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Multiple scattering in the Compton effect. V. Bounds on errors associated with multiple-scattering corrections

Elaine Braun-Keller and Irving R. Epstein*
Department of Chemistry, Brandeis University, Waltham, Massachusetts 02154
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The operator formalism developed in the previous paper is used to derive upper and lower bounds on the maximum error associated with multiple-scattering corrections to experimental Compton profiles. In some cases it may be possible to use these bounds to deduce the amount of multiple scattering in the experimental profile.

I. INTRODUCTION

In previous papers in this series,[1-3] we analyzed the nature and the importance of multiple scattering in the Compton effect. We then developed an operator formalism[4] which led to procedures for treating experimental Compton profiles so as to remove the effects of multiple scattering, leaving the true single scattered profile.[5]

There are at least two ways to test the accuracy of a single scattered profile J_s which has been derived from an experimental profile J_E by correction for multiple scattering. One may obtain J_S from a calculation (e.g., Hartree-Fock, band theory, etc.) and compare this profile with the J_S which results from correcting the experimental profile. This approach should be appropriate for small molecules for which there exist very accurate wave functions and profiles. For large molecules or solids, however, where accurate calculations may not be available, comparing the corrected J_E with the calculated J_S may not yield a very informative result. Also, some correction procedures[5(b)] use a calculated J_S to generate the corrections to J_E. Here again, comparison of the corrected and calculated profile will not afford a meaningful test of the results. An alternative method is to perform the experiment on samples of different thicknesses. If the corrected profiles are nearly independent of sample thickness, then one assumes that the corrected profiles are accurate. Such tests are useful, but will give no information about certain types of systematic error in the correction procedure, e.g., using an incorrect operator[4] to generate the multiple from the single scattered profile.

In this paper we show that, using the formalism developed in paper IV, it is possible to obtain an upper and a lower bound to the maximum error in J_S. These bounds are derived in the next section and are calculated explicitly for a simple model experiment in Sec. III. We find that for certain types of correction procedures, the bounds approach zero if x, the fraction of multiple scattering, is known exactly. We show how the bounds may be used to estimate x if a good calculated J_S is available.

II. DERIVATION OF BOUNDS

As in paper IV, we assume that the experimental profile J_E is known, and that we wish to calculate from it the single scattered profile J_S. The profiles are assumed to be related by the equation

$$J_E = (1-x)J_S + x\hat{O}J_S\,, \tag{1}$$

where $x<1$ is the fraction of multiple scattering and the operator $\hat{O}$ applied to the normalized single scattered profile J_S generates the normalized multiple scattered profile J_M. Here we shall consider only double scattering. In this case $\hat{O}$ takes the form[4]

$$\hat{O}J_S(\lambda) \equiv J_D(\lambda) = \left\langle \int F_{\lambda_0}^{\theta_1}(\lambda')F_{\lambda'}^{\theta_2}(\lambda)\,d\lambda' \right\rangle, \tag{2}$$

where λ' is the intermediate wavelength and $F_{\lambda_1}^{\theta}(\lambda_2)$ is the normalized single scattered profile observed at scattering angle θ and wavelength λ_2 when the incident photons have wavelength λ_1. The single scattered profile of interest $J_S(\lambda)$ is, in this notation, $F_{\lambda_0}^{\theta_p}(\lambda)$, where θ_p is the experimental scattering angle and λ_0 is the wavelength of the incident beam. The angular brackets signify an average over the scattering angles, i.e.,

$$\langle g(\Omega_1,\Omega_2)\rangle \equiv \int P^{\theta_p}(\Omega_1,\Omega_2)g(\Omega_1,\Omega_2)\,d\Omega_1\,d\Omega_2\,, \tag{3}$$

where P^{θ_p} is the probability that a photon is scattered first through solid angle Ω_1, then through solid angle Ω_2, and emerges with total (observed) scattering angle θ_p. In Eq. (2) and in the equations that follow, we adopt the following convention for all profiles which have solid angles as arguments:

$$f(\Omega_1) = \frac{b(\theta_p)}{b(\theta_1)} f\left(a(\theta_p) + \frac{b(\theta_p)}{b(\theta_1)}[\lambda' - a(\theta_1)]\right), \tag{4a}$$

$$f(\Omega_2) = \frac{\lambda_0 b(\theta_p)}{\lambda' b(\theta_2)} f\left(a(\theta_p) + \frac{\lambda_0 b(\theta_p)}{\lambda' b(\theta_2)}\,[\lambda - \lambda' + \lambda_0 - a(\theta_2)]\right), \tag{4b}$$

where

$$a(\theta)=\lambda_0+(2h/mc)\sin^2\tfrac{1}{2}\theta\,,\qquad b(\theta)=(2\lambda_0/mc)\sin\tfrac{1}{2}\theta\,. \tag{4c}$$

The factors multiplying the f functions on the right side of Eq. (4) are required to insure that

$$\int J_S(\Omega_1)\,d\lambda'=\int J_S(\Omega_2)\,d\lambda=\int J_S(\lambda)\,d\lambda=1\,.$$

That is, $J_S(\Omega_1)$ and $J_S(\Omega_2)$ are the intermediate single scattered profiles appropriately normalized, shifted and scaled[4] to take account of the fact that observations are made only on photons of incident wavelength λ_0 at a scattering angle θ_p.

We define two norms. For real valued functions f defined on $(-\infty,\infty)$, let

$$\|f\|_p^x=\left(\int_{-\infty}^{\infty}|f(x)|^p\,dx\right)^{1/p}\quad(p\text{ a positive integer}) \tag{5}$$

and

$$\|f\|_\infty^x=\sup_x\{|f(x)|\}\,. \tag{6}$$

We refer to these as the L^p and L^∞ norms, respectively. Since our Compton profiles are normalized and are non-negative, we have

$$\|J_E\|_1=\|J_S\|_1=\|J_D\|_1=1\,. \tag{7}$$

Let $J_S^c(\lambda)$ be the single scattered profile which has been calculated from an "exact" experimental profile $J_E^e(\lambda)$ by some correction procedure. $J_S^c(\lambda)$ is an approximation to the exact single scattered profile $J_S^e(\lambda)$. We wish to investigate the error in the single scattered profile $\delta(\lambda)$ defined by

$$J_S^c(\lambda)+\delta(\lambda)=J_S^e(\lambda)\,. \tag{8}$$

In particular, we shall seek to calculate bounds on the largest absolute value of the error

$$\|\delta\|_\infty^\lambda=\|J_S^e-J_S^c\|_\infty^\lambda\,. \tag{9}$$

To obtain our bounds, we shall need Hölder's inequality[6]:

$$\int f(x)g(x)\,dx\le\|f\|_p^x\|g\|_q^x\,, \tag{10}$$

where

$$1/p+1/q=1\,,$$

and the triangle inequality:

$$\|f+g\|_p^x\le\|f\|_p^x+\|g\|_p^x\,. \tag{11}$$

The above inequalities hold for all real-valued functions f and g provided only that all terms on the right exist. Finally, if $f(x,y)$ is a function of two variables let $\|f(x,\cdot)\|_p^y<\infty$ denote the L^p norm taken with respect to the y variable when x is held fixed (it is thus a function of x). Then (Minkowski's integral inequality[7])

$$\left\|\int_x f(x,y)\,dx\right\|_p^y\le\int_x\left\|f(x,\cdot)\right\|_p^y dx\,. \tag{12}$$

Substituting Eqs. (2) and (8) in Eq. (1), we obtain

$$\begin{aligned}J_E^e(\lambda)&=(1-x)J_S^e(\lambda)+x\left\langle\int J_S^e(\Omega_1)J_S^e(\Omega_2)d\lambda'\right\rangle\\&=(1-x)J_S^c(\lambda)+(1-x)\delta(\lambda)\\&\quad+x\left\langle\int J_S^c(\Omega_1)J_S^c(\Omega_2)\,d\lambda'+\int J_S^c(\Omega_1)\delta(\Omega_2)\,d\lambda'\right.\\&\quad\left.+\int\delta(\Omega_1)J_S^c(\Omega_2)\,d\lambda'+\int\delta(\Omega_1)\delta(\Omega_2)\,d\lambda'\right\rangle.\end{aligned} \tag{13}$$

Starting from J_S^c, we can also *calculate* an experimental profile J_E^c, e.g., using a Monte Carlo technique, by applying the operator $\hat{O}$ to J_S^c as in Eq. (1):

$$J_E^c(\lambda)=(1-x)J_S^c(\lambda)+x\left\langle\int J_S^c(\Omega_1)J_S^c(\Omega_2)\,d\lambda'\right\rangle \tag{14}$$

Note that when δ is identically zero, i.e., when J_S^c is exact, then $J_E^c(\lambda)=J_E^e(\lambda)$.

Subtracting Eq. (14) from Eq. (13), we obtain the difference between the measured and calculated experimental profiles:

$$\begin{aligned}\epsilon(\lambda)&=J_E^e(\lambda)-J_E^c(\lambda)\\&=(1-x)\delta(\lambda)\\&\quad+x\left\langle\int J_S^c(\Omega_1)\delta(\Omega_2)\,d\lambda'\right.\\&\quad\left.+\int\delta(\Omega_1)J_S^c(\Omega_2)\,d\lambda'+\int\delta(\Omega_1)\delta(\Omega_2)\,d\lambda'\right\rangle.\end{aligned} \tag{15}$$

In the Appendix, we show that if our calculated single scattered profile is well approximated by a single Gaussian

$$J_S^c(\lambda)=\frac{1}{\gamma\sqrt{\pi}\,b(\theta_p)}\exp\left(-\frac{\lambda-a(\theta_p)}{\gamma b(\theta_p)}\right)^2, \tag{16}$$

then application of the inequalities (10)–(12) to Eq. (15) leads to upper and lower bounds on $\|\delta\|_\infty^\lambda$. The results obtained are

$$\left\{\max\left(0,\frac{-xBC+[x^2B^2C^2-(1-x)(xAB-\|\epsilon\|_\infty^\lambda)]^{1/2}}{1-x}\right)\right\}^2\le\|\delta\|_\infty^\lambda\le\left\{\frac{xBC-[x^2B^2C^2-(1-x)(xAB+\|\epsilon\|_\infty^\lambda)]^{1/2}}{1-x}\right\}^2, \tag{17}$$

where

$$A = \langle \| J_S^c(\Omega_1) \|_2^{\lambda'} \rangle , \quad (18a)$$

$$B = \left(\frac{1}{2\pi}\right)^{1/4} \left\langle \left(\frac{\lambda_0}{2\gamma b(\theta_2)}\right)^{1/2} \left(\lambda_0 - \frac{2h}{mC}\sin^2\frac{\theta_2}{2}\right)^{-1/2} \right\rangle , \quad (18b)$$

$$C = [2\langle b(\theta_p)/b(\theta_1)\rangle]^{1/2} . \quad (18c)$$

Note that aside from the appearance of the profile-width parameter γ in Eq. (18b), the quantities B and C are completely determined by the geometry and initial wavelength of the experiment.

Under most experimental conditions currently employed, the wavelength shift in the first scattering is sufficiently small that the integral in Eq. (2) is well approximated[4] by a convolution of two single-scattered profiles:

$$\hat{O} J_S(q) = J_D(q) \approx \langle J_S(\Omega_1) * J_S(\Omega_2) \rangle \quad (19)$$

if $(\lambda' - \lambda_0)/\lambda_0 \ll 1$.

If Eq. (16) is valid, then application of the convolution inequalities[6]

$$\| f * g \|_\infty^\lambda \le \| f \|_1^\lambda \cdot \| g \|_\infty^\lambda , \quad (20a)$$

$$\| f * g \|_\infty^\lambda \le \| f \|_\infty^\lambda \cdot \| g \|_1^\lambda , \quad (20b)$$

$$\| f * g \|_1^\lambda \le \| f \|_1^\lambda \cdot \| g \|_1^\lambda , \quad (20c)$$

to Eq. (15) affords a new set of bounds on $\|\delta\|_\infty^\lambda$. While these bounds are not as sharp as those of Eq. (17), they are independent of any assumption about the shape of J_S, such as the Gaussian approximation of Eq. (16). These "convolution" bounds also appear to give a more well-defined minimum for the determination of x by the method described in Sec. IV A.

If we define

$$\tau = \langle \sin\tfrac{1}{2}\theta_2 / \sin\tfrac{1}{2}\theta_p \rangle ,$$

$$\delta_1 = \frac{-(1+x) + [(1+x)^2 + 4x\|\epsilon\|_1^\lambda]^{1/2}}{2(1+x)} ,$$

typical convolution bounds are given by

$$\frac{\|\epsilon\|_\infty^\lambda - x\tau\delta_1 \|J_S^c\|_\infty^\lambda}{1 - x + x\tau(1+\delta_1)} \le \|\delta\|_\infty^\lambda \le \frac{\|\epsilon\|_\infty^\lambda + x\tau\delta_1 \|J_S^c\|_\infty^\lambda}{1 - x - x\tau(1+\delta_1)} . \quad (21)$$

Seven other sets of upper and lower bounds may also be found[8] by applying different combinations of the inequalities (20a) and (20b) to Eq. (15). Which of these afford the greatest lower and least upper bounds depends upon the detailed shape of the profile.

III. MODEL CALCULATION

To test the sharpness of the bounds, the above expressions were calculated for the model system treated in paper IV, a single electron surrounded by a planar ring of electrons. In this model, the angular averaging becomes trivial, since only a single pair of scattering angles (Ω_1, Ω_2) can occur.

With an assumed scattering angle $\theta_p = 150°$ and $x = 0.1$, we calculated J_E^e for a Gaussian J_S^e of half-width 0.833 ($\gamma = 1$) assuming only single and double scattering. An approximate J_S^c was generated by performing one iteration of the Newton-Raphson procedure described in paper IV. This profile was then used in Eq. (1) to produce J_E^c. In Table I we give $J_S^c(\lambda)$, $J_S^e(\lambda)$, and $\delta(\lambda)$. The greatest lower and least upper bounds calculated from Eq. (17) are

$$0 < \|\delta\|_\infty^\lambda < 0.17$$

as compared with the observed result $\|\delta\|_\infty^\lambda = 0.11$. This model is investigated further in the following section.

TABLE I. Exact and calculated single scattered profiles for a model experiment.

λ (Å)	J_S^e	J_S^c	δ
0.715	0.5565	0.5565	0.0
0.720	1.402	1.402	0.0
0.725	3.119	3.121	0.002
0.730	6.131	6.136	0.005
0.735	10.65	10.66	0.010
0.740	16.34	16.36	0.02
0.742	18.73	18.76	0.03
0.744	21.05	21.09	0.04
0.746	23.19	23.24	0.05
0.748	25.05	25.10	0.05
0.750	26.53	26.59	0.06
0.752	27.55	27.61	0.06
0.753	27.86	27.93	0.07
0.754	28.04	28.11	0.07
0.755	28.08	28.16	0.08
0.756	27.98	28.06	0.08
0.757	27.74	27.83	0.09
0.758	27.37	27.46	0.09
0.759	26.87	26.97	0.10
0.760	26.25	26.35	0.10
0.762	24.68	24.79	0.11
0.764	22.75	22.86	0.11
0.770	15.82	15.92	0.10
0.775	10.20	10.29	0.09
0.780	5.812	5.871	0.06
0.785	2.925	2.960	0.04

IV. DISCUSSION AND FURTHER APPLICATIONS

Examination of the two iterative approaches to the multiple scattering correction derived in paper IV shows that if those procedures are carried to convergence, then $\|\delta\|_\infty$ is identically zero. This observation has a number of consequences. First, it implies that such iterative procedures are the best correction methods, since *if* x is known exactly and the iteration is carried to self-consistency, then J_S is obtained with a vanishingly small error.

This will also be the case, however, if an incorrect value of x is used in the above correction procedures. That is, for a given J_E, there exists an infinity of solutions (x, J_S) satisfying Eq. (1). Any such solution will yield $\|\delta\|_\infty = 0$. Thus, the bounds derived here will not be of direct applicability in such cases.[9] However, if x is obtained independently, either by using the ratio of elastic to inelastic scattering[5(a)] or by extrapolating tabulated estimates of the dependence of x on sample content and thickness,[10] then reliable bounds may be calculated. Alternatively, if J_S^c is derived either by an extrapolation procedure[5(c)] or by a method which starts from a theoretical profile,[5(b)] then our error analysis can be applied directly. If a self-consistent iterative correction procedure is used, then other methods of utilizing the error bounds may also prove fruitful.

A. Estimation of x

If we are given the experimental profile J_E and the true single scattered profile J_S, then there is a unique value of x which satisfies the operator equation (1). For this value of x, the error bounds calculated using J_S, J_E, and x should be a minimum. Therefore, if we have a good calculated profile (e.g., from a molecular orbital calculation), we can vary x and calculate the bounds on $\|\delta\|_\infty^\lambda$ until a minimum is obtained. Hence the error bounds provide an independent method of estimating x.

In Fig. 1 we show the results obtained by treating the model discussed in the previous section in this manner. We have used the true single scattered profile, varied x from its exact value of 0.10, and computed the upper bound on $\|\delta\|_\infty^\lambda$. The variation in the error is sufficiently marked to define the true x. Of course, in a real case the exact J_S will not be known and we expect the minimum in the curve to be somewhat less pronounced. The results of the same calculation for the convolution operator bounds are shown in Fig. 2. The result is much more dramatic, although the bounds themselves are not very good.

B. Higher-order scattering

Our treatment thus far has assumed that essentially all the multiple scattering is double scattering, i.e., that triple and higher order scattering are negligible. As we point out in paper IV, a more rigorous treatment would replace $x\hat{O}$ in Eq. (1) by $\sum_{i=2}^{\infty} x_i \hat{O}_i$ where $\hat{O}_i$ is an operator which generates the ith order scattered profile from J_S.

Our derivations of error bounds on $\|\delta\|_\infty^\lambda$ can easily be augmented in this manner, though the algebra becomes somewhat tedious. Perhaps a more practical approach to including higher-order scattering in the estimate of error bounds is to carry out the correction using standard techniques which allow only for double (or for thick samples, triple as well) scattering, but to obtain J_E^c from J_S^c by including higher orders of scattering. The bounds are then calculated using the double-scattering-on-

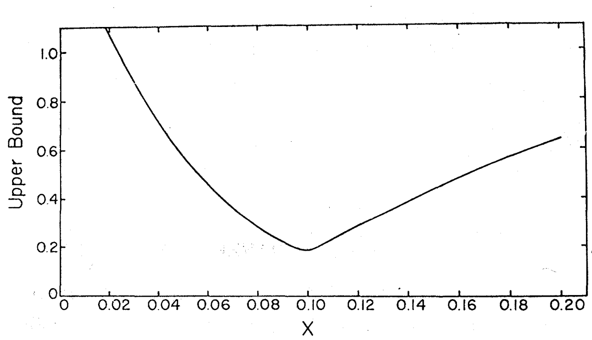

FIG. 1. Variation in upper bound to the error $\|\delta\|_\infty$ in the single scattered profile as x is varied from its true value 0.10.

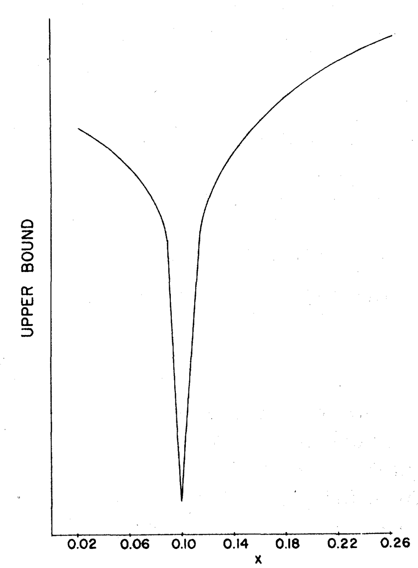

FIG. 2. Variation in upper bound to the error $\|\delta\|_\infty$ in the single scattered profile as x is varied from its true value 0.10. Convolution operator.

ly formulas derived here, and they give an estimate of the errors caused by neglect of higher-order scattering. The higher-order x_i need not be calculated explicitly, but may be estimated either in the course of the Monte Carlo calculation of J_E^c or from the fractions of lower-order scattering and the fact that x_{i+1}/x_i reaches a constant value in most samples for $i \geq 2$.[3] The single calculation required of J_E^c including higher-order scattering is easily performed by currently available Monte Carlo programs.[3,5(a),5(b)]

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APPENDIX. DERIVATION OF UPPER AND LOWER BOUNDS

Taking the L^∞ norm of Eq. (15) and applying the triangle inequality, we have

$$\|\epsilon\|_\infty^\lambda \leq (1-x)\|\delta\|_\infty^\lambda + x\left(\left\|\left\langle \int J_S^c(\Omega_1)\delta(\Omega_2)\,d\lambda'\right\rangle\right\|_\infty^\lambda + \left\|\left\langle \int \delta(\Omega_1)J_S^c(\Omega_2)\,d\lambda'\right\rangle\right\|_\infty^\lambda + \left\|\left\langle \int \delta(\Omega_1)\delta(\Omega_2)\,d\lambda'\right\rangle\right\|_\infty^\lambda\right). \quad \text{(A1)}$$

We use the Minkowski inequality (12) to move the L^∞ norms on the right-hand side of Eq. (A1) inside the angular averages. Application of inequality (10) to the integration over λ' then gives

$$\|\epsilon\|_\infty^\lambda \leq (1-x)\|\delta\|_\infty^\lambda + x(\langle \| \|J_S^c(\Omega_1)\|_p^{\lambda'} \| \|\delta(\Omega_2)\|_q^{\lambda'} \|_\infty^\lambda\rangle + \langle \| \|\delta(\Omega_1)\|_p^{\lambda'} \| \|J_S^c(\Omega_2)\|_q^{\lambda'} \|_\infty^\lambda\rangle + \langle \| \|\delta(\Omega_1)\|_p^{\lambda'} \| \|\delta(\Omega_2)\|_q^{\lambda'} \|_\infty^\lambda\rangle). \quad \text{(A2)}$$

Several inequalities may be obtained from Eq. (A2) with different choices for p and q. Some may be immediately discarded. Consider, for example, $p=\infty$, $q=1$. We have

$$\|J_S^c(\Omega_2)\|_1^{\lambda'} = \int \frac{\lambda_0 b(\theta_p)}{\lambda' b(\theta_2)} J_S^c\left(a(\theta_p) + \frac{\lambda_0 b(\theta_p)}{\lambda' b(\theta_2)} \times [\lambda - \lambda' + \lambda_0 - a(\theta_2)]\right) d\lambda'$$

$$= \frac{\lambda_0 b(\theta_p)}{b(\theta_2)} \int \frac{1}{\lambda'} J_S^c\left(\alpha + \frac{\beta}{\lambda'}\right) d\lambda' \quad \text{(A3)}$$

where

$$\alpha = a(\theta_p) - \lambda_0 b(\theta_p)/b(\theta_2), \quad \text{(A4a)}$$

$$\beta = [\lambda_0 b(\theta_p)/b(\theta_2)][\lambda + \lambda_0 - a(\theta_2)]. \quad \text{(A4b)}$$

If J_S^c is a Gaussian of the form $\exp(-x^2/\gamma^2)$, then as $\lambda' \to \infty$, the integrand in Eq. (A3) approaches $\exp(-\alpha^2/\gamma^2)/\lambda'$, and the integral diverges. Thus the inequality (A2) will not yield a useful result in this case.

The case $p=1$, $q=\infty$ is also unproductive. However, by choosing $p=q=2$, we are able to obtain a more meaningful inequality. We need to evaluate all of the angular averages in Eq. (A2). In order to do this, we approximate J_S^c by a single Gaussian:

$$J_S^c(\lambda) = \frac{1}{\gamma\sqrt{\pi}\, b(\theta_p)} \exp\left[-\left(\frac{\lambda - a(\theta_p)}{\gamma b(\theta_p)}\right)^2\right]. \quad \text{(A5)}$$

Then, setting

$$\alpha' = [\alpha - a(\theta_p)]/\gamma, \quad \text{(A6a)}$$

$$\beta' = \beta/\gamma, \quad \text{(A6b)}$$

where α and β are defined in Eq. (A4), we have

$$J_S^c(\Omega_2) = \frac{\lambda_0}{\gamma\sqrt{\pi}\, b(\theta_2)} \frac{1}{\lambda'} e^{-(\alpha'+\beta'/\lambda')^2}$$

The L^2 norm is therefore

$$\|J_S^c(\Omega_2)\|_2^{\lambda'} = \frac{\lambda_0}{\gamma\sqrt{\pi}\, b(\theta_2)}\left[\int_{\lambda_0}^{\infty} \frac{e^{-2(\alpha'+\beta'/\lambda')^2}}{\lambda'^2} d\lambda'\right]^{1/2} = \frac{\lambda_0}{\gamma\sqrt{\pi}\, b(\theta_2)}\left[\int_0^{1/\lambda_0} e^{-2(\alpha'+\beta' t)^2} dt\right]^{1/2}. \quad \text{(A7)}$$

While the integral in Eq. (A7) may be evaluated explicitly to yield

$$\|J_S^c(\Omega_2)\|_2^{\lambda'} = \frac{\lambda_0}{\beta'\gamma\sqrt{2\pi}\, b(\theta_2)} \times \left[\operatorname{erf}\left(\frac{\alpha' + \beta'/\lambda_0}{\sqrt{2}}\right) - \operatorname{erf}\left(\frac{\alpha'}{\sqrt{2}}\right)\right],$$

we find it easier to use the upper bound obtained by replacing the upper limit of the integral by $+\infty$. We thus have

$$\|J_S^c(\Omega_2)\|_2^{\lambda'} \leq \frac{\lambda_0}{\gamma\sqrt{\pi}\, b(\theta_2)}\left[\frac{1}{2\beta'}\left(\frac{\pi}{2}\right)^{1/2}\right]. \quad \text{(A8)}$$

Recalling the definition of β' [Eqs. (A4) and (A6)], we obtain

$$\|J_S^c(\Omega_2)\|_2^{\lambda'} \leq \left(\frac{1}{2\pi}\right)^{1/4}\left(\frac{\lambda_0}{2\gamma b(\theta_2)}\right)^{1/2} \frac{1}{[\lambda + \lambda_0 - a(\theta_2)]^{1/2}}. \quad \text{(A9)}$$

We now need to find the L^∞ norm of Eq. (A9) with respect to λ. Since $a(\theta_2)$ and $b(\theta_2)$ do not depend upon λ and since $\lambda_0 < \lambda < \infty$, the sup of the right-hand side of Eq. (A9) must occur at $\lambda = \lambda_0$. Therefore, using Eq. (4c), we have

$$\| \| J_S^c(\Omega_2) \|_2^{\lambda'} \|_\infty^\lambda = \left(\frac{1}{2\pi}\right)^{1/4} \left(\frac{\lambda_0}{2\gamma b(\theta_2)}\right)^{1/2} \left(\frac{1}{\lambda_0 - (2h/mc)\sin^2(\theta_2/2)}\right)^{1/2}.$$

Next, we evaluate $\|\delta(\Omega_1)\|_2^{\lambda'}$. Setting $p=1$, $q=\infty$, we have Hölder's inequality (10):

$$\begin{aligned}\|\delta(\Omega_1)\|_2^{\lambda'} &= \left(\int [J_S^c(\Omega_1) - J_S^e(\Omega_1)]^2 d\lambda'\right)^{1/2} \\ &= \left(\int [J_S^c(\Omega_1) - J_S^e(\Omega_1)][J_S^c(\Omega_1) - J_S^e(\Omega_1)] d\lambda'\right)^{1/2} \\ &\le (\|J_S^c(\Omega_1) - J_S^e(\Omega_1)\|_1^{\lambda'} \|J_S^c(\Omega_1) - J_S^e(\Omega_1)\|_\infty^{\lambda'})^{1/2}. \end{aligned} \tag{A10}$$

By the definition of δ,

$$\|J_S^c(\Omega_1) - J_S^e(\Omega_1)\|_\infty^{\lambda'} = \|\delta(\Omega_1)\|_\infty^{\lambda'}. \tag{A11}$$

Because of the normalizing factors which were included in Eq. (4), we must have

$$\|J_S^c(\Omega_1)\|_1^{\lambda'} = \|J_S^e(\Omega_1)\|_1^{\lambda'} = \|J_S^e\|_1^\lambda = 1 \tag{A12a}$$

and

$$\|\delta(\Omega_1)\|_1^{\lambda'} = \|\delta\|_1^\lambda. \tag{A12b}$$

The change of variables in Eq. (4) together with this preservation of normalization also implies that

$$\|\delta(\Omega_1)\|_\infty^{\lambda'} = [b(\theta_p)/b(\theta_1)]\|\delta\|_\infty^\lambda. \tag{A13}$$

Combining Eqs. (A11)–(A13) with Eq. (A10), we now have

$$\begin{aligned}\|\delta(\Omega_1)\|_2^{\lambda'} &\le \left[\frac{b(\theta_p)}{b(\theta_1)}\|\delta\|_\infty^\lambda \|J_S^c(\Omega_1) - J_S^e(\Omega_1)\|_1^{\lambda'}\right]^{1/2} \\ &\le \left[\frac{b(\theta_p)}{b(\theta_1)}\|\delta\|_\infty^\lambda (\|J_S^c(\Omega_1)\|_1^{\lambda'} + \|J_S^e(\Omega_1)\|_1^{\lambda'})\right]^{1/2} \\ &= \left[\frac{2b(\theta_p)}{b(\theta_1)}\|\delta\|_\infty^\lambda\right]^{1/2}, \end{aligned} \tag{A14}$$

where $\|\delta\|_\infty^\lambda$ is the quantity we seek.

Finally, we must estimate $\|\|\delta(\Omega_2)\|_2^{\lambda'}\|_\infty^\lambda$. We obtain a bound by assuming that our calculated single scattered profile is sufficiently accurate that

$$\|\delta(\Omega_2)\|_2^{\lambda'} = \|J_S^c(\Omega_2) - J_S^e(\Omega_2)\|_2^{\lambda'} < \|J_S^c(\Omega_2)\|_2^{\lambda'}. \tag{A15}$$

We have now found all of the quantities necessary to evaluate Eq. (17). We summarize: (a) $\|J_S^c(\Omega_1)\|_2^{\lambda'}$, found by numerical integration;

(b) $\|\|\theta(\Omega_2)\|_2^{\lambda'}\|_\infty^\lambda < \|\|J_S^c(\Omega_2)\|_2^{\lambda'}\|_\infty^\lambda$;

(c) $\|\delta(\Omega_1)\|_2^{\lambda'} < \left[2\frac{b(\theta_p)}{b(\theta_1)}\|\delta\|_\infty^\lambda\right]^{1/2}$;

(d) $\|J_S^c(\Omega_2)\|_2^{\lambda'}\|_\infty^\lambda < \left(\frac{1}{2\pi}\right)^{1/4}\left(\frac{\lambda_0}{2\gamma b(\theta_2)}\right)^{1/2} \times \left(\lambda_0 - \frac{2h}{mc}\sin^2\frac{\theta_2}{2}\right)^{-1/2}$.

If we set

$$A = \langle \|J_S^c(\Omega_1)\|_2^{\lambda'}\rangle, \tag{18a}$$

$$B = \left(\frac{1}{2\pi}\right)^{1/4}\left\langle\left(\frac{\lambda_0}{2\gamma b(\theta_2)}\right)^{1/2}\left(\lambda_0 - \frac{2h}{mc}\sin^2\frac{\theta_2}{2}\right)^{-1/2}\right\rangle, \tag{18b}$$

$$C = \left[2\left\langle\frac{b(\theta_p)}{b(\theta_1)}\right\rangle\right]^{1/2}, \tag{18c}$$

then Eq. (A2) becomes

$$\|\epsilon\|_\infty^\lambda < (1-x)\|\delta\|_\infty^\lambda + x[AB + 2BC(\|\delta\|_\infty^\lambda)^{1/2}]. \tag{A16}$$

Equation (A16) is a quadratic in $(\|\delta\|_\infty^\lambda)^{\frac{1}{2}}$ and it may be solved to yield the lower bounds

$$(\|\delta\|_\infty^\lambda)^{1/2} \gtrless \frac{-xBC \pm [x^2B^2C^2 - (1-x)(xAB - \|\epsilon\|_\infty^\lambda)]^{1/2}}{1-x}. \tag{A17}$$

Closer examination of Eq. (A16) shows that if $\|\epsilon\|_\infty^\lambda < xAB$ then the inequality will hold for any value of $\|\delta\|_\infty^\lambda$, and the only lower bound available in this case is the obvious

$$\|\delta\|_\infty^\lambda \ge 0. \tag{A18}$$

If $\|\epsilon\|_\infty^\lambda \ge xAB$, then the quadratic has two real roots δ_+ and δ_-, with $\delta_- < 0 < \delta_+$ and $|\delta_-| > |\delta_+|$. For the greatest lower bound on $\|\delta\|_\infty^\lambda$ we must choose δ_+, the positive root in Eq. (A18).

Upper bounds on $\|\delta\|_\infty^\lambda$ are obtained by writing Eq. (15) in the form

$$(1-x)\delta(\lambda) = \epsilon(\lambda) - x\left\langle\int J_S^c(\Omega_1)\delta(\Omega_2)d\lambda' + \int \delta(\Omega_1)J_S^c(\Omega_2)d\lambda' + \int \delta(\Omega_1)\delta(\Omega_2)d\lambda'\right\rangle. \tag{A19}$$

Applying the inequalities (10)–(12) in the same manner used to derive the lower bounds, we obtain

$$(1-x)\|\delta\|_\infty^\lambda < \|\epsilon\|_\infty^\lambda + x[AB + 2BC(\|\delta\|_\infty^\lambda)^{1/2}]$$

or

$$(\|\delta\|_\infty^\lambda)^{1/2} \lesseqgtr \frac{xBC \pm [x^2B^2C^2 + (1-x)(xAB + \|\epsilon\|_\infty^\lambda)]^{1/2}}{1-x} \tag{A20}$$

with A, B, C as defined in Eqs. (18). In this case, the roots of Eq. (A20) will always be real with $\delta_- < 0 < \delta_+$ and $|\delta_+| > |\delta_-|$. Now, since we seek the least upper bound, we choose δ_-, the negative root of Eq. (A20).

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