Inverse Scattering Theory: Strategies Based on the Volterra Inverse Series for Acoustic Scattering†

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We consider the necessity of half-off-shell transition-matrix elements (near-field) information on iterative approaches to the inverse acoustic scattering problem. We then show that, because of the manner in which half-off-shell effects enter, the recently introduced Volterra inverse series correctly predicts the first two moments of the interaction, while the Fredholm inverse series is correct only for the first moment. Finally, we demonstrate that the Volterra approach provides a method for *exactly* obtaining interactions that can be written as a sum of delta functions.

I. Introduction

The inverse scattering problem is ubiquitous in science, engineering, and medicine, and, thus, is of enormous importance. Examples include medical imaging of various types, seismic exploration, radar, sonar, nondestructive testing in industry, civil engineering, airport and homeland security, etc. The two predominant approaches for the acoustic and electromagnetic inverse scattering problems are (i) choosing a model and adjusting imbedded parameters to best produce the observed scattering, or (2) reverting the Born expansion of the acoustic or electromagnetic Lippmann−Schwinger integral equation to obtain the interaction responsible for the scattering. The first method generally requires extremely robust algorithms for solving (repeatedly) the scattering problem. It is typically limited by the specific form chosen to model the interaction. Currently, the most robust version of this approach is perhaps that of Rabitz and co-workers[1], who used sensitivity analysis with the forward scattering approach. The second approach was first formulated by Jost and Kohn[2] and pursued vigorously by Moses,[3] Razavy,[4] and Prosser.[5] By far, the majority of actual applications have been restricted to the first-order term. The most extensive studies of the higher order terms in recent years are those of Weglein and co-workers.[6] The difficulties with the inverse Born series approach concern questions of whether (i) the series converges, (ii) more than on-shell transition-matrix (T-matrix) elements are needed (i.e., more than “far-field” measurements). A straightforward examination of terms in the inverse Born series certainly shows that the expressions involve half-off-shell T-matrix elements. These are generally evaluated in terms of far-field quantities, using an ansatz discussed by Moses,[3] Razavy,[4] and Prosser.[5]

Recently we have introduced an approach to the inverse scattering series that completely solves the problem of convergence.[7] This is achieved by renormalizing the Lippmann−Schwinger equation from a Fredholm structure to a Volterra structure. It was proved that the resulting inverse Born series converges absolutely and uniformly, *independent* of the strength of the interaction.[7,8] However, the issue of how to deal with the need for half-off-shell scattering information remains outstanding. We base our strategy for solving the inverse problem on exploiting the superior convergence properties of the Volterra-based inverse series, in combination with the introduction of a parametrization of the interaction, which allows for a greatly simplified determination of the interaction parameters. This enables us to take account of half-off-shell (near field) effects.

It is also important to note, and we emphasize the fact, that use of a Volterra-based inversion requires either (i) measurement of both the reflection and transmission amplitudes, to achieve the simplest form of inversion, or (ii) the solution of more-complicated, nonlinear algebraic equations if only the reflection amplitude is measured. In Section II of this paper, we present a simple analysis that shows clearly the need to deal with half-off-shell or near-field effects to treat the problem. In Section III, we present a general analysis of the moments of the Fredholm and Volterra Born approximations compared to the moments of the true interaction. This shows that the Volterra-based Born expansion yields one higher moment before the half-off-shell effects come into play. In Section IV, we then consider inversion of the scattering produced by any interaction that can be expressed as a sum of Dirac delta functions (a model interaction that is shown in Appendix B to be of practical utility). This interaction also illustrates the convergence properties of the Volterra series. For simplicity, we restrict ourselves to a scalar scattering wave (i.e., acoustic scattering); however, the analysis is valid also for more-complicated electromagnetic scattering. In Section V, we discuss the data required for implementation of the Volterra-based inversion. Finally, in Section VI, we give our conclusions.

II. Analysis of the Moses−Razavy−Prosser Ansatz for Half-Off-Shell Transition Amplitudes

The Born-type inverse scattering series is most simply obtained from the abstract Lippmann−Schwinger equation

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$$T_k = V + VG_{0k}^{+}T_k \tag{1}$$

where V is the (local) interaction, T_k is the transition operator, and G_{0k}^{+} is the free (unperturbed) causal Green's operator,

$$G_{0k}^{+} = \frac{k^2}{k^2 - H_0 + i\epsilon} \tag{2}$$

modified for the acoustic (and electromagnetic) case by the multiplicative factor, k^2. This factor arises because, unlike for the quantum scattering case, the scattering interaction is of the form k^2V. This extra factor causes important changes in the scattering behavior compared to the quantal case as is elaborated in the Appendix A. Here, k^2 is essentially the square of the spatial wavenumber parameter; H_0 describes the unperturbed wave propagation. Also, we explicitly indicate that the abstract operators T_k and G_{0k}^{+} are dependent on k as a parameter. The scattering amplitude for the process $k \to k'$ then is given (using Dirac notation for compactness) in terms of

$$\langle k'|T_k|k\rangle = \langle k'|V|k\rangle + \langle k'|VG_{0k}^{+}T_k|k\rangle \tag{3}$$

Taking advantage of the local character of V, we then have that

$$\langle k'|V|k\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}z\, \mathrm{e}^{i(k-k')z}V(z) \tag{4}$$

It is important to note that the matrix element $\langle k'|V|k\rangle$ of the true local interaction is dependent *only* on the difference ($k - k'$). Conversely, if $\langle k'|V|k\rangle$ is only a function of $k - k'$, then V is local. If $V(z)$ is real, then we also have that

$$\langle k'|V|k\rangle = \langle k|V|k'\rangle^* \tag{5}$$

It is easily established that $\langle k'|V|k\rangle$ and $\langle k'|T_k|k\rangle$ cannot be simultaneously dependent only on the difference ($k - k'$), because if that were the case, eq 1 could be written as

$$\begin{aligned}\langle k'|T_k|k\rangle &= \langle k'|V|k\rangle + \\ &\quad \int \mathrm{d}k''\, \tilde{V}(k''-k')\langle k''|G_{0k}^{+}|k''\rangle \tilde{T}_k(k-k'') \\ &= \langle k'|V|k\rangle + \int \mathrm{d}y\, \tilde{V}(k-k'-y)\langle k''|G_{0k}^{+}|k''\rangle \tilde{T}_k(y) \\ &= \langle k'|V|k\rangle + \\ &\quad \int \mathrm{d}y\, \tilde{V}(k-k'-y)\frac{k^2}{(2k-y)y+i\epsilon}\tilde{T}_k(y)\end{aligned} \tag{6}$$

The last line, which results from substitution of the Green's function of eq 2 into the previous line, clearly shows that the integral—and, hence, the LHS of this equation—is not solely a function of $k - k'$, which is a contradiction. For inversion, we write eq 1 as an equation for $\langle k'|V|\ k\rangle$:

$$\langle k'|V|k\rangle = \langle k'|T_k|k\rangle - \langle k'|VG_{0k}^{+}T_k|k\rangle \tag{7}$$

Using the resolution of the identity

$$1 = \int \mathrm{d}k''\, |k''\rangle\langle k''| \tag{8}$$

this equation becomes

$$\langle k'|V|k\rangle = \langle k'|T_k|k\rangle - \int \mathrm{d}k''\, \frac{\langle k'|V|k''\rangle\langle k''|T_k|k\rangle}{k^2 - k'' + i\epsilon} \tag{9}$$

which is an exact equation. We first observe that, if we take $|k'| = |k|$ so that $\langle k'|T_k|k\rangle$ corresponds to an *on-shell* matrix element, then $\langle k'|V|k''\rangle$ still involves both on-shell and half-on-shell T-matrix elements.

As we have seen, although V is taken to be a local operator, it *cannot* be true, generally, that T_k is local (or, more precisely, $\langle k'|T_k|k\rangle$ is not solely a function of $k - k'$). The essence of the Moses−Razavy−Prosser ansatz is

$$\langle k''|T_k|k\rangle \approx \langle k''|V_1|k\rangle \qquad (\text{for } -\infty < k'' < \infty) \tag{10}$$

where

$$V_1(z) \equiv \int_{-\infty}^{\infty} \mathrm{d}(2k)\, \mathrm{e}^{-2ikz}\langle -k|T_k|k\rangle \tag{11}$$

That is, half-off-shell elements of T_k can be obtained as on-shell matrix elements of the T-operator for *different* values of k. However, eqs 10 and 11 imply that T_k is equivalent to a *local* operator, which, generally, cannot be true. We note that this analysis also applies to the Volterra inverse integral equation. One can, in general, write the Volterra Green's operator, $\tilde{G}_{0k}$, as G_{0k}^{+} plus a solution of the homogeneous free Green's function[7,8] equation. Such homogeneous solutions can *always* be written as a sum of separable, totally on-shell operators that have the form

$$O_k = \sum_n |\phi_{nk}\rangle\langle\chi_{nk}| \tag{12}$$

where

$$(k^2 - H_0)|\phi_{nk}\rangle = (k^2 - H_0)|\chi_{nk}\rangle = 0 \tag{13}$$

Then,

$$G_{0k}^{+} = \tilde{G}_{0k} + O_k \tag{14}$$

and

$$\begin{aligned}T_k &= V + V\tilde{G}_{0k}T_k + VO_kT_k \\ &= V[1 + O_kT_k] + V\tilde{G}_{0k}T_k\end{aligned} \tag{15}$$

We define $\tilde{T}_k$ by

$$T_k = V + V\tilde{G}_{0k}\tilde{T}_k \tag{16}$$

where

$$T_k = \tilde{T}_k(1 + O_kT_k) \tag{17}$$

Again, one easily can show that $\tilde{T}_k$ is generally nonlocal, and a parallel analysis to that for T_k holds. The major distinction between using eq 3 to generate an inverse series for $\langle k'|V|k\rangle$ and using similar matrix elements of eq 16, expressed as

$$V = \tilde{T}_k - V\tilde{G}_{0k}\tilde{T}_k \tag{18}$$

is that the iterative solution of eq 16 for V is guaranteed to converge absolutely and uniformly no matter how strong V is.[7,8] Thus, whether one bases an inversion on T_k or $\tilde{T}_k$, *both* require the equivalent of half-on-shell information for their implementation. We next examine the behavior of these two inversion alternatives, with regard to their relations to the moments of the true interaction.

III. Analysis of Moments of the Interaction

The moments of the interaction are defined as

$$V[n] \equiv \int_{-\infty}^{\infty} \mathrm{d}z\, z^n V(z) \tag{19}$$

It is clear from eqs 7 and 18 that $V[n]$ is exactly given by

$$V[n] \equiv \int_{-\infty}^{\infty} \mathrm{d}z z^n \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} \langle -k|V|k\rangle \tag{20}$$

leading to

$$V[n] = \int_{-\infty}^{\infty} \mathrm{d}z z^n \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} [\langle -k|T_k|k\rangle - \langle -k|VG_{0k}^{+}T_k|k\rangle] \tag{21}$$

or

$$V[n] = \int_{-\infty}^{\infty} \mathrm{d}z\, z^n \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} [\langle -k|\tilde{T}_k|k\rangle - \langle -k|V\tilde{G}_{0k}\tilde{T}_k|k\rangle] \tag{22}$$

It is generally assumed that $\langle -k|T_k|k\rangle$ and $\langle -k|\tilde{T}_k|k\rangle$ are obtained experimentally by a far-field measurement. Again, defining

$$V_1(z) \equiv \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} \langle -k|T_k|k\rangle \tag{23}$$

and

$$\tilde{V}_1(z) \equiv \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} \langle -k|\tilde{T}_k|k\rangle \tag{24}$$

we have

$$V[n] = V_1[n] - \int_{-\infty}^{\infty} \mathrm{d}z\, z^n \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} \langle -k|VG_{0k}^{+}T_k|k\rangle \tag{25}$$

and

$$V[n] = \tilde{V}_1[n] - \int_{-\infty}^{\infty} \mathrm{d}z\, z^n \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{-2ikz} \langle -k|V\tilde{G}_{0k}\tilde{T}_k|k\rangle \tag{26}$$

We shall now prove that, generally, $\tilde{V}_1[n]$ is exact (i.e., $\tilde{V}[n] = \tilde{V}_1[n]$) through $n = 1$ while $V_1[n]$ is only correct for $n = 0$. To do this, we substitute into these equations the coordinate representation matrix elements of G_{0k}^{+} and $\tilde{G}_{0k}$, which are given respectively by[8]

$$G_{0k}^{+}(z|z') = \frac{-ik}{2} \mathrm{e}^{ik|z'-z|} \tag{27}$$

and

$$\tilde{G}_{0k}(z|z') = k \sin(k[z' - z]) H(z' - z) \tag{28}$$

Here, $H(z' - z)$ is the Heaviside function,

$$H(z) = 1 \qquad (\text{for } z > 0) \tag{29a}$$

$$= 0 \qquad (\text{for } z \le 0) \tag{29b}$$

After judicious insertion of identity resolutions, we easily obtain the following results:

$$V[n] = V_1[n] + \frac{i}{2} \int_{-\infty}^{\infty} \mathrm{d}z\, z^n \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z'' \times \mathrm{e}^{-2ikz} \mathrm{e}^{ikz} V(z') k \mathrm{e}^{ik|z'-z''|} \langle z''|T_k|k\rangle \tag{30}$$

and

$$V[n] = \tilde{V}_1[n] - \int_{-\infty}^{\infty} \mathrm{d}z\, z^n \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z'' \times \mathrm{e}^{-2ikz} \mathrm{e}^{ikz} V(z') k \sin(k[z'' - z']) H(z'' - z') \langle z''|\tilde{T}_k|k\rangle \tag{31}$$

Next, we interchange the order of the dz and dk integrals and note that

$$\int_{-\infty}^{\infty} \mathrm{d}z\, z^n \mathrm{e}^{-2ikz} = \left(\frac{i}{2}\right)^n \frac{\partial^n}{\partial k^n} \int_{-\infty}^{\infty} \mathrm{d}z\, \mathrm{e}^{-2ikz} \tag{32a}$$

$$= 2\pi \left(\frac{i}{2}\right)^n \frac{\partial^n}{\partial k^n} \delta(2k) \tag{32b}$$

Consequently, eqs 30 and 31 become

$$V[n] = V_1[n] + \frac{\pi i^{n+1}}{2^n} \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z''\, V(z') \frac{\partial^n}{\partial k^n} \times \{\mathrm{e}^{ikz} k \mathrm{e}^{ik|z'-z''|} \langle z''|T_k|\, k\rangle\}_{k=0} \tag{33}$$

and

$$V[n] = \tilde{V}_1[n] - \frac{\pi i^n}{2^{n-1}} \int_{-\infty}^{\infty} \mathrm{d}z' \int_{-\infty}^{\infty} \mathrm{d}z''\, V(z') H(z'' - z') \frac{\partial^n}{\partial k^n} \times \{\mathrm{e}^{ikz'} \sin[k(z'' - z')] \langle z''|T_k|k\rangle\}_{k=0} \tag{34}$$

Now, the essential point to note is that, when $n = 0$, the second terms in *both* eqs 33 and 34 vanish, because there is *no* derivative and $k = 0$. Therefore, we conclude that

$$V[0] = V_1[0] = \tilde{V}_1[0] \tag{35}$$

However, when $n = 1$, there is a nonzero contribution from the second term on the right-hand side (RHS) of eq 33 since one term contains $(\partial/\partial k)(k) = 1$ and the remaining factors generally are nonzero. The second term on the RHS in eq 34 remains zero, because

$$\frac{\partial}{\partial k}\{k \sin[k(z'' - z')]\}_{k=0} = 0 \tag{36}$$

and we thus conclude that

$$V[1] = \tilde{V}[1] \tag{37}$$

Thus, the approximation to the interaction produced by the Volterra formalism yields correct values for $V[0]$ and $V[1]$, whereas the Fredholm-based Born series yields the correct values only for $V[0]$. In another paper, we will present a complete inversion scheme based on the moments of V, using the iterated Volterra−Born series.[9]

We now turn to consider the Volterra-based inversion for interactions that can be expressed as sums of Dirac delta functions.

IV. Volterra-Based Inverse Scattering Treatment for Sums of Dirac Delta Functions

Rodberg and Thaler[10] have presented an interesting derivation of Fredholm's method for solving the Lippmann−Schwinger equation that involves writing the interaction as a sum of Dirac delta functions. Essentially, they argue that, because

$$V(z) = \int_{-\infty}^{\infty} \mathrm{d}z'\, \delta(z' - z) V(z') \tag{38}$$

holds for reasonable interaction functions, one can write $V(z)$ as a limit:

$$V(z) = \lim_{\Delta j \to 0} \sum_j \Delta_j \delta(z_j - z) V(z_j) \tag{39}$$

Although care must be exercised with such an argument (see Appendix B), it suggests that a useful model, especially for a scattering interaction that has an effective compact support and is also effectively band-limited (of course, both are not rigorously possible simultaneously), can be taken to be

$$V(z) = \sum_{j=1}^{J} \Delta_j \delta(z_j - z) V(z_j) \tag{40}$$

where J is the finite number of delta functions needed to represent the interaction adequately. (Using Hermite distributed approximating functionals (HDAFs, or $\delta_M(z - z_j|\sigma)$) to replace the delta functions, we can obtain the smooth, well-behaved interaction form

$$V(z) = \sum_j \delta_M(z - z_j|\sigma) V(z_j) \tag{41}$$

about which we later make some brief comments in Appendix B. In this paper, we shall focus primarily on eq 40.)

We recall that the Volterra-based solution of the $1 - D$ scalar Helmholtz equation is[7]

$$\tilde{\psi}_k(z) = \frac{e^{ikz}}{2\pi} + k\int_{-\infty}^{\infty} dz' \sin[k(z' - z)] H(z' - z) V(z') \tilde{\psi}(z') \tag{42}$$

For the interaction described by eq 40, this is easily seen to give

$$\tilde{\psi}_k(z) = \frac{e^{ikz}}{2\pi} + k\sum_{j=1}^{J} \sin[k(z_j - z)] H(z_j - z) \Delta_j V(z_j) \tilde{\psi}(z_j) \tag{43}$$

We assume, without loss of generality, that

$$z_j > z_{j-1} \tag{44}$$

In terms of the full Green's operator, we have that

$$\tilde{\psi}_k(z) = \langle z|k\rangle + \langle z|\tilde{G}V|k\rangle \tag{45}$$

which, making use of the well-known expansion

$$\tilde{G} = \sum_{j=0} (\tilde{G}_0 V)^j \tilde{G}_0 \tag{46}$$

results in

$$\begin{aligned}\tilde{\psi}_k(z) &= \langle z|k\rangle + \sum_{n=1} \langle z|(\tilde{G}_0 V)^n|k\rangle \\ &= \langle z|k\rangle + \sum_{n=1} \int_{z<\zeta_1}^{\infty} d\zeta_1 \int_{\zeta_1<\zeta_2}^{\infty} d\zeta_2 ... \int_{z<\zeta_1}^{\infty} d\zeta_n \times \\ &\quad \langle z|\tilde{G}_0 V|\zeta_1\rangle\langle\zeta_1|\tilde{G}_0 V|\zeta_2\rangle ... \langle\zeta_{n-1}|\tilde{G}_0 V|\zeta_n\rangle\langle\zeta_n|k\rangle\end{aligned} \tag{47}$$

Here, for clarity, we have used ζ instead of z as the symbol to represent the ordered coordinate integration variables. This formula is general; however, if we now introduce the interaction of eq 40, the integrals can be trivially evaluated to yield

$$\tilde{\psi}_k(z) = \langle z|k\rangle + \sum_{n=1} \sum_{z<\zeta_1}^{z_J} \sum_{\zeta_1<\zeta_2}^{z_J} ... \sum_{\zeta_{n-1}<\zeta_n}^{z_J} \langle z|\tilde{G}_0 V|\zeta_1\rangle\langle\zeta_1|\tilde{G}_0 V|\zeta_2\rangle ... \langle\zeta_{n-1}|\tilde{G}_0 V|\zeta_n\rangle\langle\zeta_n|k\rangle \tag{48}$$

where ζ_1 through ζ_n are now elements of an ordered subset of the z-points where the δ-functions of the interaction are located. Let $N_z \le J$ be the number of such points greater than z; the number of ordered sets of ζ-points satisfying the limits on the summations then is given by the binomial coefficient $(N_z!/n!(N_z - n)!)$. The sum $\sum_{z<\zeta_1}^{z_J} \sum_{\zeta_1<\zeta_2}^{z_J} ... \sum 1_{\zeta_{n-}<\zeta_n}^{z_J}$, which, for conciseness, we write as $\sum_{\zeta_1,\zeta_2,...\zeta_n}$, is the sum over all $(N_z!/n!(N_z - n)!)$ sets. Finally, we have that

$$\begin{aligned}\tilde{\psi}_k(z) &= \langle z|k\rangle + \sum_{n=1}^{N_z} \sum_{\zeta_1,\zeta_2,...\zeta_n} \langle z|\tilde{G}_0 V|\zeta_1\rangle\langle\zeta_1|\tilde{G}_0 V|\zeta_2\rangle ... \\ &\quad \langle\zeta_{n-1}|\tilde{G}_0 V|\zeta_n\rangle\langle\zeta_n|k\rangle \\ &= \langle z|k\rangle + \sum_{n=1}^{N_z} (k\Delta)^n \sum_{\zeta_1,\zeta_2,...\zeta_n} \sin(k[\zeta_1 - z]) V(\zeta_1) \times \\ &\quad \sin(k[\zeta_2 - \zeta_1]) V(\zeta_2) ... \\ &\quad \sin(k[\zeta_n - \zeta_{n-1}]) V(\zeta_n)\langle\zeta_n|k\rangle\end{aligned} \tag{49}$$

It is clear that the number of terms contributing to $\tilde{\psi}_k(z)$, for any value of z, is $1 + \sum_{n=1}^{N_z}(N_z!/n!(N_z - n)!) = 2^{N_z}$, which is finite (again assuming the number of delta functions in the interaction to be finite). Thus, for $z \ge z_J$, $N_z = 0$ and only one term contributes to $\tilde{\psi}_k(z)$. That is,

$$\tilde{\psi}_k(z) = \langle z|k\rangle \tag{50}$$

Similarly, for $z_J > z \ge z_J - 1$, $N_z = 1$ and we have

$$\tilde{\psi}_k(z) = \langle z|k\rangle + k\Delta_J \sin(k[z_J - z]) V(z_J)\langle z_J|k\rangle \tag{51}$$

and, for $z_{J-1} > z \ge z_{J-2}$, $N_z = 2$ and

$$\begin{aligned}\tilde{\psi}_k(z) &= \langle z|k\rangle + k\Delta_J \sin(k[z_J - z]) V(z_J)\langle z_J|k\rangle + \\ &\quad k\Delta_{J-1} \sin(k[z_{J-1} - z]) V(z_{J-1})\langle z_{J-1}|k\rangle + \\ &\quad k^2\Delta_{J-1}\Delta_J \sin(k[z_{J-1} - z]) V(z_{J-1}) \sin(k[z_J - z]) V(z_J)\langle z_J|k\rangle\end{aligned} \tag{52}$$

etc. As one progresses in this manner from the transmission to the reflection region, the number of terms proliferate, but they are individually quite simple. Finally, in the reflection region, the number of terms in the wave function is two raised to the number of scattering points in the interaction. Obviously, if we had such a progression of $\tilde{\psi}_k$ values, it would be trivial to solve for the various $V(z_j)$ values sequentially, starting from the transmission end.

It is instructive to express this result using an $(N_z + 1)$-dimensional vector representation, where one component represents the point z and the other N_z components represent the delta-function points in the interaction on the transmission side of z. To this end, we introduce a set of $N_z + 1$ orthogonal unit vectors $|0\}$, $|1\}$, $|2\}$...$|N_z\}$, where $|0\}$ is the unit vector associated with z. Here, we use Dirac notation with $|j\}$ representing the jth unit vector in this *finite* dimensional space. We then have $\{s|t\} = \delta_{s,t}$ and the identity matrix in this space is given by

$$1 = \sum_{s=0}^{N_z} |s\}\{s| \tag{53}$$

We next define the matrix $\boldsymbol{Y}$ by

$$\{j|\boldsymbol{Y}|l\} = \sin(k[z_l - z_j])V(z_l)\Delta_l \tag{54}$$

Then,

$$\tilde{\psi}_k(z) = \{0|[1 + kY|1\}\{1|][1 + kY|2\}\{2|]... [1 + kY|N_z\}\{N_z|]\sum_{l=0}^{N_z} |l\}\langle z_l|k\rangle \tag{55}$$

which provides an explicit summation of the Volterra−Born series for this interaction. Physically, we see that each scattering center (i.e., delta function) in the interaction either produces a reflection or has no effect. Hence, the wave function at any point is only aware of the scattering centers that lie to the transmission side. The Volterra−Born series at a point z is simply a finite sum of the 2^{N_z} possibilities. Finally, if we knew $\tilde{\psi}_k(z)$ in the reflection region at as many values of k as there are scattering points in the interaction, we could, in principle, solve the resulting (highly nonlinear) equations for $V(z_j)$.

One could, of course, follow exactly the same procedure in the Fredholm case, starting with

$$\psi_k^+(z) = \langle z|k\rangle + \langle z|G^+V|k\rangle \tag{56}$$

However, in this case, there is no Heaviside function in the coordinate representation of the Green's operator, and, consequently, the counterpart to eq 48 does not have an ordered sum. The result is that the sum of terms contributing to $\psi_k^+(z)$ for any value of z is infinite. This simple interaction illustrates the comparative convergence properties of the Fredholm−Born and Volterra−Born series.

We next note that the $\tilde{\mathrm{T}}$-matrix element is

$$\langle -k|\tilde{T}_k|k\rangle = \langle -k|V|\tilde{\psi}_k\rangle = \sum_{j=1}^{J} e^{ikz_j}V(z_j)\Delta_j\tilde{\psi}_k(z_j) \tag{57}$$

From eq 24, we have

$$V_1(z) = \int_{-\infty}^{\infty} dk\, e^{-2ikz}\sum_{j=1}^{J} e^{ikz_j}V(z_j)\Delta_j\tilde{\psi}_k(z_j) \tag{58}$$

and, thus, from eq 52, we see that the general form of $\tilde{\psi}_k(z_j)$ is

$$\tilde{\psi}_k(z_j) = \langle z_j|k\rangle + R(k) \tag{59}$$

where the various terms in $R(k)$ have two types of k-dependence. First, each is proportional to a linear or higher power of k, and, second, each contains phase-factor exponentials (resulting from decomposition of the sine functions). Hence, the k-integral of each term can be evaluated explicitly. The integral of the $\langle z_j|k\rangle$ terms simply reproduce the original interaction (corresponding to the first-order Born approximation), and, because

$$k^l e^{-2ikz} = \left(\frac{i}{2}\right)^l \frac{\partial^l}{\partial z^l} e^{-2ikz} \tag{60}$$

the terms arising from $R(k)$ contain first- or higher-order derivatives (with respect to z) of delta functions. For example, the special case of $J = 3$ is

$$\begin{aligned} V_1(z) = \sum_{j=1}^{3}\Delta_j V(z_j)\delta(z - z_j) + \\ \frac{1}{4}\sum_{j=1}^{2}\sum_{j'>j}\Delta_j\Delta_{j'}V(z_j)V(z_{j'})[\delta'(z_{j'} - z) - \delta'(z_j - z)] + \\ \frac{\Delta_1\Delta_2\Delta_3}{16}[\delta''(z_3 - z) - \delta''(z_2 - z) + \\ \delta''(z_1 - z) - \delta''(z_1 + z_3 - z_2 - z)] \end{aligned} \tag{61}$$

If there are more sampling points in the interaction, the structure remains analogous, but there occur higher-order derivatives of the Dirac delta functions. Finally, we note that, formally,

$$\int_{z_j-\Delta_j/2}^{z_j+\Delta_j/2} dz\, \delta^p(z - z_j) = 0 \qquad (p \geq 1) \tag{62}$$

It follows that averaging V_1 in the neighborhood of a sampling point averages all of the higher terms to zero and we find that

$$\int_{z_j-\Delta_j/2}^{z_j+\Delta_j/2} dz\, V_1(z) = \Delta_j V(z_j) \tag{63}$$

After the $V(z_j)$ values are known, one knows the interaction.

Of course, such averaging is a formal exercise for a interaction that is a sum of delta functions, because both $V(z)$ and $V_1(z)$ are not true functions. They only have meaning in terms of delta sequences. However, the operational procedure can be applied to real data to construct an HDAF approximation, where the HDAF is interpreted as a member of a delta sequence. Thus, the suggested procedure would be to take the on-shell (far-field) amplitudes $\langle -k|\tilde{T}_k|k\rangle$ and evaluate $\tilde{V}_1(z)$ using eq 24. One then would use some averaging procedure, such as that indicated in eq 63, to obtain approximate expressions for $\Delta_j V(z_j)$ on a sufficiently dense set of points to construct an acceptable approximation to the true interaction, using eq 41.

V. Implementation of the Volterra-Based Inversion

As is evident from eq 63, if we have the modified reflection coefficient $\langle -k|\tilde{T}|k\rangle$, we can evaluate the $V(z_j)$ parameters approximately by a suitable averaging procedure. However, experiments are generally performed under conditions that do *not* make direct measurement of $\langle -k|\tilde{T}|k\rangle$ possible. However, as shown previously, this quantity is easily calculated from the physical reflection $\langle -k|T|k\rangle$ and transmission $\langle k|T|k\rangle$ amplitudes.[7] Thus, immediate use of eqs 57, 58, and 63 requires an additional measurement, compared to a Fredholm-based inversion. This is the price one pays to obtain the simplified Volterra expressions. It is significant, nevertheless, that even if one *cannot* measure the transmission $\langle k|T|k\rangle$, the Volterra-based inversion can still be performed, albeit with substantially greater required effort.

To see how this can be done, we consider the Lippmann−Schwinger equation:

$$\psi_k^+(z) = e^{ikz} - \frac{ik}{2}\int_{-\infty}^{\infty} dz'\, e^{ik|z-z'|}V(z')\psi_k^+(z') \tag{64}$$

For the interaction form of eq 40, this yields

$$\psi_k^+(z) = e^{ikz} - \frac{ik\Delta}{2}\sum_j e^{ik|z-z_j|}V(z_j)\psi_k^+(z_j) \tag{65}$$

We find the transmission coefficient to be

$$t_k = 1 - \frac{ik}{2}\int_{-\infty}^{\infty} \mathrm{d}z\, \mathrm{e}^{-ikz} V(z)\psi_k^+(z)$$
$$= 1 - \frac{ik\Delta}{2}\sum_j \mathrm{e}^{-ikz_j} V(z_j)\psi_k^+(z_j) \quad (66)$$

Similarly, the reflection coefficient is

$$r_k = -\frac{ik\Delta}{2}\sum_j \mathrm{e}^{ikz_j} V(z_j)\psi_k^+(z_j) \quad (67)$$

The Volterra normalization is such that $\tilde{t}_k \equiv 1$. To achieve this, we note that

$$t_k \tilde{\psi}_k(z) = \psi_k^+(z) \quad (68)$$

Then, by eq 66,

$$t_k = \frac{1}{1 + \frac{ik\Delta}{2}\sum_j \mathrm{e}^{-ikz_j} V(z_j)\tilde{\psi}_k(z_j)} \quad (69)$$

and

$$\frac{r_k}{t_k} = \tilde{r}_k \quad (70)$$

Thus,

$$r_k\left[1 + \frac{ik\Delta}{2}\sum_j \mathrm{e}^{-ikz_j} V(z_j)\tilde{\psi}_k(z_j)\right] = \tilde{r}_k \quad (71)$$

and

$$\tilde{V}_1(z) = \int_{-\infty}^{\infty} \mathrm{d}(2k)\frac{2i}{k}\tilde{r}_k \mathrm{e}^{-2ikz} \quad (72)$$

yielding

$$\tilde{V}_1(z) = \int_{-\infty}^{\infty} \mathrm{d}(2k)\, \mathrm{e}^{-2ikz}\frac{2i}{k} r_k\left[1 + \frac{ik\Delta}{2}\sum_j \mathrm{e}^{-ikz_j} V(z_j)\tilde{\psi}_k(z_j)\right] \quad (73)$$

To use this expression, we substitute for $\tilde{\psi}_k(z_j)$ using eq 55 and perform the averages in eq 63 to generate a system of nonlinear algebraic equations for the $\tilde{\psi}_k(z_j)$ parameters. The only experimental data then are the r_k values.

VI. Conclusions

In this paper, we have considered the problem of taking account of half-off-shell matrix elements of *either* T_k or $\tilde{T}_k$. We considered the moments of the interaction expressed in terms of T_k and $\tilde{T}_k$ and proved that $\tilde{V}_1[n]$, $n = 0, 1$ is *exact*, whereas *only* $V_1[0]$ is exact. This suggests that an inversion based on the Volterra scheme should be preferred, because of the different manner in which the half-off-shell effects enter. This is further supported by the superior convergence properties of the Volterra-based inverse scattering series. We illustrated these convergence properties using a simple model interaction that is expressed as a sum of Dirac delta functions. It was shown that a *formal* local average of $\tilde{V}_1$ in the neighborhood of a delta-function sampling point yields *exactly* the desired sampling value, $\Delta_j V(z_j)$. This is, of course, not exactly true for a real interaction. However, as argued by Rodberg and Thaler,[10] we expect that a sufficiently dense sampling, combined with an HDAF replacement of the Dirac delta functions, should yield a reasonable approximation.[11] It has the advantage that the averaging process is, in essence, taking account of the half-off-shell contributions, because it averages them exactly to zero for any interaction constructed as a sum of Dirac delta functions. Our next step will be to develop and test methods based on this approach on a one-dimensional model. This delta-function approach, strictly speaking, is dependent on taking a specific form for the interaction, but its application can be *very* general when the interaction parameters are determined as discussed.

Appendix A: The Modification of G_{0k}^+ by the Factor of k^2

Recall that the acoustic and electromagnetic wave scattering (in 1 − D) is of the form k^2V. The Lippmann−Schwinger equation is

$$|\psi_k^+\rangle = |k\rangle + G_{0k}^+(k^2V)|\psi_k^+\rangle \quad (74)$$

The transition operator is then defined as

$$T_k|k\rangle = V|\psi_k^+\rangle$$
$$= (V + VG_{0k}^+ k^2 T_k)|k\rangle \quad (75)$$

It is then convenient to absorb the k^2-factor into the Green's function, as was done in eq 2. This k^2-factor has a consequence of making a Born-expansion solution for T_k a low-k approximation.[6] This is in sharp contrast to quantum scattering for which it is well-known that the Born series always converges for sufficiently large values of k.[8,12] In the Volterra case, this k^2-factor cannot prevent convergence, regardless of how large k is.

Appendix B: Representation of $V(z)$ Using Dirac Delta Functions

In a series of studies,[11] it has been shown that a well-behaved function can be represented to controllable accuracy by an HDAF approximation. From this point of view, the model interaction form

$$V(z) = \sum_j \delta_M(z - z_j|\sigma)V(z_j) \quad (76)$$

(see eq 37), with a suitable choice of the embedded parameters $V(z_j)$, can be made to approximate *any* realistic interaction closely. (Of course, a limitless number of delta-function approximations could be utilized; however, as we later discuss, there are advantages to the HDAF approximation.) If V is effectively compact (and band-limited), then only a finite number of $V(z_j)$ parameters are needed. The Born expansion of the wave function is given by

$$\psi_k(z) = \langle z|k\rangle + \sum_{n=1}\langle z|(G_0V)^n|k\rangle \quad (77)$$

where $\psi_k(z)$ and G_0 can represent either $\psi_k^+(z)$ and G_0^+ or $\tilde{\psi}_k(z)$ and $\tilde{G}_0$. Because V is a local operator,

$$\langle z|(G_0V)^n|\, k\rangle = \int_{-\infty}^{\infty} \mathrm{d}z''\, \langle z|(G_0|z''\rangle V(z'')\langle z''|(G_0V)^{n-1}|k\rangle \quad (78)$$

and, hence, for this model interaction, we have

$$\langle z|(G_0V)^n|k\rangle = \sum_j\{\int_{-\infty}^{\infty}dz''\ \langle z|(G_0|z''\rangle\delta_M(z''-z_j|\sigma)\times \langle z''|(G_0V)^{n-1}|k\rangle\}V(z_j) \quad (79)$$

Now, $\delta_M(z''-z_j|\sigma)$, as a member of a delta sequence, is highly localized around z_j. In fact, the degree of localization can be controlled by our choice of the width parameter, σ. The flexibility of the interaction form, $V(z)$, of eq 76 to represent any realistic interaction is dependent on it being "well-tempered", as has been discussed elsewhere.[11] This essentially requires that, as σ is decreased, the number of z_j-points must be increased. By suitably localizing $\delta_M(z''-z_j|\sigma)$ relative to how the rapidly the rest of the integrand varies, we can write

$$\int_{-\infty}^{\infty}dz''\ \langle z|(G_0|z''\rangle\delta_M(z''-z_j|\sigma)\langle z''|(G_0V)^{n-1}|k\rangle \simeq \int_{-\infty}^{\infty}dz''\ \langle z|(G_0|z_j\rangle\delta_M(z''-z_j|\sigma)\langle z_j|(G_0V)^{n-1}|k\rangle \quad (80)$$

to arbitrary accuracy while still keeping the number of z_j-points in eq 79 finite. Because

$$\int_{-\infty}^{\infty}dz''\ \delta_M(z''-z_j|\sigma) = 1 \quad (81)$$

we then have

$$\langle z|(G_0V)^n|k\rangle \simeq \sum_j\langle z|(G_0|z_j\rangle\langle z_j|(G_0V)^{n-1}|k\rangle\}V(z_j) \quad (82)$$

This is clearly tantamount to making a delta-function approximation for $V(z)$. Repeating this process for $\langle z_j|(G_0V)^{n-1}|k\rangle$ etc., we can ultimately reduce the Born expansion of the wave function to a form equivalent to that obtained starting with a interaction that is a sum of delta functions. In this sense, the delta-function interaction is quite general, but its application (i.e., in the context of the aforementioned discussion, fixing σ and the number of sample points) sensitively is dependent on the particular problem. From the basic theory of Fourier transforms, we know that the variation of the integrand in eq 80 is controlled by its bandwidth in Fourier transform space, and, in turn, the bandwidth controls the width of the spacing between z_j-points through the Nyquist relationship. Clearly, one wants the bandwidth to be as small as can be reasonably chosen, to make the sample point spacing as large as possible. At the same time, the aforementioned discussion also makes clear that one wants to minimize the spread of the delta-function approximation about the point z_j in eq 80. The problem of *simultaneously* minimizing the bandwidth and the spread of the delta-function approximation in z-space is addressed through the choice of the delta-function approximation of the form used in eq 76. It has been shown elsewhere that, in the sense of the Heisenberg Uncertainty Principle, the HDAF approximation (i.e., $\delta_M(z-z_j|\sigma)$) is the best one can do.[13]

The aforementioned discussion examines the conditions under which an interaction that is a sum of delta functions can adequately represent the true interaction. However, it does *not* justify the procedure of eq 63 per se, because this averaging procedure, which is strictly correct for a delta-function interaction, is dependent explicitly on the fact that the delta-function interaction is not well-tempered. Precisely how this procedure should be implemented/modified for a realistic interaction is a subject for further research.

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