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Integral representation for the Glauber scattering amplitude for direct Coulomb ionization by charged particles

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An integral representation is developed for the scattering amplitude for ionization by charged particles in the Glauber approximation. Unlike previous results based on a series expansion in the momentum of the ejected electron, $\vec{k}_e$, the present results are rigorously convergent for all physical values of $\vec{k}_e$. Results calculated by this method agree with earlier results for ionization of atomic hydrogen by electron impact using Padé approximants to approximately sum the series. Total cross sections for the ionization of atomic hydrogen by proton impact are presented and compared to experimental data. This technique is applicable to the ionization of neutral atoms whose participating electron is represented by a hydrogenic wave function, and the remaining electrons are ignored.

I. INTRODUCTION

The theory of direct Coulomb ionization of atoms by charged particle impact has no rigorous solution. Furthermore, most practical solutions are moderately tedious. For example in the Born approximation, while total cross sections for excitation to bound states have been expressed in closed forms, ionization total cross sections require two numerical integrations. On the other hand, the success of the Born approximation and its utility in a variety of practical applications is encouraging.

The Glauber approximation, which represents an improvement to the Born approximation, has been successful in predicting total and differential cross sections for both elastic and inelastic charged particle scattering by atomic systems.[1] Recently the Glauber approximation has been applied[2-4] to the ionization of atomic hydrogen by electron impact, the simple system in which this approximation has been tested most extensively. The results are in agreement with the experimental data for incident energies greater than 30 eV and are superior to the corresponding Born results.

In order to apply the Glauber approximation it is convenient to expand the scattering amplitude in spherical harmonics according to

$$f(\vec{q},\vec{k}_e)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}(\vec{q},k_e)\,Y_l^m(\hat{k}_e)\,, \qquad (1)$$

where the sum is over the angular momentum of the ejected electron which carries off momentum $\vec{k}_e$, $\vec{q}$ being the momentum transfer.[5,6] The functions $f_{lm}(\vec{q},k_e)$ were represented[2] as a power series in k_e, which was divergent for $k_e>1$. The method of Padé approximants was used to obtain an approximate analytic continuation of the power-series representation of $f_{lm}(\vec{q},k_e)$ to $k_e>1$. As there are no general convergence theorems for Padé approximants, the usefulness of the approximation would be improved, from the point of view of mathematical rigor and computational ease, if an alternate representation of the scattering amplitude $f(\vec{q},\vec{k}_e)$ could be obtained avoiding the use of analytic continuation by Padé approximants. To this end, we have obtained a one-dimensional representation of the functions f_{lm} which are convergent for all physical values of $\vec{q}$ and $\vec{k}_e$. Recently, Narumi, Tsuji, and Miyamoto[3] as well as Thomas,[4] have presented results based on an alternate representation for $f_{lm}(\vec{q},k_e)$.

In Sec. II integral expressions for the functions $f_{lm}(\vec{q},k_e)$ are obtained which are rigorously convergent for all real values of k_e. Section III contains a comparison of the present results with those previously obtained as well as new results of calculations for the ionization of atomic hydrogen by proton impact.

II. DERIVATION

The scattering amplitude for the ionization of hydrogen by an incident charge Z_1 within the Glauber approximation may be written[5] in the center-of-mass system as

$$f(\vec{q},\vec{k}_e)=\frac{-i\mu Z_1}{2\pi\eta}\int \chi_c^{-*}(\vec{k}_e,\vec{r})\left[1-\left(\frac{|\vec{b}-\vec{s}\,|}{b}\right)^{2i\eta}\right]\times u_0(\vec{r})e^{i\vec{q}\cdot\vec{b}}\,d^2b\,d^2s\,dz\,. \qquad (2)$$

In this expression μ is the reduced mass of the incident projectile and hydrogen nucleus and $\eta=-Z_1/v_0$, where v_0 is the relative incident velocity of Z_1. The coordinates of the incident projectile are $(\vec{b},\vec{x})$ while those of the electron are $(\vec{s},\vec{z})$. As has been previously discussed, the $\vec{x}$ axis rather than being taken along $\vec{v}_0$ is chosen such that $\vec{x}\cdot\vec{q}=0$.

The function $\chi_C^{-*}(\vec{k}_e,\vec{r})$ is a Coulomb function representing the wave function of the ionized electron, and is given by[7]

$$\chi_C^{-*}=(2\pi)^{-3/2}e^{-\gamma\pi/2}\Gamma(1+i\gamma)e^{-i\vec{k}_e\cdot\vec{r}}\times {}_1F_1(-i\gamma,1,i(k_e r+\vec{k}_e\cdot\vec{r})) \quad (3a)$$

$$=(\tfrac{1}{2}\pi)^{-1/2}e^{-\gamma\pi/2}\sum_{l=0}^{\infty}(-2ik_e r)^l\frac{\Gamma(l+1+i\gamma)}{(2l+1)!}\times e^{ik_e r}{}_1F_1(l+1+i\gamma,2l+2,-2ik_e r)\times\sum_{m=-l}^{l}Y_l^{m*}(\hat{k}_e)Y_l^m(\hat{r}) \quad (3b)$$

where

$$\gamma=-Z_2^*/k_e$$

and where Eq. (3b) is the partial-wave expansion of the Coulomb function χ_C^{-*} in angular momentum states of the ejected electron.

The function $u_0(\vec{r})$ is the initial state of the hydrogen atom which we consider throughout to be the ground state, though generalization to other initial states is straightforward:

$$u_0(\vec{r})=2\lambda^{3/2}e^{-\lambda r}\,Y_0^0(\hat{r})=(\lambda^{3/2}/\sqrt{\pi})e^{-\lambda r}\ .$$

For the sake of generality, in the derivation that follows we have considered the nuclear charge Z_2^*, which appears in the charge parameter of the Coulomb function, and the nuclear charge λ, which appears in the ground-state wave function, to be distinct quantities. When considering charged-particle ionization of hydrogen this is, of course, unnecessary as $\lambda=Z_2^*=1$.

Analogous to the method developed by McGuire *et al.*[5] the partial-wave expansion of the Coulomb function χ_C^{-*} is used to expand the scattering amplitude of Eq. (2) as

$$f(\vec{q},\vec{k}_e)=\frac{-2i\mu\lambda^{3/2}Z_1}{(2\pi)^{3/2}\eta}\sum_{l=0}^{\infty}C_l(-ik_e)^l\times\sum_{m=-l}^{l}I_{lm}(\vec{q},k_e)Y_l^m(\hat{k}_e)\,, \quad (4a)$$

where

$$I_{lm}=\frac{1}{\sqrt{\pi}}\int r^l e^{-\lambda r}e^{-ik_e r}{}_1F_1(l+1+i\gamma,2l+2,-2ik_e r)\times Y_l^{*m}(\hat{r})\phi(\eta)e^{i\vec{q}\cdot\vec{b}}\,d^2b\,d^3r \quad (4b)$$

and

$$\phi(\eta)=1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta},\quad C_l=\frac{2^l e^{-\pi\gamma/2}\Gamma(l+1+i\gamma)}{(2l+1)!}\ .$$

The previous representation of $f(\vec{q},\vec{k}_e)$ was then obtained by using methods developed by Thomas and Gerjuoy[8] to reduce the functions I_{lm} to a power series in k_e. Employing an alternate reduction procedure, we have obtained a one-dimensional integral representation of the functions I_{lm} of Eq. (4b), which avoids the convergence problems encountered when using the power series

By making use of a selection rule given by Thomas and Gerjuoy,[8] it may be shown that $I_{lm}=0$ if $l+m$ is not an even integer. Using the requirements on l and m above, the spherical harmonics $Y_l^{m*}(\hat{r})$ may be expressed[9] as

$$Y_l^{m*}(\hat{r})=\frac{(-1)^m}{2\sqrt{\pi}}\sin^m\theta e^{-im\phi}\sum_{j=0}^{(l-m)/2}c_{lm}^j\cos^{2j}\theta \qquad (m\geq 0) \quad (5)$$

The mathematical development given below is valid for $m\geq 0$. Evaluation of I_{lm} for $m<0$ may easily be done using the $m>0$ results and Eq. (4b) with the relation

$$Y_l^{-m*}(\hat{r})=(-1)^m Y_l^m(\hat{r})\ .$$

The factor of 1 which appears in $\phi(\eta)$ of Eq. (4b) may be shown[8] not to enter the calculation whenever the bound-state electron wave function is orthogonal to each partial-wave continuum wave function. Hence, rewriting

$$e^{-im\phi}\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}e^{i\vec{q}\cdot\vec{b}}=e^{-im\phi}\left(1+\frac{r^2\sin^2\theta}{b^2}-\frac{2r\sin\theta\cos(\phi_b-\phi)}{b^2}\right)^{i\eta}\exp[iqb\cos(\phi_q-\phi_b)]$$

$$=e^{-im\phi}e^{-im\phi_q}\left(1+\frac{r^2\sin^2\theta}{b^2}-\frac{2r\sin\theta}{b^2}\cos\phi\right)^{i\eta}\exp(iqb\cos\phi_b+im\phi_b)\,,$$

the function I_{lm} may be expanded as

$$I_{lm}=-\frac{(-1)^m}{2\pi}e^{-im\phi_q}\sum_{j=0}^{(l-m)/2}c_{lm}^j\int r^{l+2}e^{-ar}{}_1F_1(l+1+i\gamma,2l+2,-2ik_e r)(1+z^2-2z\cos\phi)^{i\eta}\times\exp(iqb\cos\phi_b+im\phi_b)e^{-im\phi}\sin^{1+m}\theta\cos^{2j}\theta\,dr\,db\,d\theta\,d\phi\,d\phi_b\,, \quad (6)$$

$$a=\lambda-ik_e\,,\qquad z=(r\sin\theta)/b\ .$$

The angular integration over ϕ_b is readily done using the integral representation[10] of the Bessel function

$$\int_0^{2\pi} \exp(iqb\cos\phi_b + im\phi_b)d\phi_b = 2\pi i^m J_m(qb)\,. \quad (7)$$

Noting that $\sin(m\phi)$ is an odd function, the angular integration over the azimuthal angle ϕ then becomes[11]

$$\int_0^{2\pi} (1+z^2-2z\cos\phi)^{i\eta}\cos(m\phi)\,d\phi = \frac{2\pi\Gamma(m-i\eta)}{m!\,\Gamma(-i\eta)}\,G(z)\,, \quad (8a)$$

$$G(z) = \begin{cases} z^m\,{}_2F_1(-i\eta, m-i\eta, m+1, z^2)\,, & z<1\,,\\ z^{-m+2i\eta}\,{}_2F_1(-i\eta, m-i\eta, m+1, z^{-2})\,, & z>1\,. \end{cases} \quad (8b)$$

Making the transformation $b \to b\sin\theta$, the integral of Eq. (6) becomes

$$I_{lm} = \frac{-2\pi(-i)^m\Gamma(m-i\eta)}{\Gamma(-i\eta)m!}\sum_{j=0}^{(l-m)/2} c_{lm}^j\, e^{-im\phi_q} \times\int r^{l+2}e^{-ar}\,{}_1F_1(l+1+i\gamma, 2l+2, -2ik_e r) \times G(r/b)J_m(qb\sin\theta)b\sin^{m+3}\theta\cos^{2j}\theta\, db\, dr\, d\theta \quad (9a)$$

$$= \sum_{j=0}^{(l-m)/2} c_{lm}^j I_{lm}^j \quad (9b)$$

and replacing a factor of $\sin^2\theta$ by $1-\cos^2\theta$,

$$I_{lm} = \sum_{j=0}^{(l-m+2)/2} d_{lm}^j g_{lm}^j\,, \quad \text{where } I_{lm}^j = g_{lm}^j - g_{lm}^{j+1}\,. \quad (9c)$$

The final angular integration over θ may now be carried out yielding[12] spherical Bessel functions j_ν,

$$\int_0^{\pi} J_m(qb\sin\theta)\sin^{1+m}\theta\cos^{2j}\theta\,d\theta = 2(2j-1)!!(qb)^{-j}j_{j+m}(qb)\,, \quad (10)$$

which are expanded in a finite series in inverse powers of (qb) as[13]

$$j_{j+m}(qb) = \frac{1}{2qb}\sum_{n=0}^{j+m}\frac{a_{m+j}^n}{(qb)^n}\left[e^{iqb} + (-1)^{m+j-n-1}e^{-iqb}\right]. \quad (11)$$

Though individual terms of this series become unbounded as $qb \to 0$, the sum may be shown to behave as $(qb)^{j+m}$ near $qb = 0$.

Making the transformation $b \to br/q$, the integral for g_{lm}^j becomes

$$g_{lm}^j = \frac{-2\pi(-i)^m\Gamma(m-i\eta)}{\Gamma(-i\eta)m!}\,\frac{(2j-1)!!}{q^2}\,e^{-im\phi_q}\sum_{n=0}^{j+m} a_{m+j}^n \times\int r^{l+3-j-n}b^{-n-j}\,{}_1F_1(l+1+i\gamma, 2l+2, -2ik_e r) \times G(q/b)\left[e^{-cr} + (-1)^{m+j-n-1}e^{-dr}\right]dr\,db\,, \quad (12)$$

where

$$c = a - iqb\,, \quad d = a + iqb\,.$$

Final reduction of the scattering amplitude to a one-dimensional integral is made by integrating over r using the relation[14]

$$\int_0^\infty r^n e^{-tr}\,{}_1F_1(l+1+i\gamma, 2l+2, -2ik_e r)\,dr = \Gamma(n+1)t^{-n-1}\,{}_2F_1(l+1+i\gamma, n+1, 2l+2, -2ik_e/t)\,. \quad (13)$$

The double sum over the set of coefficients d_{lm}^j, $(2j-1)!!$, a_{m+j}^n and the sign factor $(-1)^{m+j-n-1}$ may be reduced in a straightforward fashion to a single sum over a set of coefficients, namely,

$$A_{lm}^p = \sum_{j=0}^{p}(2j-1)!!\,d_{lm}^j a_{m+j}^{p-j}\,,$$

where the sum excludes values of d_{lm}^j and a_{m+j}^{p-j} which are not defined by Eqs. (9c) and (11).

Following this reduction the integral, I_{lm} becomes

$$I_{lm} = \frac{-2\pi(-i)^m\Gamma(m-i\eta)}{\Gamma(-i\eta)m!}e^{-im\phi_q}\sum_{p=0}^{l+2}(l+3-p)!\,\frac{1}{q^2}\int_0^\infty G(q/b)\left[A_{lm}^p c^{-p-4}(c/b)^p\,{}_2F_1(l+1+i\gamma, l+4-p, 2l+2, -2ik_e/c) + (-1)^{m+p+1}A_{lm}^p d^{-l-4}(d/b)^p\,{}_2F_1(l+1+i\gamma, l+4-p, 2l+2, -2ik_e/d)\right]db \quad (14a)$$

$$= \frac{-2\pi(-i)^m\Gamma(m-i\eta)}{\Gamma(-i\eta)m!\,q^2}e^{-im\phi_q}\sum_{p=0}^{l+2}I_{lm}^p\,. \quad (14b)$$

Collecting terms the scattering amplitude may now be expressed as

$$f(\vec{q}, \vec{k}_e) = \frac{4\pi\mu\lambda^{3/2} Z_1}{(2\pi)^{3/2} q^2} \sum_{l=0}^{\infty} k_e^l C_l \sum_{m=-l}^{l} (-1)^{(l+m)/2} \frac{\Gamma(m-i\eta)}{m!\,\Gamma(1-i\eta)}\, e^{-im\phi_q} \sum_{p=0}^{l+2} I_{lm}^p Y_l^m(\hat{k}_e)\,.$$

It should be noted that the integrand of Eq. (14a) approaches zero in a well-behaved manner as b goes to zero. The apparent divergence in Eq. (14a) comes from the use of the expansion of the spherical Bessel function of Eq. (11) previously discussed. It may also be seen that as b becomes large, all hypergeometric functions in the integrand of Eq. (11) tend to unity so that the integrand becomes rapidly damped by the inverse powers of b, c, and d.

III. CROSS SECTIONS

Total cross sections for electron ionization of atomic hydrogen were computed using the integral expressions of the preceding section. These cross sections were found to agree to approximately 1% with the previously calculated results[2] employing Padé approximants. As the functional dependence of the integrand of Eq. (11) is separated in q and k_e, many of the functional evaluations necessary to compute total and differential cross sections may be saved, which speeds evaluation. The time necessary for evaluation of a total cross section using either method is 1 to 2 minutes on an IBM 370-158 computer.

The ionization of an atomic system by heavy charged particles includes a much larger range of momenta of the ejected electron, k_e, in cross-section calculations than is the case with electrons. For these large values of k_e the calculation of $f(\vec{q}, \vec{k}_e)$ using Padé approximants[2] becomes numerically impractical and inefficient. The method just presented has no such drawback, and here we present new calculations for the ionization of atomic hydrogen by proton impact. The results of this calculation are shown in Fig. 1 with numerical results given in Table I. Peach[15] has done a similar partial-wave expansion calculation for proton ionization of hydrogen within the Born approximation and finds that the first four partial waves, in the energy range considered here, give the correct Born result to within a few percent. We include in the sum of Eq. (15) partial-wave values for $l \leq 4$, and for total cross sections we expect this to represent the preponderance of the sum in the energy range considered where all partial waves are included, although more partial waves may be needed to compute differential cross sections accurately. The results of the Born calculation are also included in the figure as well as the experimental values obtained by Gilbody and Ireland[16] and Fite *et al.*[17] As with the result of electrons[2] on hydrogen, the present results predict a peak at higher incident energies than does the Born approximation.

Comparison with experimental data for $p+\mathrm{H}$ is inconclusive, in contrast with the $e+\mathrm{H}$ case where the data clearly favor the Glauber results over Born results. While it is possible that the data are in error, it is also possible that our calculation is incomplete, especially in the vicinity of the peak of the cross section. We have, for example,

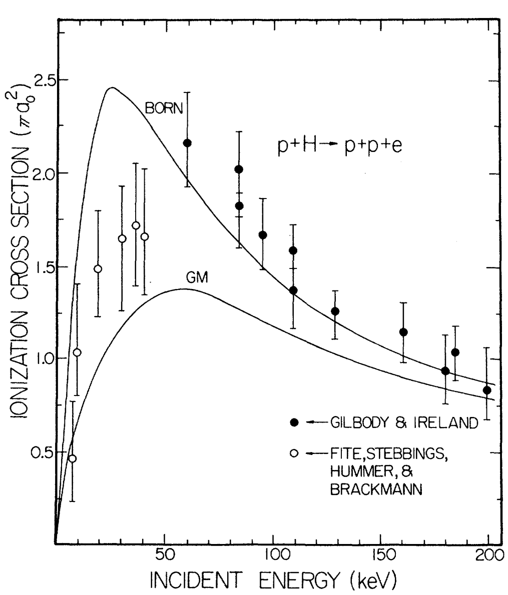

FIG. 1. Total cross sections for the ionization of atomic hydrogen by proton impact vs projectile energy. Data were extracted from Refs. 16 and 17.

TABLE I. Total cross sections for the ionization of atomic hydrogen by proton impact as a function of the energy of the projectile.

E_0 (keV)	Ionization cross sections (πa_0^2) This work	Born approx.
10	0.63	1.64
25	1.03	2.46
30	1.15	2.44
35	1.25	2.39
40	1.31	2.31
50	1.37	2.13
55	1.38	2.05
60	1.37	1.96
75	1.32	1.74
100	1.19	1.45
150	0.96	1.09
200	0.79	0.88

treated the protons as distinguishable, and have not properly treated contributions corresponding to electrons traveling off near[18] the projectile. It is unfortunate that these contributions are, in general, difficult to include in the Glauber approximation.

Our integral expression for the Glauber scattering amplitude may be applied to the ionization of neutral atoms other than atomic hydrogen by using a one-electron approximation. Once the wave function of the participating electron is determined the other atomic electrons are ignored. This approach, of course, introduces additional approximations, often not negligible, into the calculation. Consequently, additional and more detailed data for the ionization of atomic hydrogen, together with additional data for other atomic targets, may be useful in testing and extending our understanding of atomic ionization.

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