Inverse Scattering Theory: Renormalization of the Lippmann−Schwinger Equation for Quantum Elastic Scattering with Spherical Symmetry†

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We present a new inverse scattering series for quantum elastic scattering in three spherical dimensions. The new series, which converges absolutely, independent of the strength of the scattering interaction, results from a renormalization transformation of the Lippmann−Schwinger Fredholm integral equation to a Volterra form. A new feature of the formulation is that it does *not* require the determination of phase shifts and it can be applied even to integral cross-section measurements. The approach is illustrated by application to a simple example problem.

I. Introduction

There have been several general approaches to the inverse scattering problem in quantum mechanics. The earliest of those was pioneered by Jost and Kohn[1] and Moses,[2] and it is based on the Born−Neumann perturbation expansion of the Lippmann−Schwinger integral equation describing quantum scattering. Additional work on the approach includes that of Razavey,[3] Prosser,[4] and most importantly, in the context of the seismic inverse problem, Weglein and co-workers.[5] The key mathematical issue in the approach concerns the convergence of the resulting inverse scattering series, and this can be deferred, at least for some aspects of the problem, by considering certain subseries.[5]

The other general approach has been that pursued, for example, by Marchenko,[6] Gel'fand, and Levitan[7] and R. G. Newton.[8] In these approaches, alternative integral equations (of the Volterra type) are derived, leading to extremely robust behavior under iteration (i.e., absolute convergence independent of interaction strength). So far as we can tell, the principle difficulty associated with these approaches is in the nature of the input data required for their implementation. Indeed, it is true in general for quantum scattering that experiment does not readily provide the quantities that are directly involved in the inversion equations.[8] This is in part a consequence of the fact that in quantum mechanics probabilities rather than amplitudes are observed, thereby leading to ambiguities in phases. The present paper is not primarily directed at dealing with this issue, although our results are interesting from this aspect. We shall assume that either measurements of angular distributions are available experimentally because these *do* provide the sort of phase information that one desires or that one has access to integral cross sections for a range of collision energies.

The approach that we shall pursue has its origin in the first class of methods.[1−5] These methods are most simply formulated in terms of the solution, by iteration, of the Lippmann−Schwinger equation for the transition amplitude. Thus, for structureless particle scattering in 3-D, one has

$$T = V + VG_0^+T \tag{1}$$

where

$$G_0^+ = \frac{1}{E - K + i\epsilon} \tag{2}$$

$$H = K + V \tag{3}$$

denote the noninteracting Green function and the Hamiltonian, H, which is the sum of K, the kinetic energy, and V, the interaction responsible for the scattering. We view eq 1 now as an integral equation for V (rather than for T):

$$V = T - VG_0^+T \tag{4}$$

Then a power series solution for V in terms of T has the form

$$V = T - TG_0^+T + TG_0^+TG_0^+T - ...$$

$$= \sum_j^\infty V_j \tag{5}$$

Such an expression is problematic because it requires knowledge of the off-shell T-matrix elements (which are generally not available because they are equivalent to near-field measurements of the wave function). However, for the case of a local potential, we must interpret eq 5 as a sum of local, effective interactions that (provided the series converges) add up to the true, local interaction. Thus, consider the first-order term:

$$V_1 = T \tag{6}$$

An arbitrary off-shell matrix element of this is then of the form

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$$\langle \vec{k}'|V_1|\vec{k}\rangle = \langle \vec{k}'|T|\vec{k}\rangle \tag{7}$$

$$= \frac{1}{(2\pi)^3}\int \mathrm{d}\vec{k} e^{-\mathrm{i}\vec{k}'\cdot\vec{r}} V_1(\vec{r}) \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} \tag{8}$$

$$= \tilde{V}_1(\vec{k} - \vec{k}') \tag{9}$$

Thus, because of the local character assumed for V (and therefore also for V_j, $j = 1, 2,...$), we can obtain approximately all needed T-matrix elements for eq 5 once $V_1(\vec{r})$ is determined.[1−5] This results from the inverse Fourier transform of eq 9, where in particular we consider backward-scattered amplitudes.[8] Then $\vec{k}' = -\vec{k}$ and

$$V_1(2\vec{k}) = \langle -\vec{k}|\, T|\vec{k}\rangle \tag{10}$$

$$V_1(\vec{r}) = 2\int \mathrm{d}\vec{k}\ \mathrm{e}^{-2\mathrm{i}\vec{k}\cdot\vec{r}} V_1(2\vec{k}) \tag{11}$$

Notice that all of the matrix elements of T can be obtained from $\tilde{V}_1(2\vec{k})$ approximately from the condition that

$$\langle \vec{k}'|T|\vec{k}''\rangle = \tilde{V}_1(2\vec{k}) \tag{12}$$

where

$$\vec{k} = \frac{1}{2}[k'' - k'] \tag{13}$$

Thus, eq 5 can also be expressed approximately in the form

$$V = V_1 - V_1 G_0^+ V_1 + V_1 G_0^+ V_1 G_0^+ V_1 - ... \tag{14}$$

This is all well and good except that it can lead only to well-defined results if the perturbation expansion (eq 9) converges. Unfortunately, this is extremely difficult to ascertain in general, and it depends on the strength of interaction, V, the existence of bound states in the spectrum of H, the energy of the collision process, and so forth.[8] In general, the expansion does not converge if the interaction is too strong (or if it supports bound states).

The goal of the present paper is to provide an alternative inverse scattering series approach that is guaranteed to converge absolutely, independent of the strength of the interaction. The paper is organized as follows. In the next section, we derive a renormalized inverse scattering series and discuss its convergence. In section III, we discuss the information required to apply the new inversion, and in section IV, we illustrate the approach by applying it to a simple model scattering system. In section V, we discuss our results.

II. Renormalization of the Lippmann−Schwinger Equation

We begin by remembering that eqs 1−14 also apply in an appropriately modified form if one considers the various partial wave components. For simplicity, we shall restrict ourselves to spherically symmetric interactions in this paper, but the method is general.[9] The radial Lippmann−Schwinger equation is well known to be[8,10]

$$\psi_{lk}^+(r) = j_l(kr) - \frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r'\, r'^2\, h_l^+(kr_>)\, j_l(kr_<)\, V(r')\, \psi_{lk}^+(r')$$

$$= j_l(kr) + \int_0^\infty \mathrm{d}r'\, r' G_{l0k}^+(r, r')\, V(r')\, \psi_{lk}^+(r') \tag{15}$$

where $r_>(r_<)$ is the usual greater (lesser) component of the pair (r, r'), j_l is the lth regular spherical Bessel function, h_l^+ is the lth spherical Hankel function with the outgoing wave condition, ψ_{lk}^+ is the lth partial wave component of the scattering boundary condition solution to the Schrödinger equation, and G_{l0k}^+ is defined by the second equality in eq 15. Specifically,

$$\psi_{\vec{k}}^+(\vec{r}) = \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int \mathrm{d}\vec{r}'\, \frac{\mathrm{e}^{\mathrm{i}k|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} V(r')\, \psi_{\vec{k}}^+(\vec{r}') \tag{16}$$

$$\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} = \sum_l \sum_m \mathrm{i}^l Y_{lm}(\hat{r})\, Y_{lm}^*(\hat{k})\, j_l(kr) \tag{17}$$

$$-\frac{1}{4\pi}\frac{\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}\,'}}{|\vec{r} - \vec{r}'|} = -\frac{2mk}{\hbar^2}\sum_l \sum_m Y_l^m(\hat{r})\, Y_l^m(\hat{r}')^*\, h_l^+(kr_>)\, j_l(kr_<) \tag{18}$$

$$\psi_{\vec{k}}^+(\vec{r}) = \sum_l \sum_m i^l Y_{lm}(\hat{r})\, Y_{lm}^*(\hat{k})\, \psi_{lk}^+(r) \tag{19}$$

The asymptotic form of $\psi_{lk}^+(r)$ (for any $r > r_{\max}$ such that $V(r) = 0$) is

$$\psi_{lk}^+(r) \to j_l(kr) + T_l^{(1)}\, h_l^+(kr) \tag{20}$$

where

$$T_l^{(1)} \equiv -\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 j_l(kr)\, V(r)\, \psi_{lk}^+(r) \tag{21}$$

With this definition, the (unitary) S matrix, S_l, satisfies

$$S_l = 1 + 2\mathrm{i}T_l^{(1)} \tag{22}$$

implying that

$$T_l^{(1)} = \mathrm{e}^{\mathrm{i}\eta_l} \sin \eta_l \tag{23}$$

Here, η_l is the usual phase shift, and

$$S_l = \mathrm{e}^{2\mathrm{i}\eta_l} \tag{24}$$

It will also prove necessary to define an additional quantity:

$$T_l^{(2)} \equiv -\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 n_l(kr)\, V(r)\, \psi_{lk}^+(r) \tag{25}$$

We note that in general $T_l^{(2)}$ is not a directly measured quantity nor is it immediately obtainable from measured quantities. Finally, the differential scattering amplitude, $f(\theta)$, is

$$f(\theta) = \frac{1}{k}\sum_l (2l + 1) P_l(\cos\theta) T_l \tag{26}$$

where θ is the angle between the incident relative momentum vector, $\vec{k}$, and the direction of observation, $\hat{r}$. For mathematical simplicity, we shall also assume that the interaction has "compact support" (i.e., it is zero outside the range of $r_{\max}$):

$$V(r) = 0 \qquad r > r_{\max} \tag{27}$$

In general, however, our results will hold for interactions that are not too singular at $r = 0$ and that tend to zero faster than $1/r^2$ as $r \to \infty$. Following Sams and Kouri[11] and Kouri and Vijay,[12] we rewrite eq 15 as

$$\psi_{lk}^{+}(r) = j_l(kr)\left[1 - \frac{2mk}{\hbar^2}\int_0^\infty dr'\, r'^2 h_l^{+}(kr')\, V(r')\, \psi_{lk}^{+}(r')\right] - \frac{2mk}{\hbar^2}\int_0^r dr'\, r'^2 [n_l(kr)\, j_l(kr') - j_l(kr)\, n_l(kr')] V(r')\, \psi_{lk}^{+}(r') \quad (28)$$

But

$$h_l^{+}(kr') = n_l(kr) + i j_l(kr) \quad (29)$$

so we write eq 28 as

$$\psi_{lk}^{+}(r) = j_l(kr)[1 + T_l^{(2)} + iT_l^{(1)}] - \frac{2mk}{\hbar^2}\int_0^r dr'\, r'^2 [n_l(kr)\, j_l(kr') - j_l(kr)\, n_l(kr')] V(r')\, \psi_{lk}^{+}(r') \quad (30)$$

We recognize that the factor $[1 + T_l^{(2)} + iT_l^{(1)}]$, although unknown, is simply a constant normalization so that

$$\psi_{lk}^{+}(r) = u_{lk}(r)[1 + T_l^{(2)} + iT_l^{(1)}] \quad (31)$$

where

$$u_{lk}(r) = j_l(kr) + \int_0^r dr'\, r'^2 \tilde{G}_{l0k}(r, r')\, V(r')\, u_{lk}(r') \quad (32)$$

$$\tilde{G}_{l0k}(r, r') = -\frac{2mk}{\hbar^2}[n_l(kr)\, j_l(kr') - j_l(kr)\, n_l(kr')] \quad (33)$$

Equation 32 for $u_{lk}(r)$ has the tremendous virtue, compared to the Lippmann−Schwinger equation for $\psi_{lk}^{+}(r)$, of being a Volterra integral equation,[8,13] and under iteration, it converges absolutely and uniformly for all appropriately measurable interactions because the kernel, $\tilde{G}_{l0k}(r, r')\, V(r')$, is triangular, implying that the Fredholm determinant is identically one.[8] Consequently, it has no zeros, and the Fredholm solution encounters no singular points. This is the best possible mathematical situation that one can ever have!

However, we still must address the problem of how to make use of eq 31 because $T_l^{(2)}$ is not readily available. Before dealing with this, we note that by analogy to our earlier work on acoustic scattering[12] we can introduce a partial wave transition operator, T_l,

$$V\psi_{kl}^{+} = T_l j_l \quad (34)$$

$$T_l = V + VG_{l0k}^{+} T_l \quad (35)$$

and the Volterra-based auxiliary operators

$$\tilde{G}_{l0k} = G_{l0k}^{+} + \frac{2mk}{\hbar^2}|j_l\rangle\langle h_l^{+}| \quad (36)$$

or in the coordinate representation,

$$\tilde{G}_{l0k}(r, r') = G_{l0k}^{+}(r_<, r_>) + \frac{2mk}{\hbar^2} j_l(kr)\, h_l^{+}(kr') \quad (37)$$

Then we define $\tilde{T}_l$ such that

$$Vu_{kl} = \tilde{T}_l j_l \quad (38)$$

$$\tilde{T}_l = V + V\tilde{G}_{l0k}\tilde{T}_l \quad (39)$$

We see that

$$T_l = \tilde{T}_l\left(1 - \frac{2mk}{\hbar^2}|j_l\rangle\langle h_l^{+}|T_l\right) \quad (40)$$

$$= \tilde{T}_l\left(1 - \frac{2mk}{\hbar^2}|j_l\rangle\langle n_l|T_l - \frac{2mik}{\hbar^2}|j_l\rangle\langle j_l|T_l\right) \quad (41)$$

It follows that

$$T_l^{(1)} = \tilde{T}_l^{(1)}[1 + T_l^{(2)} + iT_l^{(1)}]$$
$$T_l^{(2)} = \tilde{T}_l^{(2)}[1 + T_l^{(2)} + iT_l^{(1)}] \quad (42)$$

We then see that

$$T_l^{(1)} = \frac{\tilde{T}_l^{(1)}}{1 - \tilde{T}_l^{(2)} - i\tilde{T}_l^{(1)}} \quad (43)$$

This relation enables us to express the perturbation expansion of V in terms of $\tilde{T}_l^{(1)}$ and $\tilde{T}_l^{(2)}$ and then ultimately in terms of $\tilde{T}_l^{(1)}$. We stress, however, that from eq 39

$$V = \tilde{T}_l - V\tilde{G}_{l0k}\tilde{T}_l \quad (44)$$

$$= \tilde{T}_l - \tilde{T}_l\tilde{G}_{l0k}\tilde{T}_l + \tilde{T}_l\tilde{G}_{l0k}\tilde{T}_l\tilde{G}_{l0k}\tilde{T}_l + \ldots \quad (45)$$

which converges absolutely and uniformly independent of the strength of the interaction. We shall again restrict ourselves to local (and for this paper, spherically symmetric) interactions, $V(r)$.

We now consider how to determine the $\tilde{V}_j$, defined by

$$V = \sum_{j=1}^{\infty}\tilde{V}_j \quad (46)$$

$$\tilde{V}_1 = \tilde{T}_l \quad (47)$$

$$\tilde{V}_2 = -\tilde{V}_1\tilde{G}_{l0k}\tilde{V}_1 \quad (48)$$

$$\tilde{V}_3 = \tilde{V}_1\tilde{G}_{l0k}\tilde{V}_1\tilde{G}_{l0k}\tilde{V}_1 = -\tilde{V}_2\tilde{G}_{l0k}\tilde{V}_1 \quad (49)$$

$$\tilde{V}_j = \tilde{V}_{j-1}\tilde{G}_{l0k}\tilde{V}_1 \quad (50)$$

$$\tilde{V}_{1l}^{(1)} \equiv -\frac{2mk}{\hbar^2}\int_0^\infty dr\, r^2 j_l^2(kr)\, \tilde{V}_1(r) \quad (51)$$

$$\tilde{V}_{1l}^{(2)} \equiv -\frac{2mk}{\hbar^2}\int_0^\infty dr\, r^2 n_l(kr)\, \tilde{V}_1(r)\, j_l(kr) \quad (52)$$

We have written the upper limit as ∞ rather than r_{max} in anticipation of the fact that, provided $\tilde{V}_1(r)$ tends to zero faster than $1/r^2$, the more general result holds. It is not difficult then to show that

$$T_l^{(1)} = \frac{\tilde{V}_{1l}^{(1)}}{1 - \tilde{V}_{1l}^{(2)} - i\tilde{V}_{1l}^{(1)}} \quad (53)$$

$$T_l^{(2)} = \frac{\tilde{V}_{2l}^{(1)}}{1 - \tilde{V}_{1l}^{(2)} - i\tilde{V}_{1l}^{(1)}} \quad (54)$$

These results have some extremely interesting features. First, note that both $\tilde{V}_{1l}^{(1)}$ and $\tilde{V}_{1l}^{(2)}$ are purely real. Consequently, eq 53 guarantees satisfaction of the optical theorem because

$$\mathrm{Im}T_l^{(1)} = |T_l^{(1)}|^2 \tag{55}$$

(This also implies that one cannot eliminate $\tilde{V}_{1l}^{(2)}$ in favor of $\tilde{V}_{1l}^{(1)}$ by using the real and imaginary parts of eq 53). Second, eq 53 is sufficient to enable an inversion, provided that $T_l^{(1)}$ is known. Thus, eq 53 is viewed as an equation that is satisfied by the first-order radial function, $\tilde{V}_1(r)$:

$$T_l^{(1)}(k) = \frac{-\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 j_l^2(kr)\,\tilde{V}_1(r)}{1+\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 n_l(kr)\,\tilde{V}_1(r)\,j_l(kr)+\frac{2mik}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 j_l^2(kr)\,\tilde{V}_1(r)} \tag{56}$$

Now, of course, the inversion is not so simple because one no longer has Cartesian Fourier transforms to invert. One procedure is to express $\tilde{V}_1(r)$ in some basis set (e.g., Bessel functions); an alternative is to use the distributed approximating functionals.[14] In any case, it may be necessary to obtain $\tilde{V}_1(r)$ on a numerical grid. We conclude that the fundamental results are eqs 53 and 54, along with[12]

$$\tilde{V}_{j+1} = -\tilde{V}_j \tilde{G}_{l0k} \tilde{V}_1 \qquad j \geq 1 \tag{57}$$

We now discuss the implementation of this approach in terms of measurable quantities.

III. Experimental Data Requirements for Implementation of the Volterra-Based Inverse Series

In quantum mechanical elastic scattering, the optimum measurements are the differential angular distributions, which are determined by $|f(\theta)|^2$. Because of azimuthal symmetry, we in fact consider $2\pi|f(\theta)|^2 \sin\theta$:

$$\frac{\mathrm{d}\sigma(\theta)}{\mathrm{d}\theta} = \sin\theta\,\frac{2\pi}{k^2}\Big|\sum_l (2l+1)P_l(\cos\theta)T_l^{(1)}\Big|^2 \tag{58}$$

Clearly, if a sufficient number of scattering angles are measured, then one can (in principle) determine the $T_l^{(1)}$. An alternative that avoids having to determine the individual $T_l^{(1)}$ is to use eq 56 directly, along with an appropriate representation of $\tilde{V}_1(r)$ to derive a system of inhomogeneous (nonlinear) algebraic equations that can be solved. For example, if we expand $\tilde{V}_1(r)$ in a basis $\{\phi_p(r)\}$,

$$\tilde{V}_1(r) = \sum_p \tilde{V}_{1p}\phi_p(r) \tag{59}$$

it is easily seen that

$$\frac{\mathrm{d}\sigma(\theta)}{\mathrm{d}\theta} = \sin\theta\,\frac{2\pi}{k^2}\left|\frac{\sum_l (2l+1)P_l(\cos\theta)\sum_p \tilde{V}_{1p}J_{lp}}{1-\sum_{p'}\tilde{V}_{1p'}H_{1p'}}\right|^2 \tag{60}$$

where

$$J_{lp} = -\frac{2mk}{\pi^2}\int_0^\infty \mathrm{d}r\, r^2 j_l^2(kr)\,\phi_p(r) \tag{61}$$

and

$$H_{lp} = -\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 h_l^+(kr)\,j_l(kr)\,\phi_p(r) \tag{62}$$

In general, eq 60 would be solved by a least-squares method, using more θ values than the number of terms in the expansion over p (eq 59). The redundancy is useful for averaging out noise. Another alternative is to use angular measurements at a small number of θ's but for a range of collision energies ($E = p^2k^2/2m$) to obtain an over-determined set of simultaneous nonlinear algebraic equations to solve.

Another interesting approach can be based on integral cross-section measurements. Thus, the integral cross section at energy E is well known to be

$$\sigma(E) = \frac{4\pi}{k^2}\sum_l (2l+1)|\,T_l|^2 \tag{63}$$

leading to the expression

$$\sigma(E) = \frac{4\pi}{k^2}\sum_l (2l+1)\left|\frac{\sum_p \tilde{V}_{1p}J_{lp}}{1-\sum_{p'}\tilde{V}_{1p'}H_{1p'}}\right|^2 \tag{64}$$

One must evaluate $\sigma(E)$ at enough energies to generate the requisite algebraic equations for the $\tilde{V}_{1p}$. In expressions 60 and 64, it is clear that lower-energy measurements will be numerically less complicated because the partial wave expansion will converge with fewer angular momentum states. However, we also expect that (at least for potentials with a repulsive core) the short-range part of the potential will be less accurate than the longer range part if one uses low-energy data.

It is important to note that in the case of the integral cross-section approach one makes no use of phase-dependent effects; indeed, only the $|\,T_l|^2$ enter the expression. Neither the basis set nor DAF approaches necessarily require any knowledge of the phase of the T_l, but one speculates that an inversion based on angular measurements will be more robust (in terms of accuracy) than one based on integral cross-section measurements. This remains to be tested. If either the integral or differential cross-section approach proves to be feasible, then this will represent an extremely attractive feature compared to approaches that require a determination of the individual partial-wave phase shifts[8]

Finally, we point out that once $\tilde{V}_1(r)$ is known all higher-order $\tilde{V}_j(r)$ can be computed in the coordinate representation using eq 57. We notice that the same radial functions, $\tilde{V}_j(r)$, result no matter which partial wave is considered. This is a consequence of the assumed spherical symmetry of the original potential. This provides an internal consistency condition that must be satisfied.

Of course, the above ideas, although formally correct, still must be tested on actual experimental data. An important issue is that of the effects of noise and inaccuracies in the data. In this regard, DAF-based methods may offer advantages.[14,15] For the problem at hand, it is convenient to use the spherical form of the 3-D non-Cartesian DAF. In doing so, we can represent a function $f(\vec{R})$, defined in 3-D, by

$$f(\vec{R}) = \int \mathrm{d}\vec{R}'\, I_{\sigma,\mu}(R'^2)\, f(\vec{R}+\vec{R}') \tag{65}$$

Here,

$$I_{\sigma,\mu}(R'^2) = \mathrm{e}^{-\bar{R}'^2} L_s^{(\mu)}(\bar{R}'^2) \tag{66}$$

where $\bar{R}' = (1/\sqrt{2\sigma})R'$, $L_s^{(\mu)}$ are related to the associated Laguerre polynomials of degree μ, and the integral is over all space. The expansion becomes exact in either the limit $\sigma \rightarrow 0$ or $\mu \rightarrow \infty$. The gradient of the function is given in similar approximation by replacing $I_{\sigma,\mu}(R'^2)$ with $\bar{R}'e^{-\bar{R}'^2}L_p^{(\mu)}(\bar{R}'^2)$, where $L_p^{(\mu)}$ is a different polynomial of degree μ.[14] Similar equations hold for higher derivatives.

Because for the case at hand we know that the potential is spherically symmetric about the origin, it is convenient to write the integral in the form

$$V(\vec{R}) = \int d\vec{r} I_{\sigma,\mu}(R'^2)\, V(\vec{r}) \tag{67}$$

where $\vec{R}' = \vec{r} - \vec{R}$. Using spherical polar coordinates, we have

$$V(R) = 2\pi \int_0^\infty dr\, r^2 \int_\pi^\infty d\theta \sin\theta\, I(R'^2)\, V(r) \tag{68}$$

where by the law of cosines

$$R'^2 = r^2 + R^2 - 2rR\cos\theta \tag{69}$$

Thus we can write $V(R)$ in the form

$$V(R) = \int_0^\infty dr\, W(R, r)\, V(r) \tag{70}$$

where

$$W(R, r) = 2\pi r^2 \int_0^\infty d\theta \sin\theta\, I(R'^2) \tag{71}$$

is a known function. We now discretize the integral on a grid, using the trapezoidal rule, to obtain

$$V(R) \approx \Delta r \sum_{j'=1}^{\infty} W(R, r_{j'})\, V_{j'} \tag{72}$$

where Δr is the uniform grid spacing and $V_{j'}$ is the value of the potential on the j' grid point. Finally, we combine eq 72, for $V_1(R)$, with eqs 56 and 58 to obtain

$$\frac{d\sigma}{d\theta} = \sin\theta \frac{2\pi}{k^2} \left| \sum_l (2l+1) \frac{P_l(\cos\theta) \sum_j V_1(r_j)\, J_l(r_j)}{1 - \sum_j V_j(r_j)\, H_l(r_j)} \right|^2 \tag{73}$$

where

$$J_l(r_j) = -\frac{2\mu k}{\hbar^2} \int_0^\infty dR\, R^2 j_l^2(kR)\, W(R, r_j)$$

and

$$H_l(r_j) = -\frac{2\mu k}{\hbar^2} \int_0^\infty dR\, R^2 j_l(kR)\, h_l^+(kR)\, W(R, r_j)$$

Clearly, one will obtain expressions for $d\sigma/d\theta$ and $\sigma(E)$ that are entirely analogous to those resulting from the basis set expansion approach. Both methods require the solution of nonlinear algebraic equations, and the same experimental data is employed.

IV. Simple Example

By far the simplest scattering problem to solve from the point of view of the Lippmann−Schwinger equation is for a local, Dirac delta function potential.[3,12] In our first study of inverse acoustic scattering, we found that the Volterra-based series converged to the exact result in a single term. A simple 3-D analogue is the spherically symmetric potential

$$V(r) = \lambda \delta(r - r_0) \tag{74}$$

It is easily shown that the exact transition amplitude is

$$T_l^{(1)} = \frac{-\frac{2mk}{\hbar^2}\lambda r_0^2\, j_l^2(kr_0)}{1 + \frac{2mk}{\hbar^2}\lambda r_0^2\; n_l(kr_0)\, j_l(kr_0) + \frac{2mik}{\hbar^2}\lambda r_0^2\, j_l^2(kr_0)} \tag{75}$$

Given such detailed input, we can use eq 56 directly:

$$\frac{\lambda r_0^2\, j_l^2(kr_0)}{1 + \frac{2mk}{\hbar^2}\lambda r_0^2\, n_l(kr_0)\, j_l(kr_0) + \frac{2mik}{\hbar^2}\lambda r_0^2\, j_l^2(kr_0)} = \frac{\int_0^\infty dr\, r^2 j_l^2(kr)\, \tilde{V}_1(r)}{1 + \frac{2mk}{\hbar^2}\int_0^\infty dr\, r^2\, n_l(kr)\, \tilde{V}_1(r)\, j_l(kr) + \frac{2mik}{\hbar^2}\int_0^\infty dr\, r^2 j_l^2(kr)\, \tilde{V}_1(r)} \tag{76}$$

Obviously, the solution is (independent of the partial wave considered)

$$\tilde{V}_1(r) = \lambda \delta(r - r_0) \tag{77}$$

Next, we must evaluate the higher-order terms in the expansion of $V(r)$ in terms of the $\tilde{V}_j(r)$. By eq 57,

$$\tilde{V}_2(r) = -\tilde{V}_1 \tilde{G}_{l0k} \tilde{V}_1 \tag{78}$$

$$= -\lambda \delta(r - r_0) \int_0^\infty dr'\, \tilde{G}_{l0k}(r, r')\, \lambda \delta(r' - r_0) \tag{79}$$

$$= -\lambda \delta(r - r_0)\, \tilde{G}_{l0k}(r_0, r_0) \tag{80}$$

Clearly, because of the behavior of $\tilde{G}_{l0k}(r_0, r_0)$, $\tilde{V}_2(r)$ is identically zero, no matter what the value of l. Furthermore, by eq 57, all higher $\tilde{V}_j$'s are also zero. We conclude that

$$V(r) = \sum_j \tilde{V}_j(r) \equiv \lambda \delta(r - r_0) \tag{81}$$

Thus, the Volterra-based inverse series again converges to the exact result in a single term.

Of course, in general, one does not know the individual T_l's. In this model problem, the differential scattering amplitude is

$$f(\theta) = -\frac{2mk\, r_0^2}{\hbar^2} \frac{\sum_l (2l+1)\, P_l(\cos\theta)\, j_l^2(kr_0)}{1 + \frac{2mk}{\hbar^2}\lambda\, r_0^2\; h_l^+(kr_0)\, j_l(kr_0)} \tag{82}$$

and the cross section is the square of its modulus. The convergence of this partial wave series results from the property of the Bessel functions, $j_l(kr_0)$, that $j_l(kr_0) \rightarrow 0$ for $l > kr_0$. Again, one can in principle obtain sufficient equations and obtain the exact result. The basic conclusion is the same, namely, that the Volterra inversion converges to the exact result in a single term.

V. Discussion of Results

In this paper, we have presented a new approach to the inverse scattering problem in quantum mechanics. Although attention

was focused on purely elastic scattering by a spherically symmetric potential, the method is quite general. Indeed, it can be applied not only to quantum scattering but also to many other types of processes. Any process that can be described by a Lippmann−Schwinger-type causal (or anticausal) integral equation should be amenable to the approach. The method is based on a renormalization transformation of the Lippmann−Schwinger Fredholm equation to obtain a Volterra integral equation.[11,12] In quantum scattering, such equations are well known[8,10] but principally used to analyze the analytic structure of the *S* matrix. An exception is the earlier work of Sams and Kouri,[11] who utilized the renormalization point of view to develop a noniterative numerical method for directly solving the coordinate representation of the *T* matrix. The principal benefit of the renormalization to a Volterra equation for inverse scattering is the fact that their noniterative solutions converge absolutely and (under relatively mild conditions) uniformly independent of the strength of the interaction. This feature allows us to utilize the Volterra equations in a manner similar to that pioneered by Jost and Kohn,[1] Moses,[2] and most recently Weglein,[5] but with the guarantee that the inverse series always converges.

In the case of quantum scattering in 3-D, the results are complicated by the facts that **(**a**)** the renormalization factor is no longer a directly measurable quantity as it is for acoustic scattering in 1-D,[3,5,12] **(**b**)** the different partial waves do not separate in a simple fashion, and **(**c**)** the equations that one must solve to determine the potential are nonlinear because of the intrinsic nature of quantum mechanics. However, there are no difficulties in principle with the present method. Furthermore, the present inverse series does not require the determination of phases. It can, at least in principle, be applied either to differential or integral cross-section measurements. If it indeed is the case that sufficiently accurate results can be obtained without requiring the determination of phase-sensitive quantities, then this will provide a major advantage over other inversion equations for quantum scattering.[8]

For the case of scattering by a spherically symmetric Dirac delta function potential, the convergence to the exact result is obtained with a single term. By contrast, the Born−Neumann inverse series based on the Lippmann−Schwinger equation yields the result

$$\int_0^\infty \mathrm{d}r\, r^2 V_1(r)\, j_l^2(kr) = T_l^{(1)} \tag{83}$$

for the first-order effective local interaction. It is immediate that any real V_1 obtained from the above will introduce unphysical behavior because the left side of the equation is real (i.e., eq 80 manifestly violates the optical theorem for real $V_1(r)$). Comparing this to eq 52 and using eq 75 leads to

$$-\frac{2mk}{\hbar^2}\int_0^\infty \mathrm{d}r\, r^2 V_1(r)\, j_l^2(kr) = \frac{-\frac{2mk}{\hbar^2}\lambda r_0^2\, j_l^2(kr_0)}{1+\frac{2mk}{\hbar^2}r_0^2\lambda\, h_l^+(kr_0)\, j_l(kr_0)} \tag{84}$$

A solution of this equation is easily seen to be

$$V_1(r) = \frac{\lambda\delta(r-r_0)}{1+\frac{2mk}{\hbar^2}\lambda r_0^2\; h_l^+(kr_0)\, j_l(kr_0)} \tag{85}$$

The second-order correction is

$$V_2(r) = \frac{-\lambda^2\delta(r-r_0)\, G_{l0k}^+(r_0, r_0)}{\left[1+\frac{2mk}{\hbar^2}\lambda r_0^2\, h_l^+(kr_0)\, j_l(kr_0)\right]^2} \tag{86}$$

$$\neq 0 \tag{87}$$

Thus, in this case, the first-order term of the series does not yield the exact answer in general, and it does not consist of a single nonzero term. In fact, one easily sees that one must sum the infinite series analytically to obtain the correct result for values of λ that are outside the convergence radius of the series.

Equation 83 corresponds to the first term in the Taylor expansion of the denominator on the right side of eq 84, which is analogous to the situation we encountered in our previous work on 1-D inverse acoustic scattering. Such an expansion converges only for sufficiently small λ values (as well as also depending on the value of r_0). Of course, it does permit one to sum the infinite series analytically to obtain the result that holds outside the convergence limits of the series itself.[12] As is also usual for the Born−Neumann expansion in quantum scattering, the approximation does eventually converge for high enough energy, *E* (large enough *k*).

We are currently exploring the inversion of quantum 3-D elastic scattering by a nonspherical target, as well as various other wave phenomena. Of particular interest are the cases of acoustic and electromagnetic scattering in full 3-D. In addition, we shall carry out test calculations to verify that one can use non-phase-sensitive integral cross sections to carry out an inversion. These results will be reported as they are obtained.

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References and Notes

(1) Jost, R.; Kohn, W. *Phys. Rev.* **1952**, *87*, 977.
(2) Moses, H. E. *Phys. Rev.* **1956**, *102*, 559.
(3) Razavy, M. *J. Acoust. Soc. Am.* **1975**, *58*, 956.
(4) Prosser, R. T. *J. Math. Phys.* **1969**, *10*, 1819. Prosser, R. T. *J. Math. Phys.* **1976**, *17*, 1775. Prosser, R. T. *J. Math. Phys.* **1980**, *21*, 2648.
(5) Weglein, A. B.; Matson, K. H.; Foster, D. J.; Carvalho, P. M.; Corrigan, D.; Shaw, S. A. Imaging and Inversion at Depth without a Velocity Model: Theory, Concepts and Initial Evaluation; Expanded Abstracts, Society for Exploration Geophysics 2000, Calgary, CA. Weglein, A. B.; Stolt, R. H. Migration-Inversion Revisited. *The Leading Edge*; 1999; p 950. See also the subseries approach to removing multiples from seismic data in Weglein, A. B.; Gasparotto, F. A.; Carvalho, P. M.; Stolt, R. H. *Geophysics* **1997**, *62*, 1775.
(6) Marchenko, V. A. *Math. Rev.* **1950**, *12*, 183. Marchenko, V. A. *Am. Math. Soc. Transl.* **1960**, *25*, 77.
(7) Gel'fand, I. M.; Levitan, B. M. *Math. Rev.* **1951**, *13*, 240. Gel'fand, I. M.; Levitan, B. M. *Am. Math. Soc. Transl.* **1951**, *1*, 253.
(8) Newton, R. G. *Scattering Theory of Waves and Particles*; Springer-Verlag: New York, 1982.
(9) Kouri, D. J. To be submitted for publication.
(10) Goldberger, M. L.; Watson, K. M. *Collision Theory*; Wiley: New York, 1964.
(11) Sams, W. N.; Kouri, D. J. *J. Chem. Phys.* **1969**, *51*, 4809, 4815.
(12) Kouri, D. J.; Vijay, Amrendra *Phys. Rev. E.* **2003**, *67*, 0466xx.
(13) Courant, R.; Hilbert, D. H. *Methods of Mathematical Physics*; Interscience: New York, 1953.
(14) Hoffman, D. K.; Kouri, D. J. *J. Phys. Chem.* **1993**, *97*, 4984. Hoffman, D. K.; Kouri, D. J. *J. Phys. Chem.* **1991**, *95*, 8299.
(15) Hoffman, D. K.; Gunaratne, G. H.; Zhang, D. S.; Kouri, D. J. *Chaos* **2000**, *10*, 240.
(16) Rudin, W. *Functional Analysis*, 2nd ed.; McGraw-Hill: New York, 1991.