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# Numerical method for the calculation of two-center integrals

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A numerical method has been developed to calculate the two-center integrals which can be used to evaluate the charge-transfer matrix elements arising in ion-atom collisions. The initial three-dimensional integrals are first reduced to one-dimensional integrals using a Feynman-integral technique. A special routine which uses continuation in the complex plane has been designed to evaluate the integrals in the region far away from the target to remove their rapid oscillation in this region. Then a Gauss-Laguerre integral method is used to compute this analytic continuation. The four-state charge-transfer matrix elements in proton-hydrogen scattering have been calculated to illustrate the method. The resultant coupled differential equations are solved by the Runge-Kutta method. Some cross sections for proton-hydrogen scattering have been evaluated and compared with available results.

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## I. INTRODUCTION

For many years, charge transfer in the ion-atom collision has received a great deal of attention. The most difficult problem which arises in the coupled-channel calculation of proton-hydrogen scattering is the evaluation of one-electron, two-center, three-dimensional space integrals accurately. The importance of charge-transfer processes in many applications has necessitated the development of fast and accurate methods of calculation. Toward this end, the reduction of the three-dimensional integrals to one-dimensional integrals and then computing them numerically already represents a considerable saving in computer time. Further improvement in our method is achieved through continuation in the complex plane.

The first method was given by McCarroll [1] for the $1s$-$1s$ charge transfer in the collision between a proton and atomic hydrogen. In his treatment the initial integral was reduced to a one-dimensional integral in prolate spheroidal coordinates. The resultant integrand contained a spherical Bessel function. McElroy [2] extended McCarroll's method to include excitation to higher states and found that it gave rise to a rather complicated algebra. Gallaher and Msezane [3] used another method and obtained one-dimensional integrals. Their integrands involved the sum or product of Bessel functions and are complex even for $s$-$s$ matrix elements. Wilets and Gallaher [4] reduced the problem to two-dimensional integrals, which took more computing time. Cheshire [5] solved the problem by showing that it can be expressed as the solution of a set of first-order differential equations. When high excitation states are included, the differential equations become complicated. A general formulation of Fourier transform method has been given by Shakeshaft [6]. He used Simpson's rule and found that the error can be $2\times10^{-5}$ for $1s$-$1s$ matrix elements.

In this paper, we report a numerical method which has been developed to calculate the charge-transfer matrix elements for the proton-hydrogen collision. The initial integrals have been reduced to one-dimensional integrals by using the Feynman technique and modified spherical Bessel function of the third kind. A Gaussian quadrature method has been used in the region around the target. A special integral routine has been designed to evaluate the integral in the region far away from the target. Gauss-Laguerre integral methods have been used after an analytic continuation has been performed to remove the very fast oscillations. Four-state $(1s,2s,2p_0,2p_1)$ coupled differential equations in proton-hydrogen scattering have been solved by using the Runge-Kutta method. Excitation and charge-transfer cross sections at 40-, 60-, and 100-keV proton energies have been calculated and compared with the results of Cheshire, Gallaher, and Taylor [7] and Rapp and Dinwiddie [8].

## II. METHOD

In the proton-hydrogen collision the coordinate system may be described as in Fig. 1. In the figure, **B** is the impact parameter, **R** and **r** are the position vectors of the projectile and target electron relative to the target proton, and **v** is the velocity of the incoming particle which

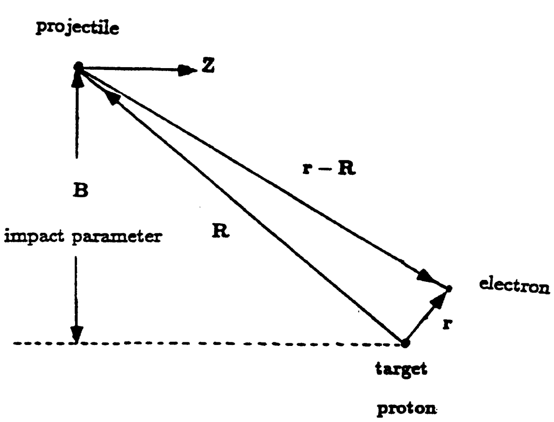


FIG. 1. Collision and coordinate system.

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is moving in the $Z$ direction. The basic integral used to evaluate the charge-transfer matrix elements is

$$I_1=\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}\frac{e^{-i\mathbf{v}\cdot\mathbf{r}}}{r}d\mathbf{r}\ , \tag{1}$$

where $f$ and $\alpha$ are real constants related to the initial and final states. Introducing a Fourier transform for $e^{-\alpha r}/r$, Eq. (1) may be written as

$$I_1=\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{i(\mathbf{k}-\mathbf{v})\cdot(\mathbf{r}-\mathbf{R})}d\mathbf{r}\frac{1}{2\pi^2}\times\int_{-\infty}^{+\infty}\frac{e^{i(\mathbf{k}-\mathbf{v})\cdot\mathbf{R}}}{k^2+\alpha^2}d\mathbf{k}\ . \tag{2}$$

After the $r$ integral has been carried out, we find that

$$I_1=\frac{2}{\pi}\int_{-\infty}^{+\infty}\frac{e^{i(\mathbf{k}-\mathbf{v})\cdot\mathbf{R}}}{(k^2+\alpha^2)(|\mathbf{k}-\mathbf{v}|^2+f^2)}d\mathbf{k}\ . \tag{3}$$

Using the Feynman identity

$$(ab)^{-1}=\int_0^1\frac{dx}{[a+(b-a)x]^2}\ , \tag{4}$$

Eq. (3) becomes

$$\begin{aligned}I_1&=\frac{2}{\pi}\int_0^1 dx\int_{-\infty}^{+\infty}\frac{e^{i(\mathbf{k}-\mathbf{v})\cdot\mathbf{R}}}{[(k^2+\alpha^2)+(|\mathbf{k}-\mathbf{v}|^2+f^2-k^2-\alpha^2)x]^2}d\mathbf{k}\\&=\frac{2}{\pi}\int_0^1 dx\int_{-\infty}^{+\infty}\frac{e^{i[\mathbf{p}+(x-1)\mathbf{v}]\cdot\mathbf{R}}d\mathbf{p}}{\{(\mathbf{p}+x\mathbf{v})^2+\alpha^2+[|\mathbf{p}+(x-1)\mathbf{v}|^2+f^2-(\mathbf{p}+x\mathbf{v})^2-\alpha^2]x\}^2}\ ,\end{aligned}$$

where $\mathbf{p}=\mathbf{k}-x\mathbf{v}$. Define $M=v^2x(1-x)+(f^2-\alpha^2)x+\alpha^2$. The denominator then reduces to

$$(\mathbf{p}+x\mathbf{v})^2+\alpha^2+[|\mathbf{p}+(x-1)\mathbf{v}|^2+f^2-(\mathbf{p}+x\mathbf{v})^2-\alpha^2]x=p^2+v^2x(1-x)+(f^2-\alpha^2)x+\alpha^2=p^2+M\ . \tag{5}$$

The remaining integral may be evaluated to finally give

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}\frac{e^{-i\mathbf{v}\cdot\mathbf{r}}}{r}d\mathbf{r}=2\pi\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}\frac{e^{-\sqrt{M}R}}{\sqrt{M}}dx\ . \tag{6}$$

To calculate charge-transfer matrix elements, a differentiation with respect to $f$, $-\alpha$, or $v$ has to be taken. A modified spherical Bessel function of the third kind, $h_n$, has been used to simplify the differentiation. The $H(n)$ functions are defined below to simplify the expressions of the formulas

$$H(n)=-i^n\frac{R^{2n+1}}{\rho^n}h_n(i\rho)\ , \tag{7}$$

where $\rho=\sqrt{M}R$. The list of formulas which can be used to calculate charge-transfer matrix elements for $s$-$s$, $s$-$p$, $p$-$p$ in the proton-hydrogen scattering are given in Appendix A. Below is such an example, which is obtained by differentiation of Eq. (6) with respect to $-\alpha$:

$$\begin{aligned}I_2&=\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}d\mathbf{r}\\&=2\pi\alpha\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)H(1)dx\ .\end{aligned} \tag{8}$$

The Gaussian quadrature method has been used in the region around the target to evaluate the one-dimensional integral. When $vZ$ increases the difficulty arises from the oscillations of the integrand. If $f$ and $\alpha$ are real, one can find that there are no singularities in the integrand in the region bounded by two vertical lines at $x=0$ and $x=1$. Therefore, using this very important remark the initial integral can be extended to the complex plane and evaluated around two lines: the positive imaginary axis and the line parallel to the positive imaginary axis starting at 1, see Fig. 2. In the first integral we replace

$$x=i\beta\ , \tag{9}$$

where

$$\beta=\frac{y}{v(Z+R)}\ . \tag{10}$$

The first contribution to the integral of Eq. (8) is

$$I_3=\frac{ie^{-ivZ}}{v(Z+R)}\int_0^\infty e^{-y}\left[1-\frac{iy}{v(Z+R)}\right]\times\frac{\exp\left[-R\sqrt{M_1}+\frac{Ry}{Z+R}\right]}{M_1}\times\left[R+\frac{1}{\sqrt{M_1}}\right]dy\ , \tag{11}$$

where

$$M_1=(v^2+f^2-\alpha^2)\frac{iy}{v(Z+R)}+\frac{y^2}{(Z+R)^2}+\alpha^2\ . \tag{12}$$

second contribution is setting

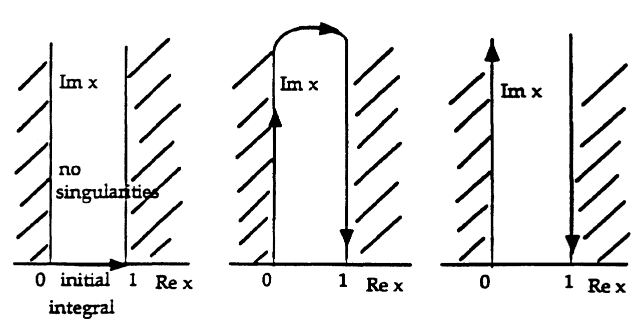


FIG. 2. Initial integrals are extended to the complex plane.

$$x = 1 + i\beta \,, \tag{13}$$

then

$$I_4 = -\frac{1}{v^2(Z+R)^2}\int_0^{\infty} e^{-y}\exp\left[-R\left[\sqrt{M_2}-\frac{y}{Z+R}\right]\right] \times \frac{y}{M_2}\left[R+\frac{1}{\sqrt{M_2}}\right]dy \,, \tag{14}$$

where

$$M_2 = \left[1+\frac{iy}{v(Z+R)}\right]\left[-\frac{ivy}{Z+R}+f^2-\alpha^2\right]+\alpha^2 \,.$$

Consequently, the integral of Eq. (8) can be evaluated as

$$I_2 = 2\pi\alpha(I_3+I_4) \,. \tag{15}$$

The other integrals in Appendix A can be analytically continued in the same way. Finally, the integrals $I_3$ and $I_4$ are evaluated by a simple Gauss-Laguerre method.

## III. RESULTS

The method given in Sec. II allows us to calculate exchange matrix elements accurately with only a few Gauss-Laguerre points in the whole collision process. This method has been used in the calculation of the charge-transfer cross sections in the proton-hydrogen scattering with $1s$, $2s$, $2p_0$, $2p_1$ hydrogen wave functions at both centers. The coupled-channel equations can be expressed (in atomic units) as

$$iv\frac{\partial a}{\partial Z} = Ta + Pb - ivS\frac{\partial b}{\partial Z} \,, \tag{16}$$

$$iv\frac{\partial b}{\partial Z} = Ga + Qb - ivS^+\frac{\partial a}{\partial Z} \,, \tag{17}$$

where $v$ is the velocity of the incoming proton $Z=vt$. The matrix elements are

$$T_{ij} = \int_{-\infty}^{+\infty}\chi_i^*(\mathbf{r})V_p\chi_j(\mathbf{r})d\mathbf{r}\exp\left[i\frac{(E_i-E_j)}{v}Z\right] \,, \tag{18}$$

$$Q_{ij} = \int_{-\infty}^{+\infty}\phi_i^*(\mathbf{r})V_t\phi_j(\mathbf{r})d\mathbf{r}\exp\left[i\frac{(E_i-E_j)}{v}Z\right] \,, \tag{19}$$

$$P_{ij} = \int_{-\infty}^{+\infty}\chi_i^*(\mathbf{r})V_t\phi_j(\mathbf{r})e^{i\mathbf{v}\cdot\mathbf{r}}d\mathbf{r}\exp\left[i\frac{(E_i-E_j)}{v}Z-\frac{ivZ}{2}\right] \,, \tag{20}$$

$$G_{ij} = \int_{-\infty}^{+\infty}\phi_i^*(\mathbf{r})V_p\chi_j(\mathbf{r})e^{-i\mathbf{v}\cdot\mathbf{r}}d\mathbf{r} \times \exp\left[i\frac{(E_i-E_j)}{v}Z+\frac{ivZ}{2}\right] \,, \tag{21}$$

$$S_{ij} = \int_{-\infty}^{+\infty}\chi_i^*(\mathbf{r})\phi_j(\mathbf{r})e^{i\mathbf{v}\cdot\mathbf{r}}d\mathbf{r} \times \exp\left[i\frac{(E_i-E_j)}{v}Z-\frac{ivZ}{2}\right] \,. \tag{22}$$

In Eqs. (18)–(22), $\chi_i(\mathbf{r})$ and $\chi_j(\mathbf{r})$ represent the wave functions around the target, and $\phi_i(\mathbf{r})$, and $\phi_j(\mathbf{r})$ are the wave functions of the projectile. $V_p$ and $V_t$ represent the residual potentials for the projectile and the target, respectively. $E_i$ and $E_j$ are the energy eigenvalues. $T_{ij}$ and $Q_{ij}$ can be evaluated analytically. Equations in Appendix A have been used to calculate $G_{ij}$, $P_{ij}$, and $S_{ij}$ numerically. The Gauss-Laguerre points for the matrix elements are dependent on the energies of the incoming proton and the initial and final charge-transfer states. Typically eight Gaussian points are needed to evaluate $1s$-$1s$ matrix elements in proton-hydrogen scattering when the proton energies are around 40 keV, and $Z$ is less than 5 (in units of $a_0$, the first Bohr radius of the hydrogen atoms the same units are used below). However, when $Z=20$ we may use Eqs. (12) and (14), as good convergence can be obtained by using only five Laguerre points. The scattering amplitudes have been obtained in the intermediate-energy range by solving the coupled-channel equations using the fourth-order Runge-Kutta method and a DEC station 5000/240 computer. Different mesh sizes have been tested in solving the equations. Here are some examples of the 40-keV results. A 2% relative error is obtained by using the mesh sizes of $\delta Z=0.076$, $(Z\le 5)$, $\delta Z=0.38$ $(Z>5)$, and $\delta Z=10$ $(Z>40)$. It takes about 1.8 min of computer CPU time. If we use $\frac{1}{4}$ of the above mesh sizes when $Z\le 5$ the relative error can be reduced to 0.1%. However, it takes about 9 min of CPU time.

Some excitation cross sections obtained by using this numerical method are compared in Table I with the

TABLE I. Cross sections ($10^{-17}$ cm$^2$) for direct excitation in proton-hydrogen scattering.

| Energy (keV) | Authors | $2s$ | $2p_0$ | $2p_1$ | $2p$ | $n=2$ |
|---|---|---|---|---|---|---|
| 40 | Cheshire | 1.591 | | | 6.905 | 8.496 |
| | Rapp | 1.52 | 3.44 | 3.75 | 7.19 | 8.71 |
| | present | 1.618 | 3.422 | 3.684 | 7.106 | 8.724 |
| 60 | Cheshire | 1.763 | | | 8.296 | 1.006(1) |
| | Rapp | 1.68 | 4.52 | 4.80 | 9.32 | 1.100(1) |
| | present | 1.770 | 4.211 | 4.722 | 8.933 | 1.070(1) |
| 100 | Cheshire | 1.371 | | | 8.618 | 9.989 |
| | Rapp | 1.30 | 3.82 | 4.90 | 8.72 | 10.02 |
| | present | 1.368 | 3.793 | 4.917 | 8.710 | 10.08 |

TABLE II. Cross sections ($10^{-17}$ cm$^2$) for charge transfer in proton-hydrogen scattering. The numbers in the brackets are the power of 10 by which the cross sections should be multiplied.

| Energy (keV) | Authors | 1s | 2s | $2p_0$ | $2p_1$ | 2p |
|---|---|---|---|---|---|---|
| 40 | Cheshire | 1.169[1] | 2.480 | | | 5.723[−1] |
| | Rapp | 1.132[1] | 2.39 | 4.6[−1] | 1.4[−1] | 6.0[−1] |
| | present | 1.157[1] | 2.558 | 4.295[−1] | 1.409[−1] | 5.704[−1] |
| 60 | Cheshire | 4.210 | 1.125 | | | 2.418[−1] |
| | Rapp | 4.07 | 1.07 | 2.2[−1] | 5[−2] | 2.6[−1] |
| | present | 4.132 | 1.158 | 1.985[−1] | 4.274[−2] | 2.412[−1] |
| 100 | Cheshire | 9.213[−1] | 2.633[−1] | | | 5.255[−2] |
| | Rapp | 8.7[−1] | 2.5[−1] | 5[−2] | 1[−2] | 5[−2] |
| | present | 8.953[−1] | 2.690[−1] | 4.590[−2] | 5.953[−3] | 5.185[−2] |

four-state results obtained by Cheshire, Gallaher, and Taylor and by Rapp and Dinwiddie, while charge-transfer cross sections are compared in Table II. As seen from Table I, our excitation cross sections are closer to those of Rapp and Dinwiddie in the energy range 40–100 keV. We note that the method of Rapp and Dinwiddie treats the important long-range coupling between the 2s and 2p states more accurately. Therefore, their treatment of the direct excitation process may have less errors. However, our charge-transfer cross sections are almost the same as those of Cheshire, Gallaher, and Taylor. Rapp and Dinwiddie pointed out that the disagreement between their data and that of Cheshire, Gallaher, and Taylor may be caused by numerical errors in both. There is no data for charge-transfer matrix elements available in both papers. Comparison of the charge-transfer cross sections in Table II shows that our calculation favors the method of Cheshire, Gallaher, and Taylor over that by Rapp and Dinwiddie. This may suggest that both the Cheshire, Gallaher, and Taylor and the present methods evaluate the charge-transfer matrix elements more accurately as compared to the method of Rapp and Dinwiddie. The advantage of our method is that we can evaluate the charge-transfer matrix elements accurately over the whole scattering range, including the region of large internuclear distances.

## IV. CONCLUSION

In this paper we have developed a numerical method for calculating two-center integrals which can be used to evaluate charge-transfer matrix elements arising in ion-atom collisions. The technique is illustrated by computing both excitation and charge-transfer cross sections for proton-hydrogen collision in a four-state approximation. Our results compare favorably with those of Cheshire, Gallaher, and Taylor and Rapp and Dinwiddie, and thereby give credence to the method.

## ACKNOWLEDGMENT

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## APPENDIX A

The formulas that are used to calculate charge-transfer matrix elements are

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}d\mathbf{r}=2\pi\alpha\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)H(1)dx\ , \tag{A1}$$

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}z\,d\mathbf{r}=2\pi\alpha\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)^2[ZH(1)-ivxH(2)]dx\ , \tag{A2}$$

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}x\,d\mathbf{r}=2\pi\alpha B\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)^2H(1)dx\ , \tag{A3}$$

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}z^2d\mathbf{r}=2\pi\alpha\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)^2\{Z^2(1-x)H(1)+x[1-2Zvi(1-x)]H(2)-v^2(1-x)x^2H(3)\}dx\ , \tag{A4}$$

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}xz\,d\mathbf{r}=2\pi\alpha B\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)^3[ZH(1)-ivxH(2)]dx\ , \tag{A5}$$

$$\int_{-\infty}^{+\infty}\frac{e^{-f|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}e^{-\alpha r}e^{-i\mathbf{v}\cdot\mathbf{r}}x^2d\mathbf{r}=2\pi\alpha\int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}}(1-x)^2[B^2(1-x)H(1)+xH(2)]dx\ , \tag{A6}$$

$$\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} d\mathbf{r} = 2\pi\alpha f \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} x(1-x) H(2) dx \,, \tag{A7}$$

$$\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} z \, d\mathbf{r} = 2\pi\alpha f \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} (1-x)^2 x [ZH(2) - ivxH(3)] dx \,, \tag{A8}$$

$$\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} x \, d\mathbf{r} = 2\pi\alpha f B \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} x (1-x)^2 H(3) dx \,, \tag{A9}$$

$$\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} xz \, d\mathbf{r} = 2\pi\alpha f B \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} x (1-x)^3 [ZH(2) - ivxH(3)] dx \,, \tag{A10}$$

$$\begin{aligned}\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} z^2 d\mathbf{r} = 2\pi\alpha f \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} x (1-x)^2 \{ & Z^2(1-x) H(2) + [x - 2x(1-x) Ziv] H(3) \\ & - x^2 (1-x) v^2 H(4)\} dx \,,\end{aligned} \tag{A11}$$

$$\int_{-\infty}^{+\infty} e^{-f|\mathbf{r}-\mathbf{R}|} e^{-i\mathbf{v}\cdot\mathbf{r}} e^{-\alpha r} x^2 d\mathbf{r} = 2\pi\alpha f \int_0^1 e^{i(x-1)\mathbf{v}\cdot\mathbf{R}} x (1-x)^2 [xH(3) + B^2(1-x) H(2)] dx \,. \tag{A12}$$

**B**, **R**, **r**, $v$, $f$, $Z$, $\alpha$, and functions $H(n)$ are defined in Sec. II.

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