Further study of a new dispersion relation for electron-atom scattering

A. K. Bhatia and A. Temkin
Laboratory for Astronomy and Solar Physics, National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, Maryland 20771
(Received 31 August 1987)

A new recently proposed dispersion relation (DR) [Temkin, Bhatia, and Kim, J. Phys. B **19**, L707 (1986)] is tested for *e*-He scattering; the results show that the new DR is *not* satisfied. Therefore we start to investigate the analytic structure of the difference amplitude, previously assumed to be nonsingular, on the negative scattering energy axis. Even under severe approximations we find that the difference amplitude contains both poles and branch points. This suggests, however, a useful approximation of these contributions to the DR which gives very satisfactory agreement in both *e*-H and *e*-He scattering. We conclude with some brief general remarks on this problem.

I. INTRODUCTION

In the case of electron-atom scattering the question of a correct dispersion relation has both fundamental theoretical and practical implications. From the theoretical point of view the problem has been—from the very beginning—to derive a dispersion relation (DR) which correctly incorporates exchange (identity of incoming and orbital electrons). The difficulty manifests itself in discerning the analytic properties of the forward-angle elastic scattering amplitude on the negative energy ($k^2<0$) scattering axis. From a practical point of view, which includes primarily being able to test the accuracy and/or consistency of measured and/or calculated cross sections, a correct DR would provide an invaluable tool in that direction.

Briefly, developments of a DR in electron scattering were initiated by Gerjuoy and Krall[1] (GK). They proposed an *e*-atom DR based on writing the scattering as a sum of direct and exchange amplitudes. They assumed that the direct amplitude was governed by an ordinary (potential-type) DR relative to a first Born amplitude with the usual type poles coming from composite bound state on the negative-energy axis.[1] The first Born direct amplitude is subtracted to ensure that on the outer circle the difference vanishes in the k^2 plane as $k^2 \rightarrow \infty$. The new ingredient of the GK treatment concerned the exchange amplitude: the hypothesis that it is governed by a similar DR in which the exchange Born amplitude has been subtracted. Here the subtraction is not for the circle at infinity (both exact and Born exchange vanish separately), but because the Born exchange itself (which can be evaluated analytically for *e*-H scattering) has nonphysical poles at $k^2<0$, whose effect was expected to be present in the exact exchange amplitude and therefore had to be subtracted out. Nevertheless, by 1975 good enough data and calculations had become available to disprove the GK-DR numerically, as was first shown convincingly in *e*-He scattering by Byron, de Heer, and Joachain.[2]

There were numerous further analyses all of which corroborated the inadequacy of subtracting the first Born exchange amplitude; however, none—except for the papers we shall now discuss—offered an explicit correction. Of the exceptions, Amusia and Kuchiev[3] attempted to sum the divergent parts of the entire exchange Born amplitude series. From a numerical point of view the results are mixed. In application to *e*-H scattering the (partially) summed series gave an analytical result[3] very similar to the exchange first Born amplitude with first-, second-, and third-order poles at $k^2=-1$. When numerically presented, they are in fact significantly less satisfactory in the range $0 \le k^2 \le 1$ than even the GK result. On the other hand, when applied to *e*-He by Kuchiev[4] the corresponding term now contains an irrational power (i.e., a branch cut on the negative-k^2 axis), and here the numerical results are quite impressive. (Both sets of results are given below.)

The second approach offering an explicit alternative to GK-DR has been given by us.[5] We proceeded from the idea that the exchange Born series is not a natural way of including exchange, recalling that the exchange Born series may not even be convergent.[6] Thus we proposed the static-exchange amplitude[7] as the basis of comparison with the full amplitude, and conjectured that the differences would be well behaved on the negative k^2 axis.

The numerical checks of our DR for *e*-H scattering,[5] depending as it does on theoretical calculation rather than reliable experimental total cross sections at intermediate energies, were not definitive. Therefore, in Sec. II we have applied our DR to *e*-He scattering, where experiment and theory in the appropriate energy ranges are sufficiently precise that a decidedly negative result cannot be blamed on uncertainties in those quantities. The application requires calculations of accurate static-exchange *e*-He phase shifts, and that calculation is the substance of Sec. II. We shall find that our DR is not satisfied.

Thus we are led to examine analytically the omitted contribution to $f-f^{(0)}$ in Sec. III; here we revert back to the case of *e*-H scattering. Using the simplest reasonable approximations, we find that this omitted term contains branch cuts as well as poles on the negative k^2 axis. (These poles and branch points do *not* arise in the corresponding e^+-H analysis.) Therefore we augment our DR with two terms, one to represent the pole and the second the branch-cut contributions from the negative k^2 axis. With such an addition, excellent satisfaction of our augmented DR both in the e-H and e-He examples is obtained.

At the end of the article we shall make some more general remarks concerning the validity of an ordinary DR for the direct scattering amplitude, and its violation for exchange.

II. APPLICATION OF DR TO e-He SCATTERING

In the k^2 plane the new (forward angle $\Longrightarrow \theta=0°$) dispersion relation[5] (DR) is (Rydberg units throughout):

$$\mathrm{Re}f(k^2,0)=\mathrm{Re}f^{(0)}(k^2,0)+\frac{1}{4\pi^2}\mathrm{P}\left[\int_0^\infty \frac{k'\sigma((k')^2)}{(k')^2-k^2}dk'^2-\int_0^\infty \frac{k'\sigma^{(0)}((k')^2)}{(k')^2-k^2}dk'^2\right] -\sum_\nu\left[\frac{\gamma_\nu(\kappa_\nu)}{k^2+|\kappa_\nu|^2}-\frac{\gamma_\nu^{(0)}(\kappa_\nu^{(0)})}{k^2+|\kappa_\nu^0|^2}\right]. \tag{2.1}$$

The scattering energy k^2 is related to the total energy E in the usual way,

$$E=\varepsilon_0+k^2\ , \tag{2.2}$$

where ε_0 (<0) is the energy of the ground state of the target atom. The *superscript* zero in (2.1) and below always refers to the corresponding quantities in the static exchange approximation. P in (2.1) represents the principal value of the integrals in question, and the sum over ν in (2.1) is the contribution from the bound state poles of the composite system. [But since there are no He$^-$ bound states, those terms will not enter the (e-He) application.]

Of the quantities that are required in (2.1) (ε_0 and ε_1 being the ground and first excited state energies of the target, respectively), then for $k^2<\varepsilon_1-\varepsilon_0$, the scattering amplitude is in the elastic region and can be conventionally written in partial wave form,

$$f(k^2,\theta)=k^{-1}\sum_\ell(2\ell+1)e^{i\eta_\ell}\sin\eta_\ell P_\ell(\cos\theta)\ . \tag{2.3}$$

In particular the forward angle scattering amplitude $f(k^2,0)$ can be trivially evaluated from very accurately calculated phase shifts of O'Malley *et al.*[8] and Nesbet,[9] which for our purposes can be considered identical. The elastic cross sections obtained from them are in turn consistent with measured cross sections in the elastic range, within the error of the experiment. On the right-hand side (rhs) of the DR we therefore also use the calculated cross section[8,9] in the elastic range, and measured cross sections[10–13] in the range 19.6 eV $<k^2<$ 700 eV range. Beyond 700 eV we use the asymptotic formula

$$\sigma_T((k')^2)=\pi\left[\frac{6.1772}{(k')^2}+\frac{24.6256}{(k')^4}-\frac{3931.47}{(k')^6}+\frac{3.01}{(k')^2}\ln[(k')^2]\right]. \tag{2.4}$$

The $(k')^{-4}$ and $(k')^{-6}$ coefficients in (2.4) are obtained by fitting to the data at $(k')^2=700$ and 800 eV. The coefficients of the first $(k')^{-2}$ and logarithmic term for e-He are taken from Ref. 14.

What has not been uniformly calculated but is needed for this application are the static-exchange scattering results. This is a one channel problem in which the phase shifts $\eta_\ell^{(0)}$ are derived from the radial functions $u_\ell^{(0)}$ with asymptotic forms

$$\lim_{r\to\infty} u_\ell^{(0)}(r)=\sin(kr-\tfrac{1}{2}\ell+\eta_\ell^{(0)})\ , \tag{2.5a}$$

which satisfy the integro-differential equations coming from

$$\langle\varphi_0 Y_{\ell 0}\,|\,H-E\,|\,\Psi_{\ell 0}^{(0)}\rangle=0\ . \tag{2.5b}$$

Here, the full partial-wave exchange approximate functions $\Psi_\ell^{(0)}$ are given by (suppressing spin variables)

$$\Psi_\ell^{(0)}=\frac{u_\ell^{(0)}(\mathbf{r}_1)}{r_1}Y_{\ell 0}(\Omega_1)\varphi_0(\mathbf{r}_2,\mathbf{r}_3)+\begin{bmatrix}1&2&3\\2&3&1\end{bmatrix}+\begin{bmatrix}1&2&3\\3&1&2\end{bmatrix}, \tag{2.6}$$

where the symbols in the last two terms represent terms with the appropriately permuted indices. There have been many calculations of this approximation starting from its inception with Morse and Allis.[7] But what has not been carefully tested in this approximation is the dependence of the phase shifts $\eta_\ell^{(0)}$ on the quality of the approximation to the ground state φ_0. To that end we have used basically four types of target functions listed in Table I. Note that none of the functions is of Hylleraas type; even W_4 contains only even powers of r_{12}. Nevertheless, for the accuracy we require we believe that these φ_0 are quite sufficient, as is explained in the next paragraph.

Selected static-exchange phase shifts are given in Table II. Here we see that the most important correlation beyond the closed shell is the radial (i.e., in-out correlation) followed by the angular correlation centered at equal radial distance (W_3). From W_4 we see that all these correlations can be represented by a single nonlinear parameter configuration interaction function providing there are enough linear parameters available.

The static-exchange cross sections obtained from these

TABLE I. Helium target state approximations.

Designation	Description	Form	Nonlinear parameters	Ground-state energy (Ry)
W_1	closed shell	$e^{-\gamma(r_1+r_2)}$	$\gamma=1.6875$	-5.6953
W_2	open shell	$e^{-(\gamma_1 r_1+\gamma_2 r_2)}+(1\rightleftarrows 2)$	$\gamma_1=2.1832$ $\gamma_2=1.1886$	-5.7513
W_3	open shell plus closed shell	$aW_2+be^{-\delta(r_1+r_2)}\cos\theta_{12}$	$\delta=2.4960$	-5.7903
W_4	correlated configuration integration	$e^{-\mu(r_1+r_2)}\sum^{8\text{ terms}} f_{lmn}$ $f_{lmn}=C_{lmn}(r_1^l r_2^m+r_1^m r_2^l)r_{12}^{2n}$	$\mu=2.15$	-5.7942
Exact energy[a]				$-5.8074\ldots$

[a]Reference 24.

phase shifts are smoothly extrapolated for $(k')^2>25$ using the formula

$$\sigma^{(0)}((k')^2)=\pi\left[\frac{4.1362}{(k')^2}-\frac{13.608\,21}{(k')^4}+\frac{305.1067}{(k')^6}\right]. \tag{2.7}$$

Here, in contrast to the asymptotic formula for the total cross section (2.4), there are no logarithmic terms due to the absence in this (static-exchange) approximation of long-range forces. Curves of total- and static-exchange cross sections are given in Fig. 1.

From these cross sections and phase shifts as described above, we can evaluate the rhs and the left-hand side (lhs) of the dispersion relation (2.1) in the elastic region of k^2. Results for the DR are given in Table III. Let us straightaway note and acknowledge that the lhs and rhs of (2.1) are decidedly *not* equal. The conclusion is clear: Our original dispersion relation (2.1) is not correct! In the next to last column of Table III we have added a term $\Delta'(k^2)$ to the rhs of (2.1),

$$\Delta'(k^2)=\frac{A}{I+k^2}+\frac{B}{k^2}\ln\left[1+\frac{k^2}{I}\right], \tag{2.8}$$

with A and B chosen so as to minimize the difference from the lhs of (2.1). I is the ionization potential for the last electron (i.e., the first ionization potential) of the target atom; in the case of He $I=1.8075$ Ry (cf. Table I). The form of $\Delta'(k^2)$ will be discussed in Sec. III; suffice it here to say that it is not an *ad hoc* "discrepancy function."

In the last column of Table III we give the rhs of the dispersion relation of Amusia and Kuchiev applied as modified to e-He scattering by Kuchiev.[4] It is important to state that the rhs of this DR is different from our DR (as well as the GK-DR). In particular it does not involve the static-exchange approximation at all. Given the fact that there are no adjustable parameters, the agreement with the lhs [which is $\mathrm{Re}f(k^2,0)$ in all these DR's] is very impressive. However, a better assessment of that DR will necessitate a consideration of e-H scattering, and that will be the subject of the next section.

With regard to static-exchange versus total cross section, note that they cross in *three* places in Fig. 1. One

TABLE II. e-He static exchange phase shifts for various target wave functions. (Results in radians.)

		Target approximation			
L	k	W_1	W_2	W_3	W_4
0	0.3	2.7130	2.4750	2.7071	2.7071
	0.5	2.4430	2.1341	2.4378	2.4326
	0.7	2.1994	1.9636	2.1959	2.1905
1	0.5	0.031 60	0.048 57	0.046 62	
	1.0	0.1538	0.1915	0.1828	
	3.0	0.3335	0.3496	0.3470	
	5.0	0.3245	0.3358	0.3358	
5	1.0	0.7443×10^{-5}	0.3084×10^{-4}	0.3641×10^{-4}	
	3.0	0.4761×10^{-2}	0.8481×10^{-2}	0.8468×10^{-2}	
	5.0	0.2243×10^{-1}	0.2918×10^{-1}	0.2917×10^{-1}	
6	3.0	0.1692×10^{-2}	0.3715×10^{-2}	0.3707×10^{-2}	
	5.0	0.1182×10^{-1}	0.1693×10^{-1}	0.1692×10^{-1}	

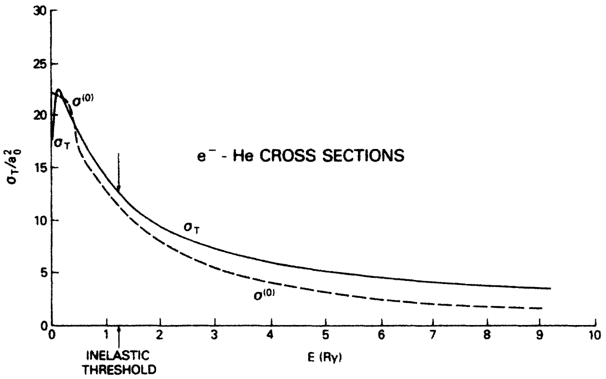

FIG. 1. e-He cross sections. Solid curve, σ_T, is total cross section based on calculations and data cited in text. Dashed curve, $\sigma^{(0)}$, is presently calculated static-exchange cross section (cf. Table II).

can expect that some unevenness of the principal value term of our DR, Eq. (2.1) in this energy region. In Table IV we present results at a finer mesh in the low-energy region and what we find is a slight deviation from monotonicity on the lhs [i.e., Re(f)] and the same for some of the individual terms of the rhs. When one combines those terms the small nonmonotonicity on the rhs cancels out. Also, our augmentation term $\Delta'(k^2)$ is monotonic; we suspect that in order to obtain a precise enough duplication of Re(f) one will require a more accurate representation of the poles and branch points on the negative k^2 axis. This will clearly represent an interesting area of future study.

III. ANALYTIC CONSIDERATIONS: e-H SCATTERING

A. Exact expressions

Having shown that the DR (2.1) is not correct, or more precisely not complete, we must examine the analytic structure of the difference amplitude,

$$\Delta f \equiv f(k^2,0) - f^{(0)}(k^2,0) , \tag{3.1}$$

particularly on the negative k^2 axis. The requirement for analytic results excludes the helium target, so we here revert back to e-H scattering. Even here what may appear as severe approximations are required, but we emphasize our basic assumptions: *it is highly unlikely (although possible) that the exact expression can be analytically less complicated than the one we shall evaluate*, based on the simplifying approximations we shall make. If we find that our approximation for Δf contains poles and branch points for k^2 negative (as we shall), then we believe the exact Δf must have at least that complicated an analytic structure.

Let us start by deriving an exact formal expression for Δf. From the Feshbach formalism[15] and the exact equations for f and $f^{(0)}$ (recall the superscript zero signifies the exchange approximation),

$$(PHP + \mathcal{V}_{\text{op}} - E)P\Psi = 0 , \tag{3.2a}$$

$$(PHP - E)P\Psi^{(0)} = 0 , \tag{3.2b}$$

we have

$$P\Psi = P\Psi^{(0)} + G_p \mathcal{V}_{\text{op}} P\Psi , \tag{3.3}$$

where $\Psi^{(0)} = P\Psi^{(0)}$ is given by (2.6), and G_p is the P-space Green's function. In the elastic range, G_p can be decomposed in partial wave form [and recall we are here confining ourselves to the two-electron (e-H) problem, and the subscripts or superscripts ($\pm$) mean singlet and triplet scattering]

$$G_p(\mathbf{r}_1,\mathbf{r}_1';\mathbf{r}_2,\mathbf{r}_2') = \sum_{\ell,m} \left[g_\ell^{(\pm)} \frac{(r_1,r_1')}{r_1 r_1'} Y_{\ell m}(\Omega_1) Y_{\ell m}(\Omega_1') \, | \varphi_0(r_2) \rangle \langle \varphi_0(r_2') | \pm (1 \rightleftarrows 2) \right] , \tag{3.4}$$

TABLE III. e-He dispersion relation. The parameters [Eq. (2.8)] are $A = -0.771\,56$ and $B = -0.143\,45$, and recall that $I = 1.8075$ (see text).

k	lhs	rhs (2.1)	rhs (2.1) + $\Delta'(k)^2$	Kuchiev[a]
0	-1.157	-0.663	-1.169	-1.090
0.1	-1.117	-0.591	-1.095	-1.024
0.2	-0.954	-0.447	-0.943	-0.870
0.3	-0.722	-0.245	-0.729	-0.674
0.4	-0.457	$+0.006$	-0.462	-0.422
0.5	-0.170	0.271	-0.178	-0.157
0.6	$+0.112$	0.527	$+0.099$	0.101
0.7	0.381	0.793	$+0.387$	0.372
0.8	0.619	1.006	0.623	0.593
0.9	0.824	1.171	0.811	0.768
1.0	0.997	1.347	1.009	0.957
1.1	1.145	1.465	1.149	1.087

[a]Kuchiev, Ref. 4.

TABLE IV. e^--He DR at low energies. All results interpolated by a spline fit from $k=0,0.1,0.2,\ldots$ results. $\mathcal{J}$ and $\mathcal{J}_0$ are the integrals on the right-hand side of Eq. (2.1).

k	lhs=Re(f)	Re(f_0)	$\mathcal{J}$	$-\mathcal{J}_0$	$\Delta'(k^2)$	rhs
0	−1.157	−1.468	2.584	−1.779	−0.506	−1.169
0.25	−1.160	−1.465	2.552	−1.729	−0.506	−1.148
0.05	−1.154	−1.457	2.557	−1.731	−0.505	−1.136
0.075	−1.140	−1.445	2.558	−1.727	−0.505	−1.119
0.100	−1.117	−1.429	2.558	−1.720	−0.504	−1.095
0.125	−1.086	−1.408	2.555	−1.709	−0.502	−1.064
0.150	−1.048	−1.383	2.550	−1.695	−0.500	−1.028
0.175	−1.004	−1.354	2.544	−1.679	−0.498	−0.987
0.200	−0.954	−1.320	2.534	−1.661	−0.496	−0.943
0.225	−0.905	−1.282	2.522	−1.641	−0.493	−0.894
0.250	−0.844	−1.240	2.506	−1.618	−0.490	−0.842
0.275	−0.784	−1.196	2.489	−1.594	−0.487	−0.788
0.300	−0.722	−1.148	2.471	−1.568	−0.484	−0.729
0.325	−0.658	−1.098	2.453	−1.541	−0.480	−0.666
0.350	−0.593	−1.045	2.433	−1.512	−0.476	−0.600

where the radial Green's functions $g_\ell^{(\pm)}(r_1,r_1')$ satisfies

$$[\mathcal{L}_{\rm ex}^{(\pm)}(\ell)-k^2]g_\ell^{(\pm)}(r_1,r_1')=k^{-1}\delta(r_1-r_1') \ . \qquad (3.5)$$

$\mathcal{L}_{\rm ex}^{(\pm)}(\ell)$ is the radial static-exchange operator[16] operating the radial Green's functions $g_\ell^{(\pm)}(r_1,r_1')$: specified in the form

$$g_\ell^{(\pm)}(r_1,r_1')=u_\ell^{(\pm)}(r_<)v_\ell^{(\pm)}(r_>) \ , \qquad (3.6)$$

where $u_\ell^{(\pm)}$ and $v_\ell^{(\pm)}$ are regular and irregular solutions of the homogeneous part of (3.5) (i.e., solutions of the exchange approximation), with the irregular solution obeying the asymptotic condition

$$\lim_{r\to\infty} v_\ell^{(\pm)}(r)\propto e^{i(kr-\pi\ell/2)} \ . \qquad (3.7)$$

Then the function $P\Psi^{(\pm)}$ of (3.3) is indeed a solution of the Schrödinger equation, from whose asymptotic form we obtain our basic expression for the exact scattering amplitude $f(E,\theta)$ in terms of static-exchange amplitude

$$f(E,\theta)=f^{(0)}(E,\theta)+\sum_\ell\left\langle\frac{u_\ell(r_1)}{r_1}Y_{\ell o}(\Omega_1)\varphi_0(r_2)\mathcal{V}_{\rm op}P\Psi_\ell\right\rangle \ . \qquad (3.8)$$

[Here and below we shall drop the ($\pm$) superscripts.] The optical potential is formally given by[15]

$$\mathcal{V}_{\rm op}=PHQ\frac{1}{E-QHQ}QHP \ , \qquad (3.9')$$

which may conveniently be expanded in terms of the eigenfunctions of QHQ,

$$QHQ\Phi_m=\mathcal{E}_n\Phi_n \qquad (3.10)$$

giving rise to [cf. Eq. (3.14) below]

$$\mathcal{V}_{\rm op}=\sum_n\frac{PHQ\mid\Phi_n\rangle\langle\Phi_n\mid QHP}{E-\mathcal{E}_n} \ . \qquad (3.9'')$$

One may show that QHP in (3.9) involving the complete Hamiltonian reduces to[17] (for the two-electron problem)

$$QHP=Q(2/r_{12})P \qquad (3.11)$$

(and similarly for PHQ). Thus the optical potential is written finally

$$\mathcal{V}_{\rm op}=\sum_n\frac{P(2/r_{12})\mid Q\Phi_n\rangle\langle\Phi_nQ\mid(2/r_{12})P}{E-\mathcal{E}_n} \ . \qquad (3.9''')$$

From (3.9‴) one sees that in using the projection operators P and Q one can completely eliminate the core terms from the interaction. For the two-electron system, P and hence $Q=1-P$ are explicitly given by[18]

$$Q=1-P_1-P_2+P_1P_2 \ , \qquad (3.12a)$$

where

$$P_i=\varphi_0(r_i)\rangle\langle\varphi_0(r_i) \ . \qquad (3.12b)$$

Finally, the fact that the spectrum $\mathcal{E}_n$ is bounded from below ($\mathcal{E}_n\geq\mathcal{E}_1>\varepsilon_0=-1$) well into the scattering continuum, $k^2<k_r^2$ ($k_r^2<(\varepsilon_1-\varepsilon_0)$), implies $E-\mathcal{E}_1<0$ for finite range of scattering energies k^2 where $E=-1+k^2$. Hence,

$$E-\mathcal{E}_1\leq E-\mathcal{E}_2\leq\cdots<0 \ , \qquad (3.13a)$$

for all $k^2<k_r^2$. But (3.13a) implies

$$0>\frac{1}{E-\mathcal{E}_1}\geq\frac{1}{E-\mathcal{E}_2}\geq\cdots\geq\frac{1}{E-\mathcal{E}_n}\geq\cdots \ , \qquad (3.13b)$$

and, using the fact that $Q\mid\Phi_n\rangle\langle\Phi_n\mid Q$ is positive definite and (by completeness in Q space),

$$\sum_n Q\mid\Phi_n\rangle\langle\Phi_n\mid Q=Q \ , \qquad (3.14)$$

we have from (3.11)

$$\mathcal{V}_{\rm op} \le \frac{1}{E-\mathcal{E}_1}\left[P\frac{2}{\mathbf{r}_{12}}Q\frac{2}{\mathbf{r}_{12}}P\right] . \qquad (3.15)$$

In this form the P operators have no further effect and may therefore be omitted. We shall use (3.15) as the basis of one of our central approximations as detailed in Sec. III B.

B. Approximations

Only if one knew the partial wave functions $P\Psi_\ell$ exactly and analytically would the above formulas, specifically (3.8), be useful for the purpose of analyzing the DR rigorously. Over and above that, one would have to sum *analytically* over partial waves ℓ, because it is known that the analytic properties of the full amplitude (as a function of k^2) may be different from those of partial wave amplitude.[19] Since our motivation here is to derive an expression of least complexity (cf. italicized statement, Sec. III A) we institute the following approximations (constants of proportionality are not included here):

$$u_\ell(kr)/kr \to i^\ell j_\ell(kr) , \qquad (3.16)$$

$$\Psi^{(\pm)} = \sum_\ell \Psi_\ell^{(\pm)} \to e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2) \pm e^{i\mathbf{k}\cdot\mathbf{r}_2}\varphi_0(r_1) \equiv \Psi_B^{(\pm)} , \qquad (3.17)$$

$$\mathcal{V}_{\rm op} \to \frac{1}{E-\bar{\mathcal{E}}}\sum\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{2}{r_{12}}Q\frac{2}{r_{12}}\Psi_B^{(\pm)}\right\rangle . \qquad (3.18)$$

This gives for the forward angle ($\Longrightarrow \mathbf{k}_f = \mathbf{k}_i \equiv \mathbf{k}$) DR:

$$\tilde{f}^{\,2}(k^2,0) = f^{(0)}(k^2,0) + (k^2-\bar{k}^2)^{-1}\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{2}{r_{12}}Q\frac{2}{r_{12}}\Psi_B^{(\pm)}\right\rangle . \qquad (3.19)$$

[The tilde now emphasizes the fact that the scattering amplitude given by (3.19) is no longer exact.]

The question we want to explore is the analytic dependence of the last term on k^2 for negative values of k^2. Note first, since the mean energy $\bar{k}^2 > 0$, that in this mean energy denominator approximation the denominator $(k^2-\bar{k}^2)^{-1}$ will have no singularities for $k^2<0$, therefore we may ignore it. The remaining integral can be written with the use of Q, Eqs. (3.12) and (3.17), in an obvious notation,

$$\begin{aligned}\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)r_{12}^{-1}Qr_{12}^{-1}\Psi_B^{(\pm)}\rangle &= F_0(k^2)+F_1(k^2)+F_2(k^2)+F_{12}(k^2)\\ &\pm[G_0(k^2)+G_1(k^2)+G_2(k^2)+G_{12}(k^2)] . \qquad (3.20)\end{aligned}$$

For example,

$$\begin{aligned}F_0(k^2) &= \langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)r_{12}^{-1}r_{12}^{-1}e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\rangle ,\\ F_2(k^2) &= -\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)r_{12}^{-1}P_2r_{12}^{-1}e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\rangle .\end{aligned} \qquad (3.20a)$$

More explicitly,

$$\begin{aligned}F_0(k^2) &= \int\int e^{-i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)r_{12}^{-2}e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)d^3r_1\,d^3r_2\\ &= \int\int \varphi_0^2(r_2)r_{12}^{-2}\,d^3r_1\,d^3r_2 . \qquad (3.20b)\end{aligned}$$

Similarly,

$$F_2(k^2) = -\int[\langle\varphi_0(r_1)r_{12}^{-1}\varphi_0(r_2)\rangle_{r_2}]^2 d^3r_1 . \qquad (3.20c)$$

The infinite contribution of each of these integrals will cancel in the sum F_0+F_2, but additionally we see from (3.20b), and (3.20c) that *these terms are independent of* k. Since only these terms would arise in positron-hydrogen scattering, we also see that our approximation is consistent with the more rigorous assertions[20] that the DR for positron-atom scattering (without anomalous thresholds[21]) holds in its original form.

With regard to the remaining integrals it is important to realize that all of the remaining terms, F_1, F_{12}, as well as all the G's arise, in one way or another, because of exchange: the F's because of the extra terms in Q, Eq. (3.12), necessary to describe exchange; and the G's because of the exchange term in $\Psi_B^{(\pm)}$ as well as (3.12). All of these terms, with the exception of $F_1(k^2)$ and $G_1(k^2)=G_2(k^2)$, can be done analytically as an explicit function of k^2. Details of the latter are given in the Appendix. Here we consider $F_1(k^2)$,

$$\begin{aligned}F_1(k^2) &= -\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_2}P_1\frac{1}{r_{12}}e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\rangle\\ &= -\int d^3r_2\left|\left\langle\frac{e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)}{r_{12}}\right\rangle_{r_1}\right|^2\varphi_0^2(r_2) . \qquad (3.21a)\end{aligned}$$

Expanding $e^{i\mathbf{k}\cdot\mathbf{r}_1}$ and r_{12}^{-1} in spherical harmonics and spherical Bessel functions, $j_\ell(kr_1)$ in the usual way allows F_1 to be reduced to a discrete but infinite expansion

$$F_1(k^2) = -64\pi\sum_n(n+1)^{-1}\int_0^\infty dr_2\,r_2^2W_n^2(k,r_2)e^{-2r_2} , \qquad (3.21b)$$

where

$$W_n(k,r_2) = \int_0^\infty dr_1\,r_1^2 j_n(kr_1)e^{-r_1}(r_<^n/r_>^{n+1}) , \qquad (3.22)$$

and $r_> \equiv \max\{r_1,r_2\}$ and $r_< \equiv \min\{r_1,r_2\}$. Each W_n and hence each term of F_1 can be evaluated analytically; for example, the $n=0$ term yields

$$F_1(k^2)\big|_{n=0} = \frac{-64\pi}{(1+k^2)^2}\left[2-\frac{4(7-k^2)}{(1+k^2)(9+k^2)}+\frac{41-5k^2}{8(1+k^2)^2(4+k^2)}\right] . \qquad (3.23)$$

From (3.23) we see that this $n=0$ contribution alone has poles at $k^2=-1$, -3, and -4. However, this does not allow any analytic conclusions about the series when summed over n.

One may avoid the n summation altogether by using the integral representation of r_{12}^{-1},

$$r_{12}^{-1}=(4\pi^2)^{-1}\int d^3p\frac{e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)}}{p^2} . \tag{3.24}$$

Inserting this into (3.21), one arrives at an integral representation of F_1,

$$F_1(k^2)=\frac{256}{\pi^3}\int\int\frac{p^{-2}q^{-2}}{[1+(\mathbf{q}-\mathbf{k})^2]^2[4+(\mathbf{p}-\mathbf{q})^2]^2[1+(\mathbf{p}-\mathbf{k})^2]^2}d^3p\,d^3q . \tag{3.25}$$

We have not been able to integrate this expression analytically; hopefully in the near future we (or someone else) will be able to evaluate it or analyze its analytic structure.

From the Appendix, we see that $F_{12}(k^2)=G_{12}(k^2)$ and $G_0(k^2)$ can be evaluated in closed form,

$$F_{12}(k^2)=G_{12}(k^2)$$
$$=16\pi[(1+k^2)^{-1}-(15+k^2)/(9+k^2)^2] , \tag{3.26}$$

$$G_0(k^2)=4\pi[(\tfrac{5}{3}+k^2)/(1+k^2)^2+(\tan^{-1}k)/k] , \tag{3.27}$$

revealing poles at $k^2=-1$ and -3.

The remaining integrals are $G_1(k^2)$ and $G_2(k^2)$, which are in fact equal to each other, but cannot be done in closed form. We have reduced them to

$$G_1(k^2)=-\langle S(\mathbf{k},\mathbf{r}_2)\varphi_0(r_2)e^{i\mathbf{k}\cdot\mathbf{r}_2}I(r_2)\rangle , \tag{3.28}$$

where $S(k,r_2)$ is the same integral that arose in (3.21a),

$$S(\mathbf{k},\mathbf{r}_2)=\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_1)r_{12}^{-1}\rangle_{\mathbf{r}_1} \tag{3.29}$$

and

$$I(r_2)=\langle\varphi_0^2(r_1)r_{12}^{-1}\rangle_{\mathbf{r}_1}=r_2^{-1}-e^{-2r_2}(1+r_2^{-1}) . \tag{3.30}$$

Again one can expand the integrals in terms of spherical Bessel functions and evaluate them term by term, or one can convert them to momentum space integrals. If one expands $G_1=\sum_{n=0}G_1^{(n)}$ in analogy with (3.21b), then one can readily evaluate $G_1^{(0)}$:

$$G_1^{(0)}(k^2)=\frac{-16\pi}{k(1+k^2)^2}\left[\tan^{-1}k+\tan^{-1}(k/2)-2\tan^{-1}(k/3)-\left[\frac{1-k}{4k}\right]\ln\left[\frac{4+k^2}{1+k^2}\right]-\frac{2k}{9+k^2}+\frac{1}{2k(4+k^2)}\right] . \tag{3.31}$$

In addition to poles, $G_1^{(0)}$ is seen to contain branch points at $k^2=-1,-4$. As regards $G_1^{(1)}(k^2)$, with use of MACSYMA (copyright owned by Massachusetts Institute of Technology and Symbolics, Inc.). Dr. Drachman has kindly evaluated it for us. The result is too complicated to warrant being given here: suffice it to say it also contains branch points at the same values of $k^2=-1,-4$. Noting then that individual terms $G_1^{(n)}(k^2)$ contain branch points, we think it is very unlikely (but not impossible) that they can completely cancel out the sum corresponding to $G_1(k^2)$. Thus we conclude that $G_1(k^2)$ does contain branch points on the $k^2<0$, at least at $k^2=-1$ and $k^2=-4$.

Concerning $\tilde{f}$ as a whole, note that if certain terms cancel in one spin state [i.e., $F_{12}(k^2)-G_{12}(k^2)$ in the triplet state], they will not cancel in the other spin state. Thus there is no way that these singularities and particularly branch points can vanish in general by cancellation.

IV. AUGMENTED DR: APPLICATIONS

The foregoing analyses and numerical results convince us then that a correct DR (for e^--atom scattering) will have a multiplicity of poles and branch points on the negative k^2 axis. However, we consider it hopeless (or very difficult at best and only for the H target) to calculate them and their residues exactly. Therefore, we shall adopt a different point of view: We shall ask to what extent can one replace the analytic structure on the left-hand cut by, say, one pole and one branch point and still maintain a *useful*, if not exact, dispersion relation.

If, for example, as guided by the considerations of Sec. III, we take in the general case such a pole and branch point at $k^2=-I$, where I is the (first) ionization potential of the target atom in question, then an augmented DR would read

$$\mathrm{Re}f(k^2,0)=\mathcal{R}+\Delta'(k^2) , \tag{4.1}$$

where [repeating Eq. (2.8)]

$$\Delta'(k^2)=\frac{A}{I+k^2}+\frac{B}{k^2}\ln\left[1+\frac{k^2}{I}\right]$$

and $\mathcal{R}$ represents the right-hand side of Eq. (2.1). The test of the utility of this augmented DR is whether reasonable values of A and B can be chosen (say, by

TABLE V. DR's for e-H scattering.

Singlet					
		Right-hand side of DR's			
k	lhs	rhs (2.1)	rhs (2.1)$+\Delta'$[a]	Amusia and Kuchiev[b]	Gerjuoy and Krall[c]
0	−5.965	−6.999	−5.952	−2.684	−7.240
0.1	−4.257	−5.419	−4.392	−0.920	−5.403
0.2	−1.503	−2.397	−1.425	+1.959	−2.680
0.3	+0.292	−0.601	+0.287	3.236	−0.730
0.4	1.170	0.458	1.242	3.861	+0.262
0.5	1.544	0.943	1.613	3.782	0.770
0.6	1.723	1.086	1.640	3.742	1.049
0.7	1.846	1.425	1.869	3.762	1.267
0.8	2.027	1.636	1.978	3.701	1.514
Triplet					
		Right-hand side of DR's			
k	lhs	rhs (2.1)	rhs (2.1)$+\Delta'$[d]	Amusia and Kuchiev[b]	Gerjuoy and Krall[c]
0	−1.768	−0.819	−1.755	−5.104	−0.547
0.1	−1.484	−0.539	−1.458	−4.764	−0.281
0.2	−0.833	0.045	−0.826	−3.994	+0.281
0.3	0.006	0.778	−0.020	−2.973	+0.994
0.4	0.859	1.538	0.831	−1.897	1.702
0.5	1.576	2.159	1.551	−0.735	2.276
0.6	2.102	2.601	2.094	−0.010	2.683
0.7	2.469	2.892	2.482	+0.454	2.949
0.8	2.722	3.090	2.768	0.938	3.125

[a]The constants in Δ' singlet are $A=2.86$ and $B=-1.81$.
[b]Amusia and Kuchiev DR, Ref. 3.
[c]Gerjuoy-Krall DR. Results from Ref. 5.
[d]The constants in Δ' triplet are $A=-2.46$ and $B=1.53$.

fitting experiment to calculation) such that the lhs and rhs of (4.1) are usefully equal over the whole range (or at the very least in the elastic range) of k^2.

To test this hypothesis we apply (4.1) first to e-He scattering. The results and discussion have already been given in Sec. II in conjunction with Tables I–IV and Fig. 1. Repeating the main conclusions: With the addition of the augmentation term $\Delta'(k^2)$, very good agreement of lhs and rhs of the DR is highly satisfactory, even better than Kuchiev.[4] However, since the latter contains no adjustable parameters, this comparison by itself could be grossly misleading. We therefore will include e-H results of Amusia and Kuchiev[3] as part of the e-H application to which we now return.

In Table V we give separate singlet and triplet e-H results for several DR's. The left-hand side, $\mathrm{Re}f(E,0)$, is the same for all of them and is numerically taken from our first paper.[5] The various right-hand sides are marked in the table. Our original [rhs of Eq. (2.1)] as well as the Gerjuoy and Krall DR results are also repeated from Ref. 5. We see first that the term $\Delta'(k^2)$ can certainly be adjusted to give fine agreement in the rhs$+\Delta'$ column. On the other hand, the results of Amusia and Kuchiev[3] (AK) are seen to be quite poor. They themselves have noted that other singularities may exist on the $k^2<0$ axis. We would only stress our belief that these consist of branch points as well as poles. The existence of branch points on the $k^2<0$ axis is also consistent with the conclusions of Gerjuoy and Lee.[22]

We believe therefore that the uneven performance of the AK-DR makes it an unreliable guide for use in other systems. Our own augmented DR is not really better unless one has an independent way of determining the semiphenomenological parameters A and B. As we have shown, this is certainly the case in e-H and e-He scattering. In future work we shall consider the next sequential (Li) target: i.e., the e-Li system. Because of both theoretical and experimental problems involving e-Li scattering and some discrepant results that already exist in the literature, this promises to be a very informative investigation.

We conclude this section with the following observation that we believe gives confirmatory evidence for an ordinary DR governing the direct amplitude as opposed to the exchange amplitude. If one writes singlet and triplet amplitudes in terms of direct (f_d) and exchange (g) amplitudes,

$$\begin{aligned} f^{(+)}&=f_d+g \ , \\ f^{(-)}&=f_d-g \ , \end{aligned} \tag{4.2}$$

then it is clear the exchange amplitude (g) will cancel in the sum. It has also been argued very cogently that the direct amplitude by itself will satisfy an ordinary (i.e., one-body potential type) DR (cf. in particular Gerjuoy and Lee[22]). In Table VI we present results, taken from our Table V, for summed singlet plus triplet amplitudes: they demonstrate that the summed (singlet plus triplet) lhs is equal to the summed rhs *in each case* (to reasonable accuracy). We believe this supports not only that an ordinary DR does hold for the direct amplitude, but it also confirms the accuracy of the cross-section calculations, particularly in the intermediate energy range, on which the evaluation of the dispersion integral on the rhs is based. Note that the identity of rhs for the GK and AK dispersion relations is not a coincidence, but is guaranteed by the fact that these DR's differ only in the form of the exchange amplitude that goes into them, and which therefore cancels out the sum.

The above point has been forcefully made by our colleague, Dr. R. J. Drachman.[25] Nevertheless, in our own opinion, it is not obvious that an ordinary DR should hold for the direct scattering amplitude. The reason is the following: If one considers say e-H scattering as a sum of two separate asymmetric solutions, direct Ψ_d and exchange Ψ_e, then we know that Ψ_d has asymptotic forms

$$\lim_{r_1\to\infty} \Psi_d(\mathbf{r}_1,\mathbf{r}_2)=\left[e^{i\mathbf{k}\cdot\mathbf{r}_1}+f_d(\theta)\frac{e^{ikr_1}}{r_1}\right]\varphi_0(r_2)\ , \tag{4.3a}$$

$$\lim_{r_2\to\infty} \Psi_d(\mathbf{r}_1,\mathbf{r}_2)=g(\theta)\frac{e^{ikr_2}}{r_2}\varphi_0(r_1) \tag{4.3b}$$

[with $\Psi_e(\mathbf{r}_1,\mathbf{r}_2)=\Psi_d(\mathbf{r}_2,\mathbf{r}_1)$]. But if we are dealing with a truly asymmetric case, say positron-hydrogen scattering, then there is only a single solution, with asymptotic forms

$$\lim_{r_1\to\infty} \Psi(\mathbf{r}_1,\mathbf{r}_2)=\left[e^{i\mathbf{k}\cdot\mathbf{r}_1}+f(\theta)\frac{e^{ikr_1}}{r_1}\right]\varphi_0(r_2)\ , \tag{4.4a}$$

$$\lim_{r_2\to\infty} \Psi(\mathbf{r}_1,\mathbf{r}_2)=0\ . \tag{4.4b}$$

The comparison shows that for e^+ scattering there is no probability for the initially bound electron (coordinates $\mathbf{r}_2$) to come out [Eq. (4.4b)] below the positronium pickup threshold, whereas for e^--scattering [Eq. (4.3b)] shows that there is no way of avoiding it coming out.

TABLE VI. Summed singlet plus triplet DR's for e-H scattering.

k	lhs	rhs (2.1)	rhs (2.1)+Δ'	AK=GK
0	−7.733	−7.818	−7.799	−7.787
0.1	−5.741	−5.958	−5.932	−5.684
0.2	−2.336	−2.352	−2.336	−2.399
0.3	+0.298	+0.177	+0.190	+0.264
0.4	2.029	1.996	2.005	1.964
0.5	3.120	3.102	3.107	3.047
0.6	3.825	3.687	3.689	3.732
0.7	4.315	4.317	4.315	4.216
0.8	4.749	4.726	4.721	4.639

Thus there is a fundamental distinction between the two situations, and the apparent fact that the direct scattering amplitude satisfies an ordinary DR must have deeper significance.

ACKNOWLEDGMENTS

Special thanks are due to our colleague, Dr. William E. Behring, for his considerable work in obtaining least-squares fits to the coefficients A and B for all cases given in the Tables. We are grateful to Samuel Nelson for assistance to Dr. Behring. Discussions with R. J. Drachman are gratefully acknowledged. We also thank Mrs. E. H. Glover for programming. Computing costs for this work were funded under U.S. National Aeronautics and Space Administration Grant N⊙. NASA-RTOP-188-38-53-14.

APPENDIX: EVALUATION OF $F_{12}(k^2)$, $G_{12}(k^2)$, AND $G_0(k^2)$

We start with

$$F_{12}(k^2)=\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_{12}}P_1P_2\frac{1}{r_{12}}\varphi_0(r_2)e^{i\mathbf{k}\cdot\mathbf{r}_1}\right\rangle\ . \tag{A1}$$

Use the definition of projectors P_i, Eq. (3.12b), then

$$F_{12}(k^2)=\left|\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_{12}}\varphi_0(r_1)\varphi_0(r_2)\right\rangle\right|^2\ . \tag{A2}$$

But

$$\left\langle\varphi_0(r_2)\frac{1}{r_{12}}\varphi_0(r_2)\right\rangle_{r_2}=\frac{1}{r_1}-e^{-2r_1}\left[1+\frac{1}{r_1}\right]\ , \tag{A3}$$

hence,

$$F_{12}(k^2)=\left|\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\left[\frac{1}{r_1}-e^{-2r_1}\left[1+\frac{1}{r_1}\right]\varphi_0(r_1)\right]\right\rangle\right|^2\ , \tag{A4}$$

of which only the s-wave part of $e^{i\mathbf{k}\cdot\mathbf{r}_1}$ contributes to give finally

$$F_{12}(k^2)=16\pi\left[\frac{1}{1+k^2}-\frac{15+k^2}{(9+k^2)^2}\right]\ . \tag{A5}$$

We next consider

$$G_{12}(k^2)=\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_{12}}P_1P_2\frac{1}{r_{12}}\varphi_0(r_1)e^{i\mathbf{k}\cdot\mathbf{r}_2}\right\rangle\ , \tag{A6}$$

which, using the same projectors P_1 and P_2, reduces to

$$G_{12}(k^2)=\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_{12}}\varphi_0(r_1)\varphi_0(r_2)\right\rangle \times\left\langle\varphi_0(r_1)\varphi_0(r_2)\frac{1}{r_{12}}\varphi_0(r_1)e^{i\mathbf{k}\cdot\mathbf{r}_2}\right\rangle\ . \tag{A7}$$

Interchanging dummy variables $r_1\leftrightarrow r_2$ in the second integral shows that it is identical to the first, thus

$$G_{12}(k^2)=\left|\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\frac{1}{r_{12}}\varphi_0(r_2)\varphi_0(r_1)\right\rangle\right|^2 . \tag{A8}$$

This is identical to (A2), hence we have shown

$$F_{12}(k^2)=G_{12}(k^2) . \tag{A9}$$

We consider finally

$$G_0(k^2)=\left\langle e^{i\mathbf{k}\cdot\mathbf{r}_1}\varphi_0(r_2)\left|\frac{1}{r_{12}^2}\right|e^{i\mathbf{k}\cdot\mathbf{r}_2}\varphi_0(r_1)\right\rangle . \tag{A10}$$

Using the integral representation r_{12}^{-2},

$$r_{12}^{-2}=\frac{1}{4\pi}\int d^3p\frac{1}{p}e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)} , \tag{A11}$$

reduce (A10) to

$$G_0(k^2)=\frac{1}{4\pi}\int d^3p\frac{1}{p}\,|\,\langle\varphi_0(r)e^{-i(\mathbf{p}+\mathbf{k})\cdot\mathbf{r}}\rangle\,|^2 \tag{A12}$$

$$=16\pi\int\int\frac{p}{[1+(\mathbf{p}+\mathbf{k})^2]^4}dp\,d\Omega_p \tag{A13}$$

$$=-\frac{16\pi}{3k}\int_0^\infty dp\left[\frac{1}{[1+(p+k)^2]^3}-\frac{1}{[1+(p-k)^2]^3}\right] , \tag{A14}$$

which can be straightforwardly integrated to give

$$G_0(k^2)=4\pi\left[\frac{\tan^{-1}k}{k}+\frac{1}{1+k^2}+\frac{\frac{2}{3}}{(1+k^2)^2}\right] . \tag{A15}$$

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