1249[-1]-0.281[-1]0.945[-2]-0.276[-1] 7 -0.265[-1]0.985[-2] -0.274[-1]-0.1243[-1]10 -0.236[-1]0.107[-1] -0.270[-1]-0.123[-1]15 -0.175[-1]0.126[-1] -0.260[-1]-0.120[-1]20 -0.112[-1]0.149[-1]-0.249[-1]-0.116[-1]25 -0.555[-2]0.174[-1]-0.238[-1]-0.110[-1]30 -0.111[-2]0.195[-1] -0.227[-1]-0.104[-1]40 0.452[-2]0.219[-1] -0.209[-1]-0.886[-2]50 0.787[-2]0.209[-1]-0.199[-1]-0.714[-2]60 0.112[-1]0.169[-1] -0.196[-1] -0.534[-2]70 0.158[-1]0.105[-1]-0.199[-1] -0.347[-2]0.250[-2] 80 0.220[-1] -0.209[-1]-0.149[-2]-0.664[-2]90 0.294[-1] -0.226[-1]0.687[-3]

-0.166[-1]

-0.252[-1]

0.323[-2]

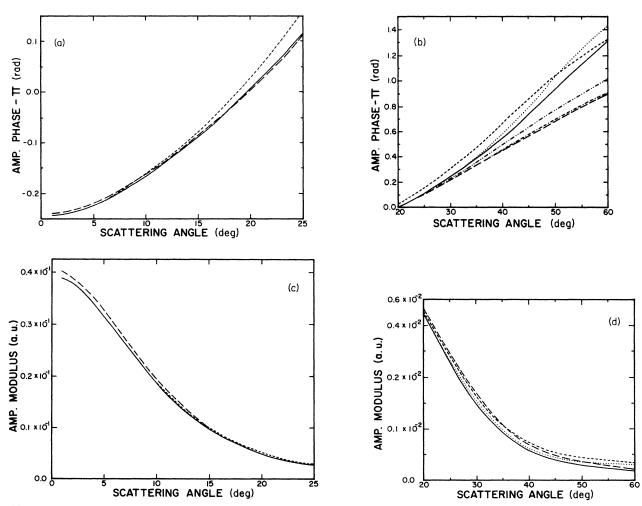


FIG. 4. (a) Same as in Fig. 2(a) at 800 eV. The second-order curve almost coincides with the exact one and is thereby not displayed. (b) Same as in Fig. 1(b) at 800 eV. (c) Same as in Fig. 2(c) at 800 eV. The second-order curve almost coincides with the exact one and is thereby not shown. (d) Same as in Fig. 2(d) at 800 eV.

100

0.375[-1]

Angles (deg)	Real part of e-e term	Imaginary part of <i>e-e</i> term	Real part of e-N term	Imaginary part of <i>e</i> -N term
1	-0.533[-4]	0.168[-4]	-0.624[-5]	0.110[-6]
2	-0.465[-4]	0.163[-4]	-0.615[-5]	0.102[-6]
3	-0.366[-4]	0.159[-4]	-0.600[-5]	0.919[-7]
5	-0.127[-4]	0.145[-4]	-0.560[-5]	0.678[-7]
7	0.869[-5]	0.144[-4]	-0.513[-5]	0.498[-7]
10	0.281[-4]	0.163[-4]	-0.446[-5]	0.462[-7]
15	0.351[-4]	0.206[-4]	-0.357[-5]	0.942[-7]
20	0.304[-4]	0.230[-4]	-0.297[-5]	0.174[-6]
25	0.242[-4]	0.234[-4]	-0.256[-5]	0.262[-6]
30	0.188[-4]	0.224[-4]	-0.227[-5]	0.349[-6]
40	0.119[-4]	0.177[-4]	-0.189[-5]	0.512[-6]
50	0.871[-5]	0.109[-4]	-0.168[-5]	0.664[-6]
60	0.787[-5]	0.258[-5]	-0.156[-5]	0.813[-6]
70	0.854[-5]	-0.666[-5]	-0.149[-5]	0.965[-6]
80	0.102[-4]	-0.165[-4]	-0.148[-5]	0.113[-5]
90	0.124[-4]	-0.267[-4]	-0.152[-5]	0.132[-5]
100	0.148[-4]	-0.369[-4]	-0.161[-5]	0.154[-5]

TABLE II. The real and imaginary parts of the electron-electron and electron-nucleus scattering terms in the second-order Glauber exchange amplitude at 1600 eV (case *I*). The numbers in the square brackets are powers of 10.

electron-electron and electron-nucleus scattering terms at 100 eV are of a comparable size despite the fact that the electron-nucleus term falls off two orders of k^{-1} faster than the electron-electron one. Only at high energy (1600 eV) when the order of falling off in k^{-1} plays an important role in the classification of the magnitude of a term that indeed we find the values of the electron-nucleus scattering term to be of either one or two orders smaller than those of the electron-electron scattering term as expected. Table III indicates that the magnitude of both the real and the imaginary parts of the second-order term at lower energy are comparable to those of the first-order one (slow convergence of the series at low energy). Furth-

ermore, the real parts of the second-order term are opposite in sign to those of the first-order one at scattering angles up to 70° (i.e., of the same sign as those of the zeroth-order one). Consequently, the contribution from the second-order term cancels out a part of the contribution from the first-order one and thereby worsens the accuracy of the approximate amplitude at low energy somewhat as was already discussed above. Because of the drastic increase in the degree of complexity of the expressions of the terms of order higher than the second in the Franco-Halpern expansion, it is difficult to check to see how far one could go on with the inclusion of these higher-order terms without encountering some divergent

TABLE III. The real and imaginary parts of the zeroth-, first-, and second-order terms of the approximate Glauber exchange amplitude at 100 eV (case *I*). The numbers in the square brackets are powers of 10.

Angles (deg)	Zeroth order	Real parts First order	Second order	Zeroth order	Imaginary parts First order	Second order
1	-0.381	0.1068	-0.575[-1]	0.1154	-0.217[-2]	-0.349[-2]
2	-0.380	0.1065	-0.572[-1]	0.114	-0.215[-2]	-0.343[-2]
3	-0.378	0.1059	-0.569[-1]	0.113	-0.213[-2]	-0.334[-2]
5	-0.371	0.104	-0.557[-1]	0.110	-0.205[-2]	-0.304[-2]
7	-0.362	0.101	-0.539[-1]	0.104	-0.196[-2]	-0.259[-2]
10	-0.344	0.959[-1]	-0.506[-1]	0.938[-1]	-0.185[-2]	-0.164[-2]
15	-0.305	0.844[-1]	-0.435[-1]	0.720[-1]	-0.194[-2]	0.559[-3]
20	-0.261	0.718[-1]	-0.361[-1]	0.492[-1]	-0.262[-2]	0.333[-2]
25	-0.216	0.599[-1]	-0.293[-1]	0.288[-1]	-0.400[-2]	0.632[-2]
30	-0.176	0.496[-1]	-0.238[-1]	0.125[-1]	-0.594[-2]	0.913[-2]
40	-0.113	0.352[-1]	-0.164[-1]	-0.768[-2]	-0.106[-1]	0.130[-1]
50	-0.716[-1]	0.276[-1]	-0.120[-1]	-0.159[-1]	-0.151[-1]	0.138[-1]
60	-0.458[-1]	0.243[-1]	-0.835[-2]	-0.179[-1]	-0.186[-1]	0.116[-1]
70	-0.300[-1]	0.234[-1]	-0.409[-2]	-0.173[-1]	-0.212[-1]	0.704[-2]
80	-0.202[-1]	0.237[-1]	0.106[-2]	-0.158[-1]	-0.230[-1]	0.101[-2]
90	-0.141[-1]	0.244[-1]	0.677[-2]	-0.142[-1]	-0.243[-1]	-0.595[-2]
100	-0.102[-1]	0.253[-1]	0.123[-1]	-0.126[-1]	-0.254[-1]	-0.134[-1]

term of the expansion series (if there should be any). It is also not obvious by a direct examination of these terms whether the expansion series converges or not. However, the numerical values obtained for the first few terms of the series as shown in Table III do seem to indicate that the series converges though somewhat more slowly at lower scattering energies. Regardless of whether some of these higher-order terms diverge or not, we believe that it may no longer be worthwhile to carry out the Franco-Halpern approximation beyond the second-order one in view of the tremendous complexity required in the derivation of these terms of order higher than the second.

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APPENDIX

This appendix shows how the function $v(\mathbf{A},d,a,b)$ reduces to closed form in the case of the Glauber exchange amplitude. The function $v(\mathbf{A},d,a,b)$ is defined as

$$v(\mathbf{A}, d, a, b) = \int_0^\infty d\theta \int_0^\infty d\phi [\mathbf{A}^2 + (d + \theta + \phi)^2]^a \\ \times [d + \theta + \phi - i \mathbf{A} \cdot \hat{\mathbf{z}}]^{-b} .$$
(A1)

After setting $\tau = \lambda = 0$ and considering $\mathbf{q} \cdot \hat{\mathbf{z}} = 0$, the function reduces to

$$v(\mathbf{q}, d, a, b) = \int_0^\infty d\theta \int_0^\infty d\phi [q^2 + (d + \theta + \phi)^2]^a \times (d + \theta + \phi)^{-b} .$$
(A2)

The integration over ϕ can be performed using a known integral formula¹³ and the function becomes

$$v(\mathbf{q},d,a,b) = -\frac{1}{\delta} \int_{d}^{\infty} dx \, x^{\delta} \, _{2}F_{1}\left[\alpha,\beta;\gamma;-\frac{q^{2}}{x^{2}}\right], \qquad (A3)$$

where

$$\delta = 2a + 1 - b$$
, $\alpha = -a$, $\beta = \frac{b - 1}{2} - a$, $\gamma = \frac{b + 1}{2} - a$.
(A4)

Two cases are to be distinguished here. If $q^2/d^2 < 1$, using a series representation for the hypergeometric function, we obtain by integrating over x,

$$v(\mathbf{q}, d, a, b) = -\frac{1}{\delta} d^{\delta+1} \sum_{n=0}^{\infty} \frac{(\alpha)_n (\beta)_n}{(\gamma)_n n!} (-1)^n \\ \times \left[\frac{q^2}{d^2}\right]^n \frac{1}{2n - (\delta+1)} .$$
 (A5)

Since $q^2/d^2 < 1$ and the signs of the consecutive terms of the series are opposite alternatively, the series in Eq. (A5) converges quite rapidly and the numerical computation of v(q,d,a,b) can therefore be done quite fast. If $q^2/d^2 > 1$, we change the variable of integration to $z=q^2/x^2$. The function becomes

$$v(\mathbf{q}, d, a, b) = -\frac{1}{2\delta} q^{\delta+1} \int_{q^2/d^2}^{\infty} F_1(\alpha, \beta; \gamma; -z) \times z^{-(\delta+3)/2} dz .$$
 (A6)

Next, we write

 $v(\mathbf{q}, d, a, b)$

$$= -\frac{1}{2\delta} q^{\delta+1} \left[\int_0^\infty {}_2F_1(\alpha,\beta;\gamma;-z) z^{-(\delta+3)/2} dz - \int_0^{q^2/d^2} {}_2F_1(\alpha,\beta;\gamma;-z) z^{-(\delta+3)/2} dz \right].$$
(A7)

The first integration can be carried out straightforwardly by applying an integral formula¹⁴

$$\int_{0}^{\omega} {}_{2}F_{1}(\alpha,\beta;\gamma;-z)z^{-(\delta+3)/2}dz$$
$$=\frac{\Gamma(\alpha+s)\Gamma(\beta+s)\Gamma(\gamma)\Gamma(-s)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(\gamma+s)}, \quad (A8)$$

where $s = (\delta + 1)/2$. For the second integral in Eq. (A7) we use a transformation formula for the hypergeometric series¹⁵ and put it in the form

$$\int_{0}^{q^{2}/d^{2}} {}_{2}F_{1}(\alpha,\beta;\gamma;-z)z^{-(\delta+3)/2}dz$$

$$=\frac{\Gamma(\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta)\Gamma(\gamma-\alpha)}\int_{0}^{d^{2}/q^{2}}t^{\delta_{1}}{}_{2}F_{1}(\alpha_{1},\beta_{1};\gamma_{1};-t)dt$$

$$+\frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)}\int_{0}^{d^{2}/q^{2}}t^{\delta_{2}}{}_{2}F_{1}(\alpha_{2},\beta_{2};\gamma_{2};-t)dt ,$$
(A9)

where

$$\delta_{1} = \alpha + s - 1, \quad \delta_{2} = \beta + s - 1,$$

$$\alpha_{1} = \alpha, \quad \beta_{1} = \alpha + 1 - \gamma,$$

$$\gamma_{1} = \alpha + 1 - \beta, \quad \alpha_{2} = \beta,$$

$$\beta_{2} = \beta + 1 - \gamma, \quad \gamma_{2} = \beta + 1 - \alpha.$$

(A10)

Finally, by using the series representation of the hypergeometric functions in Eq. (A9), we obtain, after an integration over t is carried out analytically,

$$\int_{0}^{q^{2}/d^{2}} {}_{2}F_{1}(\alpha,\beta;\gamma;-z)e^{-(\delta+3)/2}dz$$

$$=\frac{\Gamma(\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta)\Gamma(\gamma-\alpha)} \left[\frac{d^{2}}{q^{2}}\right]^{\delta_{1}+1} \sum_{n=0}^{\infty} \frac{(\alpha_{1})_{n}(\beta_{1})_{n}}{(\gamma_{1})_{n}n!} (-1)^{n} \left[\frac{d^{2}}{q^{2}}\right]^{n} \frac{1}{n+\delta_{1}+1}$$

$$+\frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)} \left[\frac{d^{2}}{q^{2}}\right]^{\delta_{2}+1} \sum_{n=0}^{\infty} \frac{(\alpha_{2})_{n}(\beta_{2})_{n}}{(\gamma_{2})_{n}n!} (-1)^{n} \left[\frac{d^{2}}{q^{2}}\right]^{n} \frac{1}{n+\delta_{2}+1} .$$
(A11)

Since both series in Eq. (A11) converge rather rapidly, the numerical computation of the second term of Eq. (A7) can also be done quite fast. In summary, when $q^2/d^2 > 1$, the closed-form expression for $v(\mathbf{q}, d, a, b)$ is

$$v(\mathbf{q},d,a,b) = -\frac{1}{2\delta} q^{\delta+1} \left[\frac{\Gamma(\alpha+s)\Gamma(\beta+s)\Gamma(\gamma)\Gamma(-s)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(\gamma+s)} - \frac{\Gamma(\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta)\Gamma(\gamma-\alpha)} \left[\frac{d^2}{q^2} \right]^{\delta_1+1} \sum_{n=0}^{\infty} \frac{(\alpha_1)_n(\beta_1)_n}{(\gamma_1)_n n!} (-1)^n \left[\frac{d^2}{q^2} \right]^n \frac{1}{n+\delta_1+1} - \frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)} \left[\frac{d^2}{q^2} \right]^{\delta_2+1} \sum_{n=0}^{\infty} \frac{(\alpha_2)_n(\beta_2)_n}{(\gamma_2)_n n!} (-1)^n \left[\frac{d^2}{q^2} \right]^n \frac{1}{n+\delta_2+1} \right].$$
(A12)

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