Differential cross sections for electron capture: A comparison of three approximations

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(Received 25 March 1988)

Closed-form expressions for 1s-1s electron-capture amplitudes for $H^+ + H$ collisions in three different approximations are compared. We find that all three approximations agree well in the region of the Thomas peak, but significant differences are noted at the minimum in the angular distributions of scattered neutral hydrogen atoms.

I. INTRODUCTION

Theoretical and experimental studies[1–4] of electron capture over the past ten years have demonstrated that the process proceeds via a second-order mechanism at high energies. Qualitatively this mechanism, the Thomas double collision mechanism,[5] is well-described semiclassically and in the second Born approximation.[2] A peak in the angular distribution of scattered neutral particles at the Thomas angle θ_T characterizes this mechanism. In the second Born approximation with plane-wave intermediate states this peak is predicted to be noticeable at energies of the order of 50 MeV for incident protons. At such high energies the cross section is so small that observation of the peak is precluded. An important advance was made by Briggs and co-workers[6] who predicted that the peak was sufficiently distinct to observe at experimental energies of the order of 10 MeV. Their result followed from a theory with better intermediate states than the simple plane waves of the second Born approximation. Observation of the peak at 2–10 MeV confirmed the insights of Ref. 6 showing that the correct intermediate states are essential to describe quantitatively the Thomas peak.

Presently there are several second-order theories[7–9] which differ from one another in the nature of the intermediate states and in the peaking approximations employed to compute the capture amplitude. Quantitatively, one of the most advanced approximations, the strong-potential Born approximation (SPB), employs eigenstates of the target as intermediate states.[4–6] The impulse approximation (IA) of Briggs[3,6,10] employs just such states but introduces peaking approximations to evaluate the amplitude. These peaking approximations are usually valid at high energies, although their use in the neighborhood of the Thomas peak is known to produce some errors.[3] Reference 4 obtains a more correct shape of the peak by evaluating the exact IA numerically.

An improved peaking approximation has been introduced in the context of the SPB approximation by McGuire and co-workers,[11] and has been applied to the Thomas peak at 3 MeV for proton-hydrogen collisions. These improved peaking approximations also apply to the IA and may remedy some of the defects of the full peaking approximation. The objective of this study is to investigate these improved peaking approximations for determinations of the Thomas peak in symmetric collisions.

Throughout this work we use a new formulation of perturbation series, referred to here as Coulomb-modified perturbation series, which are applicable when there are long-range Coulomb potentials acting in initial and/or final channels.[12] These new series are free of the singularities in higher Born terms noted by Mapleton[13] and later by Dewangen and Eichler.[14] The modified SPB amplitude obtained in Ref. 12 has a term in addition to the conventional second-order term; this term is of order $1/v^2$ smaller than the dominant terms and is neglected in our calculations. This new term has also been neglected in all previous work, including the distorted-wave Born (DWB) approximation of Burgdorder and Taulbjerg.[12,15]

Section II establishes the notation and in Sec. III we compute the capture amplitude and differential cross sections in three different approximations. The first approximation, called the fully peaked impulse approximation (PIA1), was calculated by Briggs and co-workers.[6] The second approximation called the partially peaked impulse approximation (PIA2) employs a peaking approximation used by McGuire and co-workers in a different context.[11] The third approximation, the peaked SPB, uses off-energy-shell wave functions and was computed in Ref. 11. We repeat this calculation using different techniques and obtain a simpler, although equivalent, expression for the amplitude. Differential cross sections for the reaction

$$H^+ + H \rightarrow H + H^+$$

at 10 MeV are compared.

II. NOTATION

We employ the notation of Macek and Shakeshaft.[7] Let M_P be the mass of a projectile P impinging upon a one-electron ion or atom $(e+T)$, e the electron of mass m, and T the target of mass M_T. We define the mass ratios

$$\alpha = M_T/(m+M_T), \quad \beta = M_P/(m+M_P) , \tag{2.1}$$

and the reduced masses,

$$\begin{aligned} \nu_i &= M_P(m+M_T)/(m+M_T+M_P) , \\ \nu_f &= M_T(m+M_P)/(m+M_T+M_P) . \end{aligned} \tag{2.2}$$

Let e denote the electron and let Z_T and Z_P be the charge of T and P, respectively. Let ε_i be the internal energy of $(e+T)$ in the initial state i and ε_f be the internal energy of $(e+P)$ in the final state f. We work in the center-of-mass frame of all three particles. In this frame the total energy E of the system is, in a.u. which are used throughout,

$$E=(\tfrac{1}{2}\nu_i)k_i^2+\varepsilon_i=(\tfrac{1}{2}\nu_f)k_f^2+\varepsilon_f\ , \tag{2.3}$$

where k_i is the initial momentum of P and k_F is the final momentum of $(e+P)$. With v the incident velocity of P relative to the center of mass of $(e+T)$, we have $k_i=\nu_i v$ and $k_f=\nu_f v$. We define the average momentum transfer vectors

$$\mathbf{K}=\beta\mathbf{k}_f=\mathbf{k}_i,\quad \mathbf{J}=\alpha\mathbf{k}_i-\mathbf{k}_f\ . \tag{2.4}$$

Let $\phi_i(\mathbf{r}_T)$ represent the initial internal state of $(e+T)$ and $\phi_f(\mathbf{r}_P)$ represent the final internal state of $(e+P)$. The initial- and final-state wave functions of the complete system are

$$\psi^{\pm}_{\mathbf{k},e}(\mathbf{r}_T)=[1+(\varepsilon\pm i\eta-H_0-V_{Te})^{-1}V_{Te}]\phi_{\mathbf{k}}(\mathbf{r}_T)\ , \tag{2.5}$$

where H_0 denotes the kinetic energy of the electron, $\phi_{\mathbf{k}}(\mathbf{r}_T)$ is the plane-wave function normalized on the momentum scale, and ε is the energy.

We also set $\nu_T=Z_T/v$ and $\nu_P=Z_P/v$. The parameter μ is set equal to Z_T after differentiation.

III. FORMULATION

We start with the approximate SPB amplitude given by Eq. (2.11) of Ref. 8;

$$A_{\mathrm{SPB}}=4\pi Z_P\int d^3p\,\tilde{\phi}_f(\mathbf{p})\frac{1}{|\mathbf{p}-\mathbf{K}|^2}\times\langle\psi^{-}_{\mathbf{p}+\mathbf{v},\varepsilon}(\mathbf{r})\,|\,e^{i(\mathbf{p}-\mathbf{K})\cdot\mathbf{r}}\,|\,\phi_i(\mathbf{r})\rangle\ . \tag{3.1}$$

In this paper we always employ the further approximations

$$|\mathbf{p}-\mathbf{K}|^2\approx K^2\ , \tag{3.2}$$

and

$$\psi^{+}_{\mathbf{k}_2,\varepsilon}(\mathbf{r})\approx e^{\pi\nu_T/2}\left[\frac{1-2\varepsilon/k_2^2}{4}\right]^{i\nu_T}\Gamma(1-i\nu_T)\psi^{+}_{\mathbf{k}_2}(\mathbf{r})\ . \tag{3.3}$$

Here, $\mathbf{k}_2=\mathbf{p}+\mathbf{v}$, and $\psi^{+}_{\mathbf{k}}(\mathbf{r})$ is the momentum-normalized Coulomb wave function.

These approximations give the approximate SPB amplitude Eq. (5.1) of Ref. 8, which we employ as the starting point in our calculations here;

$$A_{\mathrm{SPB}}\approx\frac{16\nu_T e^{\pi\nu_T/2}}{\pi K^2\sinh\pi\nu_T}Z_P^{7/2}Z_T^{3/2}\frac{\partial}{\partial\mu}\frac{1}{\mu^2+J^2}\times\int d^3p\frac{1}{(Z_P^2+p^2)^{2+i\nu_T}}\times\left[\frac{K^2-v^2+\mu^2+2\mathbf{p}\cdot\mathbf{J}-2i\mu v}{4(\mu^2+J^2)(v^2+2\mathbf{v}\cdot\mathbf{p}+i\eta)}\right]^{-i\nu_T}\ . \tag{3.4}$$

A. Fully peaked impulse approximation (PIA1).

In this approximation the off-shell factor in Eq. (3.3) and the $\mathbf{p}\cdot\mathbf{J}$ term are omitted and one obtains

$$A_{\mathrm{PIA1}}=32iZ_P^{5/2}Z_T^{5/2}e^{\pi\nu_T/2}\Gamma(1-i\nu_T)K^{-4}\times\left[\frac{K^2-v^2-2iZ_Tv}{K^2}\right]^{-i\nu_T}\times\left[\frac{1-i\nu_T}{K^2}+\frac{1+i\nu_T}{K^2-v^2-2iZ_Tv}\right]\ , \tag{3.5}$$

where it is understood that $-\pi<\arg(K^2-v^2-2iZ_T)<\pi$. The corresponding differential cross section is

$$\frac{d\sigma}{d\Omega_{\mathrm{PIA1}}}=2^8Z_T^5Z_P^5\frac{M^2}{v^{12}}e^{\pi\nu_T}\frac{\pi\nu_T}{\sinh\pi\nu_T}\times\exp\left[-2\nu_T\tan^{-1}\frac{2\nu_T}{x^2-1+\nu_T^2}\right]\times\frac{1}{x^{12}}\left[\frac{(2x^2-1)^2+\nu_T^2}{(x^2-1)^2+4\nu_T^2}\right]\ , \tag{3.6}$$

where

$$x=K/v,\quad x^2=\tfrac{1}{4}+M^2\sin^2\theta\ , \tag{3.7}$$

M is the heavy-particle reduced mass, and θ is the scattering angle. Equation (3.6) differs from Eq. (2.15b) of Ref. 6 but agrees with the earlier result of Ref. 3. In addition, we obtain agreement with the numerical results of Ref. 6.

The shape of the Thomas peak is largely determined by the factor in the second set of large parentheses on the right-hand side of Eq. (3.6). At $x=1$, corresponding to the Thomas angle, this factor equals $1/4\nu_T^2$ in the PIA1 approximation.

B. Partially peaked impulse approximation (PIA2).

As in the PIA1 approximation, we neglect the coefficient of the Coulomb plane wave in the expression for the approximate off-shell wave function of Eq. (3.3), but retain the factor $\mathbf{p}\cdot\mathbf{J}$ in Eq. (3.4). The integral over momentum variables is evaluated using the general expression $I(a,b,lm)$ for $a=0$ and $l=0$ given in the Appendix. We have

$$A_{\mathrm{PIA2}}=-32iZ_T^{5/2}Z_P^{5/2}e^{\pi\nu_T/2}\Gamma(1-i\nu_T)K^{-4}\times\left[\frac{K^2-v^2-2iZ_Tv-2iZ_PK}{K^2}\right]^{-i\nu_T}\times\left[\frac{1-i\nu_T}{K^2}+\frac{1+i\nu_T}{K^2-v^2-2iZ_Tv-2iZ_PK}\right]. \tag{3.8}$$

The corresponding differential cross section is

$$\frac{d\sigma}{d\Omega_{\mathrm{PIA2}}}=2^8Z_T^5Z_P^5\frac{M^2}{v^{12}}e^{\pi\nu_T}\frac{\pi\nu_T}{\sinh\pi\nu_T}\times\exp\left[-2\nu_T\tan^{-1}\frac{2\nu_T}{x^2-1+\nu_T^2}\right]\times\frac{1}{x^{12}}\left[\frac{(2x^2-1)^2+(\nu_T+2\nu_Px)^2}{(x^2-1)^2+4(\nu_T+\nu_Px)^2}\right]. \tag{3.9}$$

The expression for the cross section differs from the PIA1 only by the second factor in large parentheses. At the Thomas peak $x=1$ this factor for $Z_T=Z_P$ is just equal to $\frac{1}{16}\nu_T^2$, a factor of 4 less than in the PIA1. This reduction of the cross section at the peak is shown in Fig. 1 where the cross section in the two approximation are plotted. This reduction was also found in the exact numerical calculations of Ref. 8.

At the position of the minimum at $x^2=\frac{1}{2}$ the second factor in large parentheses has the value of $4\nu_T^2$ in the PIA1 but has the value $4(1+2)^2\nu_T^2$ for $Z_T=Z_P$ in the PIA2. This large enhancement at the minimum disagrees with the exact numerical calculations.[8] We conclude that the PIA2 is superior to the PIA1 at the Thomas peak and will give better results for integrated cross sections but does not correctly obtain the value of the cross section at the minimum.

The transverse peaking approximation of Alston[16] also gives a closed-form expression for the IA amplitude. The magnitude at the Thomas peak is higher for this approximation than for the PIA2 but is lower than the PIA1. For symmetric collisions, the transverse peaking approximation is not valid in the region of the Thomas peak, although it represents an improvement over the PIA1 amplitude.

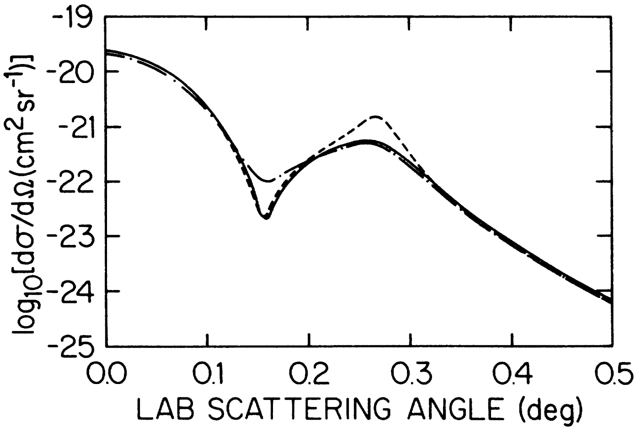

FIG. 1. Log_{10} of the differential cross section in units of $cm^2\,sr$ for electron capture in 10-MeV proton-hydrogen collisions. ——, peaked SPB; — — —, fully peaked impulse approximation (PIA1); —·—·—·, partially peaked impulse approximation (PIA2).

C. The peaked SPB approximation

For highly asymmetric collisions when $Z_T \gg Z_P$, the $\mathbf{p}\cdot\mathbf{J}$ term in Eq. (3.4) is much smaller than $B=K^2+(\mu-iv)^2$ for all values of K and omission of the $\mathbf{p}\cdot\mathbf{J}$ term is warranted. In the symmetric case, we can neglect $\mathbf{p}\cdot\mathbf{J}$ only for values of K such that B is much greater than Z_TJ. At the Thomas peak B is of the order of Z_PJ and since $Z_P\approx Z_T$ we can no longer neglect the $\mathbf{p}\cdot\mathbf{J}$ term. We still neglect $\mathbf{p}\cdot\mathbf{v}$ compared with v^2 in Eq. (3.4) but make no further approximations. The amplitude was evaluated in Ref. 11, but we use a simpler expression derived in the Appendix. We find

$$A_{\mathrm{SPB}}=-\frac{32\pi Z_P^{5/2-2i\nu_T}Z_T^{5/2}e^{\pi\nu_T}v^{2i\nu_T}\Gamma(1+3i\nu_T)\nu_T}{K^4\sinh\pi\nu_T\Gamma(2+i\nu_T)\Gamma(1+2i\nu_T)}\left[\frac{K^2-v^2+Z_T^2-2iZ_Tv-2iZ_PK}{K^2+Z_T^2}\right]^{-i\nu_T}\times\left[\left[\frac{1-i\nu_T}{K^2+Z_T^2}+\frac{1+i\nu_T}{K^2-v^2+Z_T^2-2iZ_Tv-2iZ_PK}\right]{}_2F_1(i\nu_T,i\nu_T,1+2i\nu_T;z)+\frac{4Z_PK\nu_T(1+i\nu_T)}{(1+2i\nu_T)(K^2-v^2+Z_T^2-2iZ_Tv-2iZ_PK)^2}{}_2F_1(1+i\nu_T,1-i\nu_T;2+2i\nu_T;z)\right], \tag{3.10}$$

where

$$z=\frac{K^2-v^2+Z_T^2-2iZ_Tv+2iZ_PK}{K^2-v^2+Z_T^2-2iZ_Tv-2iZ_PK}. \tag{3.11}$$

Explicit expressions for the cross section are not given since no simplifications emerge upon taking the magnitude of the SPB amplitude.

In the Thomas peak region $K=v$ so that $z\approx 0$, the hypergeometric functions equals unity, and the second term in square brackets is negligible. The value of the amplitude in this region is therefore almost identical to the PIA2 amplitude. This is shown in Fig. 1 where the solid curve represents the peaked SPB approximation. Note the close agreement with the PIA2 cross section at the Thomas peak, and, therefore with the exact IA (not shown) of Ref. 8.

No simple analytic form has been obtained for the amplitude at the minimum where $K=v/2$. Rather, we have evaluated the hypergeometric functions numerically. The cross section at the minimum thus obtained agrees with the PIA1 and the exact IA. Agreement with the PIA1 at the minimum was also noted in calculations by McGuire and co-workers.[11] Such agreement is purely fortuitous, since the SPB, exact IA, and PIA1 approximations are quite different. The Coulomb-modified SPB series of Ref. 12 includes a new term of order $1/v^2$ smaller than the dominant terms in Eq. (3.10). Since the magnitude of the cross section at the minimum depends upon terms of the order of $1/v^2$, these neglected terms will also contribute at the minimum. The only significant conclusions that can be inferred from these results is that the deep minimum does not disappear in the SPB approximation. This is important, since it indicates that the calculations of Refs. 8 and 11 do indeed give a shape for the Thomas peak which is unchanged when less restrictive approximations are used. Observations support these conclusions.[1]

Figure 2 compares the SPB cross section using Eq. (3.10) with experimental data of Vogt *et al.*[16] for 5-MeV proton-hydrogen atom collisions. The theory curve has not been averaged over the experimental angular resolution. Agreement at the Thomas peak is not as good as obtained in Ref. 17 using the peaked SPB approximation of Ref. 8 which lies above the observations. In contrast, the present approximation reduces the cross section at the peak to values which lie below the experimental data. The reduction obtained in our approximation is substantiated by experiment but the value of the resulting cross section at the peak is not. This is in qualitative agreement with calculations of McGuire and Sil quoted in Ref 17. The SPB cross section we obtain is larger and in better agreement with the data than the comparable SPB cross sections quoted in Ref. 17.

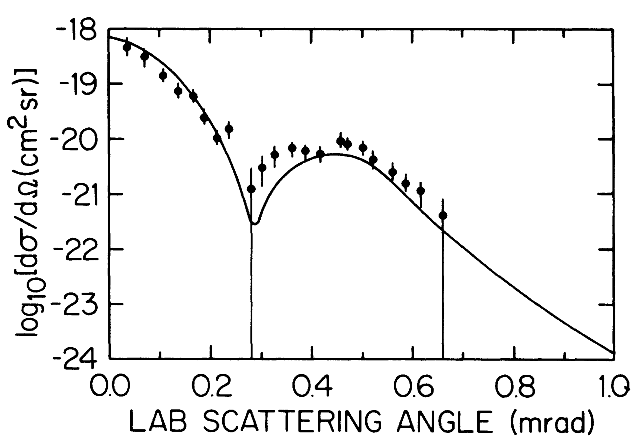

FIG. 2. Log_{10} of the differential cross section in units of $\text{cm}^2\,\text{sr}^{-1}$ for electron capture in 5-MeV proton-hydrogen collisions. The solid curve is the peaked SPB approximation of Eq. (3.10) and the data is from Ref. 17. The theory is not averaged over the experimental solid angle.

The minimum occurs because of a cancellation of the dominant terms in the expressions for the capture amplitude. At the minimum, the amplitude is sensitive to terms of order ν_T or ν_P smaller than the dominant second-order amplitude. Since some terms of this order are neglected in the impulse approximation and in the SPB amplitude, the value at the minimum is not yet accurately known. Indeed, third Born terms are of this order, and could affect the value at the minimum.

IV. CONCLUSIONS

We have reproduced, using somewhat different analytical techniques, the SPB amplitudes of Sil and McGuire.[11] Our methods give slightly simpler results for the 1*s*-1*s* capture amplitudes, in that fewer parametric derivatives are needed. We have also applied the less restrictive peaking approximation to the IA amplitude of Briggs[3] and obtain a closed-form expression. The new IA amplitude is more accurate at the Thomas peak but does not adequately describe the minimum in the angular distribution. The SPB amplitude is in good agreement with the exact IA amplitude, both at the Thomas peak and at the minimum. The agreement at the peak is expected, but the agreement at the minimum appears to be fortuitous.

ACKNOWLEDGMENT

Support for this research by National Science Foundation Grant No. PHY-8602988 is gratefully acknowledged.

APPENDIX: EVALUATION OF AN INTEGRAL

Consider the integral,

$$I(a,b,lm)=\int (Z_P^2+p^2)^{-2-a}(B+2\mathbf{p}\cdot\mathbf{J})^{-b}p^l Y_{lm}(\hat{\mathbf{p}})d^3p \; . \quad \text{(A1)}$$

With the representation,

$$(B+2\mathbf{p}\cdot\mathbf{J})^{-b}=\frac{(\pm i)^b}{\Gamma(b)}\int_0^\infty e^{\mp ix(B+2\mathbf{p}\cdot\mathbf{J})}x^{b-1}dx \; , \quad \text{(A2)}$$

where the $+$ sign in the exponential is taken if $\text{Im}(B)$ is positive, and evaluating the integrals over $\mathbf{p}$ in Eq. (A1) using standard Bessel function relations [Eqs. (10.1.47) and (11.4.44) of Ref. 18] gives the result

$$I(a,b,lm)=(\pm i)^{b+1}(-1)^l 2\pi^{3/2}J^{a+1/2}Z_P^{l-1/2-a}Y_{lm}(\hat{\mathbf{J}})$$
$$\times\frac{1}{\Gamma(b)\Gamma(2+a)}\int_0^\infty x^{b+a-1/2}e^{\mp ixB}K_{1-1/2-a}(2JZ_Px)dx,\quad 1<2\,\mathrm{Re}(a+\tfrac{3}{2})\ . \tag{A3}$$

The integral over x in Eq. (A3) is evaluated using Eqs. (6.621)–(6.623) of Ref. 19 to give the final result

$$I(a,b,lm)=2\pi^2(-1)^1(2JZ_P)^lY_{lm}(\hat{\mathbf{J}})(2Z_P)^{l-1-2-a}(B\mp 2iJZ_P)^{-b-1}$$
$$\times\frac{\Gamma(l+b)\Gamma(1-l+b+2a)}{\Gamma(b)\Gamma(1+b+a)\Gamma(2+a)}{}_2F_1(l+b,l-a;1+b+a;z)\ , \tag{A4}$$

where

$$z=\frac{B\pm 2iJZ_P}{B\mp 2iJZ_P}\ , \tag{A5}$$

and

$$\mathrm{Re}(b+a+\tfrac{1}{2})>\mathrm{Re}(1-\tfrac{1}{2}-a)\ .$$

The expression for the SPB amplitude employs $B=(\mu-iv)^2+K^2$ and requires the derivative of $I(a,b,lm)$ with respect to μ. We evaluate this derivative directly from Eq. (A1) noting that

$$\frac{\partial I(a,b,lm)}{\partial\mu}=-2b(\mu-iv)I(a,b,+1,lm)\ , \tag{A6}$$

thereby expressing the derivative in terms of the generic integral $I(a,b,lm)$. These results for $l=0$ were employed to obtain Eq. (3.9) of Sec. III.

Note that $I(a,b,lm)$ may be written in the alternative form, using Eq. (15.3.26) of Ref. 13

$$I(a,b,l)=2\pi^2(-1)^1(2JZ_P)^lY_{lm}(\hat{\mathbf{J}})(2Z_P)^{l-1-2-a}(2B)^{-1-b}$$
$$\times\frac{\Gamma(1+b)\Gamma(1-l+b+a)}{\Gamma(b)\Gamma(1+b+z)\Gamma(2+a)}{}_2F_1\left[\tfrac{1}{2}(l+b),\tfrac{1}{2}(l+b+1);1+a+b;1+\frac{4J^2Z_P^2}{B^2}\right]\ . \tag{A7}$$

This form shows that the expression for $I(a,b,lm)$ is independent of the sign in the exponential employed in the representation of Eq. (A2). In transforming Eq. (A7) back to the form Eq. (A6) one chooses the sign such that the real part of

$$(-4J^2Z_P^2/B^2)^{1/2} \tag{A8}$$

is positive.

The vector J may be complex; $\mathbf{J}=\mathbf{J}_r+i\mathbf{J}_i$. Then our final result still holds although the evaluation procedure is more complicated. We choose x such that xJ is real, and choose the sign in exponential of Eq. (A2) so that the real part of $\mp ix(B+2\mathbf{p}\cdot\mathbf{J})$ is negative, and then employ Eq. (10.1.47) of Ref. 18 as before. The integral over the magnitude of $\mathbf{p}$ is evaluated in the second step. Since the result is independent of the $\mp$ sign, the integrals over the angular variables are evaluated using orthogonality properties of the spherical harmonics. The result is identical to Eq. (A4), but the magnitude of J is understood to be given by

$$J=(\mathbf{J}\cdot\mathbf{J})^{1/2}\ ,$$

and

$$\hat{\mathbf{J}}=\mathbf{J}/J\ .$$

The important case $l=0$ was evaluated earlier in Ref. 11. These authors obtained a rather complicated result involving several terms with two parametric derivatives. In contrast, our equivalent result is expressed directly in terms of $I(a,b,lm)$, which itself has the relatively simple expression Eq. (A4).

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