The response to a perturbation in the reflection amplitude

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Abstract
We apply inverse scattering theory to calculate the functional derivative of the potential $V(x)$ and wavefunction $\psi(x, k)$ of a one-dimensional Schrödinger operator with respect to the reflection amplitude $r(k)$.

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1. Introduction

The computation of the effect of a perturbation in the potential $V(x)$ of a one-dimensional Schrödinger operator

$$H = -\partial_x^2 + V(x) \tag{1.1}$$

defined on the whole real line on the *continuous* part of the spectrum of H is a standard (albeit non-trivial) procedure in perturbation theory. For example, the response of the reflection amplitude $r(k)$ at momentum k (in a setting where there is source at $x = +\infty$) to an infinitesimal change in the potential is

$$\frac{\delta r(k)}{\delta V(x)} = \frac{(t(k)\phi(x, k))^2}{2ik}. \tag{1.2}$$

The derivation of this result is given in the appendix. Here $t(k)$ is the transmission amplitude and $t(k)\phi(x, k)$ is the solution of the Schrödinger equation

$$\left(-\partial_x^2 + V(x) - k^2\right)\Psi(x, k) = 0 \tag{1.3}$$

which satisfies the scattering boundary conditions of this problem

$$\begin{aligned}
t(k)\phi(x, k) &= t(k)\,e^{-ikx} + o(1) & x \to -\infty \\
t(k)\phi(x, k) &= e^{-ikx} + r(k)\,e^{ikx} + o(1) & x \to \infty.
\end{aligned} \tag{1.4}$$

Obtaining the kernel inverse to (1.2), i.e., the response of the Schrödinger potential $V(x)$ to a change in the reflection amplitude $r(k)$, is a much more difficult problem. It arises naturally in inverse scattering theory (IST) [1–4] in connection with the issue of stability, i.e., the notion of continuity of the inverse transform in some well-defined sense [5].

This issue of stability was studied, in the framework of the Gelfand–Levitan formulation [6] of IST, in [7]. In its most general form, one uses the Gelfand–Levitan formalism to relate the unknown one-dimensional Schrödinger operator, which is to be determined, to an appropriate prescribed comparison Schrödinger operator, which need not necessarily be the free Schrödinger operator. The kernel of the resulting Gelfand–Levitan integral equation is related to the difference of the spectral densities of the two Schrödinger operators. Then, one can study the case in which the unknown operator is infinitesimally close to the reference operator, i.e., to study the response of the potential to a perturbation in the spectral density, as was done in [7]. For example, equation (20.28) in the first reference in [7] gives the functional derivative of the Schrödinger potential with respect to the spectral density.

The problem of perturbations and stability was later studied also in the framework of the Marchenko formulation [8] of IST, in the series of papers [9]. The work in these papers constitutes a generalization of Marchenko's formulation of IST from the case in which the transformation kernel connects the unknown Schrödinger operator and the free Schrödinger operator, to the case in which the former is connected to an appropriate but otherwise arbitrary comparison Schrödinger operator. One can then study the limit in which the two operators are infinitesimally separated, as was mentioned above for the Gelfand–Levitan case. (In addition, it should be mentioned that the work in [9] uses a reformulation of Marchenko's approach as a Riemann–Hilbert problem [1, 5].) For discussions of perturbations and stability in IST in three dimensions see, e.g., [5, 10].

In this paper we obtain the response of the Schrödinger potential $V(x)$, as well as the response of the wavefunction, to a change in the reflection amplitude $r(k)$, directly from the Gelfand–Levitan–Marchenko equation[1] (formulated for the case in which the transformation kernel connects the unknown and the free Schrödinger operators), by means of elementary methods of the theory of Fredholm integral equations.

The explicit formulae we derive in this work express the *local* response of the potential and wavefunctions (see (3.13) and (3.15)) to a change in the reflection amplitude. Thus, our results add to the information which can be gleaned from the well-known trace identities of [11], the lowest of which reads

$$\int_{-\infty}^{\infty} V(x)\, dx = -\frac{2}{\pi} \int_0^{\infty} \log[1 - |r(k)|^2]\, dk - 4 \sum_{l=1}^{N} \kappa_l \qquad (1.5)$$

where $E_l = -\kappa_l^2$ are the N bound state energies (with $\kappa_l > 0$), which tell us only about that response integrated over space.

A few possibly interesting applications of the results of this paper (which include an application to supersymmetric quantum mechanics) are mentioned in the conclusions.

It would be useful at this point to introduce some additional notation and recall some basic facts, which will be used later on. For k real, $H - k^2$ is real, and therefore $\Psi^*(x, k) = \Psi(x, -k)$ for any solution of (1.3). It follows that

$$r^*(k) = r(-k) \quad \text{and} \quad t^*(k) = t(-k) \qquad (1.6)$$

in (1.4).

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[1] We refer here to equation (2.6), using the terminology of [1, 4]. In the context of scattering problems on the half-line (as, e.g., in the case of the radial equation for spherically symmetric potentials), that equation should be more appropriately referred to as the Marchenko equation.

$\Psi(x, k)$ and $\Psi^*(x, k)$ are linearly independent solutions of (1.3), and the continuous spectrum is doubly degenerate at each $k^2 > 0$. In particular, $\phi(x, k)$ and $\phi^*(x, k)$ form a basis. Since they are degenerate in energy, their Wronskian is a non-zero constant. Equating its values at $x \to \pm\infty$, we obtain the probability conservation relation

$$|r(k)|^2 + |t(k)|^2 = 1. \tag{1.7}$$

An equally suitable basis is the pair of solutions $\psi(x, k)$ and $\psi^*(x, k)$ of (1.3), in which $\psi(x, k)$ obeys the boundary condition

$$\psi(x, k) = e^{-ikx} + o(1) \qquad x \to \infty. \tag{1.8}$$

Thus, $\psi^*(x, k)$ corresponds to a setting in which there is a source at $x = -\infty$.

We see from (1.4) and (1.8) that

$$\phi(x, k) \underset{x \to \infty}{\longrightarrow} \frac{1}{t(k)} \psi(x, k) + \frac{r(k)}{t(k)} \psi^*(x, k).$$

This relation must hold for all x, since $\psi(x, k)$ and $\psi^*(x, k)$ form a basis everywhere. Adding to it the linear combination for $\phi^*(x, k)$, we may write the relation between the two bases as

$$\begin{pmatrix} \phi(x, k) \\ \phi^*(x, k) \end{pmatrix} = \begin{pmatrix} \frac{1}{t(k)} & \frac{r(k)}{t(k)} \\ \frac{r^*(k)}{t^*(k)} & \frac{1}{t^*(k)} \end{pmatrix} \begin{pmatrix} \psi(x, k) \\ \psi^*(x, k) \end{pmatrix}. \tag{1.9}$$

Note that the transformation matrix has a unit determinant. The inverse transformation is thus

$$\begin{pmatrix} \psi(x, k) \\ \psi^*(x, k) \end{pmatrix} = \begin{pmatrix} \frac{1}{t^*(k)} & -\frac{r(k)}{t(k)} \\ -\frac{r^*(k)}{t^*(k)} & \frac{1}{t(k)} \end{pmatrix} \begin{pmatrix} \phi(x, k) \\ \phi^*(x, k) \end{pmatrix}. \tag{1.10}$$

This paper is organized as follows: in the following section we present a lightning review of inverse scattering theory. In particular, we discuss the Gelfand–Levitan–Marchenko (GLM) equation and its properties. We show that its solution is simply the boundary column of its resolvent kernel.

In section 3 we compute the variational derivative of the solution of the Gelfand–Levitan–Marchenko equation with respect to the reflection amplitude. Then we derive from it the corresponding derivatives of the potential and wavefunctions (equations (3.13) and (3.15), respectively) in closed form.

In section 4 we demonstrate the consistency of our results by comparing their integrated form against known facts.

Finally, in the appendix we provide some useful technical details. In particular, we present the derivation of (1.2), and also discuss briefly the case of reflectionless potentials.

2. The Gelfand–Levitan–Marchenko equation and its solution

According to inverse scattering theory [1–4], a Schrödinger operator (1.1) whose potential $V(x)$ tends asymptotically to zero fast enough, such that $\int_{-\infty}^{\infty} |V(x)|(1 + |x|)\,dx < \infty$, and thus supports only a finite number N of bound states, is uniquely determined by the so-called scattering data. The scattering data are the reflection amplitude $r(k)$, and a finite set of $2N$ real numbers

$$\kappa_1 > \kappa_2 > \cdots \kappa_N > 0 \qquad \text{and} \qquad c_1, c_2, \ldots c_N \tag{2.1}$$

where $E_l = -\kappa_l^2$ is the lth bound state energy, and where c_l appears in the asymptotic behaviour of the lth *normalized* bound state wavefunction as $c_l \exp{-\kappa_l|x|}$ (and thus determines its 'centre of gravity').

The prescribed reflection amplitude $r(k)$ can be taken as any complex-valued function which satisfies (for k real)

$$r(-k) = r^*(k)$$
$$|r(k)| < 1 \qquad k \neq 0 \qquad\qquad\qquad (2.2)$$

and

$$r(k) = O\left(\frac{1}{k}\right) \qquad |k| \to \infty.$$

The first two conditions were already mentioned in (1.6) and (1.7), and the third one reflects the fact that $V(x)$ is a small perturbation at high energy. In addition to these conditions, there is a less obvious technical condition that the Fourier transform $B(x) = \int_{-\infty}^{\infty} \frac{r(k)}{t(k)} e^{ikx} \, dk$ should satisfy the bound $\int_{-\infty}^{\infty} (1 + |x|)|\frac{dB(x)}{dx}| \, dx < \infty$. Finally, by analyticity, the transmission amplitude $t(k)$ is completely determined by $r(k)$ as

$$\frac{t(k)}{\sqrt{1 - |r(k)|^2}} = \left(\prod_{l=1}^{N} \frac{k + i\kappa_l}{k - i\kappa_l}\right) \exp\left(\frac{1}{2\pi i} \text{P.P.} \int_{-\infty}^{\infty} \frac{\log[1 - |r(q)|^2]}{q - k} \, dq\right). \qquad (2.3)$$

Given the scattering data, IST instructs us to determine a certain real transformation kernel $K(x, y)$, bounded on the domain $y \geqslant x$, which maps the wavefunctions of the free Schrödinger operator $H_0 = -\partial_x^2$ onto those of the operator H in (1.1). For example, the left moving wave e^{-ikx} is mapped onto

$$\psi(x, k) = e^{-ikx} + \int_x^{\infty} K(x, y) e^{-iky} \, dy \qquad\qquad (2.4)$$

which is evidently the solution of (1.3) satisfying the boundary condition (1.8) mentioned above. Finally, the potential $V(x)$ in (1.1) is determined by $K(x, y)$ according to

$$V(x) = -2\frac{d}{dx} K(x, x). \qquad\qquad (2.5)$$

The kernel $K(x, y)$ is determined as the solution of the Gelfand–Levitan–Marchenko equation [1–4],

$$K(x, y) + F(x + y) + \int_x^{\infty} K(x, z) F(z + y) \, dz = 0 \qquad\qquad (2.6)$$

where the *real* function $F(x)$ is

$$F(x) = \sum_{l=1}^{N} c_l^2 e^{-\kappa_l x} + \frac{1}{2\pi} \int_{-\infty}^{\infty} r(k) e^{ikx} \, dk. \qquad\qquad (2.7)$$

For fixed x, (2.6) is a Fredholm integral equation of the second type in the unknown function $\Phi(y) = K(x, y)$,

$$\Phi(y) = f(y) + \lambda \int_x^{\infty} N(y, z) \Phi(z) \qquad\qquad (2.8)$$

with symmetric real kernel and given function

$$N(y, z) = N(z, y) = -F(y + z) \qquad f(y) = -F(x + y) = N(y, x) \quad (2.9)$$

respectively, and spectral parameter $\lambda = 1$.

It is known that (2.6) has a unique solution, i.e., the Fredholm determinant of (2.8) is not null at $\lambda = 1$ [2, 3]. It is easy to demonstrate this property in the case of reflectionless potentials (for which $r(k) = 0$ for all k), as we show in the appendix.

The unique solution of (2.8) at $\lambda = 1$ is given by

$$\Phi(y) = f(y) + \int_x^\infty R(y, z; 1) f(z) \, \mathrm{d}z \tag{2.10}$$

where $R(y, z; \lambda)$ is the resolvent kernel of (2.8). Note that for real values of λ, $R(y, z; \lambda)$ is manifestly real, when it exists.

It is useful at this point to introduce the operator $\hat{N}$ and the vectors $|\Phi\rangle$ and $|f\rangle$, which correspond to the kernel $N(y, z)$ and functions $\Phi(y)$ and $f(y)$. Thus, in obvious notation, $N(y, z) = \langle y|\hat{N}|z\rangle = -F(y + z)$, $\langle y|f\rangle = f(y) = \langle y|\hat{N}|x\rangle$ and $\Phi(y) = \langle y|\Phi\rangle$. Then, it is easy to see from (2.8) that

$$|\Phi\rangle = \frac{1}{\mathbf{1} - \hat{N}}|f\rangle = \frac{\hat{N}}{\mathbf{1} - \hat{N}}|x\rangle. \tag{2.11}$$

Similarly, from (2.10) we deduce that $R(y, z; 1) = \langle y|\hat{R}|z\rangle$, where

$$\hat{R} = \frac{1}{\mathbf{1} - \hat{N}} - \mathbf{1} = \frac{\hat{N}}{\mathbf{1} - \hat{N}}. \tag{2.12}$$

Thus, by comparing (2.11) and (2.12), we conclude that $|\Phi\rangle = \hat{R}|x\rangle$, i.e.,

$$\Phi(y) = K(x, y) = \langle y|\hat{R}|x\rangle. \tag{2.13}$$

The solution of the GLM equation (2.6) coincides with the xth column of its resolvent kernel. It is manifestly a real function of x and y.

3. The variational derivatives

In view of (2.13), it is straightforward to compute the variation of $K(x, y)$ under small perturbations in $\hat{N}$. Thus, consider a perturbation $\hat{N} \to \hat{N} + \delta\hat{N}$, which induces the variation $\hat{R} \to \hat{R} + \frac{1}{1-\hat{N}}\delta\hat{N}\frac{1}{1-\hat{N}}$. Consequently $\frac{\delta R(y,z;1)}{\delta N(a,b)} = \langle y|(\mathbf{1} + \hat{R})|a\rangle\langle b|(\mathbf{1} + \hat{R})|z\rangle$. Thus, from (2.13)

$$\frac{\delta K(x, y)}{\delta N(a, b)} = (\delta(y - a) + R(y, a; 1))(\delta(b - x) + K(x, b)). \tag{3.1}$$

In this work we are interested in variations $\delta\hat{N}$ which result from a change $\delta r(k)$ in the reflection amplitude. Due to the first condition in (2.2) we must impose $\delta r(-k) = \delta r^*(k)$. Thus, with no loss of generality, we take the positive components $r(k)$, $k \geqslant 0$ as the independent functional variables. Keeping that in mind, we obtain from (2.7) and (2.9) that

$$\frac{\delta N(a, b)}{\delta r(k)} = -\frac{1}{2\pi} \mathrm{e}^{\mathrm{i}k(a+b)}. \tag{3.2}$$

Thus, from (3.1) and (3.2) we obtain

$$\frac{\delta K(x, y)}{\delta r(k)} = \int_x^\infty \frac{\delta K(x, y)}{\delta N(a, b)} \frac{\delta N(a, b)}{\delta r(k)} \, \mathrm{d}a \, \mathrm{d}b$$
$$= -\frac{1}{2\pi} \left(\mathrm{e}^{\mathrm{i}ky} + \int_x^\infty R(y, a; 1) \mathrm{e}^{\mathrm{i}ka} \, \mathrm{d}a \right) \left(\mathrm{e}^{\mathrm{i}kx} + \int_x^\infty K(x, b) \mathrm{e}^{\mathrm{i}kb} \, \mathrm{d}b \right). \tag{3.3}$$

From (2.4) and from the reality of $K(x, y)$ and k, we recognize the last factor in (3.3) simply as $\psi^*(x, k)$. Thus,

$$\frac{\delta K(x, y)}{\delta r(k)} = -\frac{1}{2\pi} \left(\mathrm{e}^{\mathrm{i}ky} + \int_x^\infty R(y, a; 1) \mathrm{e}^{\mathrm{i}ka} \, \mathrm{d}a \right) \psi^*(x, k). \tag{3.4}$$

In order to simplify (3.4) further, we have to study the function

$$\omega(y, x; k) = \int_x^\infty R(y, a; 1) \, e^{ika} \, da. \tag{3.5}$$

Observe from (2.10) (considered with a generic given function $f(y)$), that $\Omega(y, x; k) = e^{iky} + \omega(y, x; k)$ is the unique solution of the Fredholm equation $\Omega(y, x; k) = e^{iky} + \int_x^\infty N(y, z)\Omega(z, x; k) \, dz$, from which we infer that $\omega(y, x; k)$ is the unique solution of

$$\omega(y, x; k) = -G(y, x; k) + \int_x^\infty N(y, z)\omega(z, x; k) \, dz \tag{3.6}$$

where

$$G(y, x; k) = \int_x^\infty F(y + z) \, e^{ikz} \, dz. \tag{3.7}$$

Thus, $\partial_x \omega(y, x; k)$ satisfies

$$\frac{\partial \omega(y, x; k)}{\partial x} = F(x + y)(e^{ikx} + \omega(x, x; k)) + \int_x^\infty N(y, z)\frac{\partial \omega(z, x; k)}{\partial x} \, dz. \tag{3.8}$$

From (3.5), (2.13) and the fact that $R(y, z; 1) = R(z, y; 1)$, we obtain that $\omega(x, x; k) = \int_x^\infty R(a, x; 1) \, e^{ika} \, da = \int_x^\infty K(x, a) \, e^{ika} \, da$. Thus, the inhomogeneous term in (3.8) is simply $F(x + y)\left(e^{ikx} + \int_x^\infty K(x, a) \, e^{ika} \, da\right) = F(x + y)\psi^*(x, k) = -f(y)\psi^*(x, k)$, where we used (2.4). It is the given function $f(y)$ in (2.8) multiplied by a y-independent factor $-\psi^*(x, k)$. Thus, from linearity, the unique solution of (3.8) is simply the solution of (2.8), multiplied by the same factor, namely,

$$\frac{\partial \omega(y, x; k)}{\partial x} = -K(x, y)\psi^*(x, k). \tag{3.9}$$

The initial condition for this equation at $x = y$ is obviously $\omega(y, y; k) = \int_y^\infty K(y, a) \, e^{ika} \, da = \psi^*(y, k) - e^{iky}$. Thus,

$$\omega(y, x; k) = \int_x^y \psi^*(z, k)K(z, y) \, dz + \psi^*(y, k) - e^{iky}. \tag{3.10}$$

Substituting this result into (3.4) we obtain our first main result

$$\frac{\delta K(x, y)}{\delta r(k)} = -\frac{1}{2\pi}\left(\psi^*(y, k) + \int_x^y \psi^*(z, k)K(z, y) \, dz\right)\psi^*(x, k). \tag{3.11}$$

Since $K(x, y)$ is a real kernel, we can write (3.11) alternatively as

$$\frac{\delta K(x, y)}{\delta r^*(k)} = -\frac{1}{2\pi}\left(\psi(y, k) + \int_x^y \psi(z, k)K(z, y) \, dz\right)\psi(x, k). \tag{3.12}$$

The formula for $\frac{\delta K(x,y)}{\delta r^*(k)}$ is the key for obtaining the functional derivatives of the wavefunction $\psi(x, k)$ and potential $V(x)$ with respect to the reflection amplitude $r(k)$, since the former are linear in $K(x, y)$. Thus, from (2.5) and (3.12) we obtain our second main result

$$\frac{\delta V(x)}{\delta r^*(k)} = -2\frac{d}{dx}\frac{\delta K(x, x)}{\delta r^*(k)} = \frac{1}{\pi}\frac{d}{dx}\psi^2(x, k). \tag{3.13}$$

This equation is very similar to equation (20.28) of the first reference in [7], which was derived in a different manner than ours, as was discussed in the introduction.

Similarly, from (2.4) and (3.12) we obtain

$$\frac{\delta \psi(x, k)}{\delta r^*(q)} = -\frac{1}{2\pi}\left[\int_x^\infty e^{-iky}\left(\psi(y, q) + \int_x^y \psi(z, q)K(z, y) \, dz\right) dy\right]\psi(x, q). \tag{3.14}$$

Reversing the order of integrations in the second integral according to

$$\int_x^\infty e^{-iky} \left(\int_x^y \psi(z, q) K(z, y) \, dz \right) dy = \int_x^\infty \psi(z, q) \left(\int_z^\infty e^{-iky} K(z, y) \, dy \right) dz$$

and recognizing the y-integral on the right-hand side of the last equation as $\int_z^\infty e^{-iky} K(z, y) \, dy = \psi(z, k) - e^{-ikz}$, we obtain from (3.14) our third main result

$$\frac{\delta \psi(x, k)}{\delta r^*(q)} = -\frac{1}{2\pi} \left(\int_x^\infty \psi(z, q) \psi(z, k) \, dz \right) \psi(x, q). \tag{3.15}$$

It is interesting to note that both (3.13) and (3.15) are expressed purely in terms of the wavefunction $\psi(x, k)$. Note, however, that (3.13) is local in ψ, whereas (3.15) is highly nonlocal. It would be interesting to interpret these features from a physical point of view.

4. Consistency checks of (3.13) and (3.15)

The integrated form of (3.13) should agree with the derivative $\frac{\delta}{\delta r^*(k)} \int_{-\infty}^\infty V(x) \, dx$ obtained from the trace identity (1.5). Note that (1.5) is expressed purely in terms of the positive Fourier modes of $r(k)$, the independent functional variables in our problem. Thus, taking the derivative of (1.5), we obtain

$$\frac{\delta}{\delta r^*(k)} \int_{-\infty}^\infty V(x) \, dx = -\frac{2}{\pi} \frac{\delta}{\delta r^*(k)} \int_0^\infty \log[1 - |r(q)|^2] \, dq = \frac{2}{\pi} \frac{r(k)}{|t(k)|^2} \tag{4.1}$$

where we used $|t(k)|^2 = 1 - |r(k)|^2$. This result should be confronted with the integrated form of (3.13). We obtain from the latter

$$\frac{\delta}{\delta r^*(k)} \int_{-\infty}^\infty V(x) \, dx = \frac{1}{\pi} \lim_{L \to \infty} [\psi^2(x, k)]_{-L}^L. \tag{4.2}$$

From (1.8) we observe that $\psi(L, k) \simeq e^{-ikL}$. Similarly, from (1.10) and (1.4) we deduce the asymptotic behaviour

$$\psi(-L, k) \simeq \frac{1}{t^*(k)} e^{ikL} - \frac{r(k)}{t(k)} e^{-ikL}. \tag{4.3}$$

Substituting (4.3) and $\psi(L, k) \simeq e^{-ikL}$ in (4.2), we obtain

$$\frac{\delta}{\delta r^*(k)} \int_{-\infty}^\infty V(x) \, dx = \frac{1}{\pi} \lim_{L \to \infty} \left[e^{-2ikL} \left(1 - \frac{r^2}{t^2} \right) - \frac{1}{(t^*)^2} e^{2ikL} + \frac{2r}{|t|^2} \right] \tag{4.4}$$

which coincides in the limit with (4.1) in the sense of distributions, since the first two rapidly oscillating terms on the right-hand side of (4.4), when smeared against any continuous bounded test function $U(k)$, will integrate to zero in the limit $L \to \infty$, due to the Riemann–Lebesgue lemma. Thus, (3.13) has passed its first test.

A less trivial test of (3.13) arises from comparing the complex conjugate equation of (3.13), $\frac{\delta V(x)}{\delta r(k)} = \frac{1}{\pi} \frac{d}{dx} \psi^{*2}(x, k)$ and (1.2). We see that one kernel is the inverse of the other: $\int_{-\infty}^\infty \frac{\delta r(k)}{\delta V(x)} \frac{\delta V(x)}{\delta r(q)} \, dx = \delta(k - q)$. Thus, we must verify that

$$\Gamma(k, q) = \frac{t^2(k)}{2\pi ik} \int_{-\infty}^\infty \phi^2(x, k) \frac{d}{dx} \psi^{*2}(x, q) \, dx \tag{4.5}$$

is equal to $\delta(k - q)$. Using the identity

$$\int_{-\infty}^\infty F^2 \frac{d}{dx} G^2 \, dx = \frac{1}{2} [(FG)^2]_{-\infty}^\infty + \int_{-\infty}^\infty FG(F \partial_x G - G \partial_x F) \, dx$$

with $F = \phi(x, k)$ and $G = \psi^*(x, q)$, we write (4.5) as

$$\Gamma(k, q) = \frac{t^2(k)}{2\pi i k} \left\{ \frac{1}{2} [(\phi(x, k)\psi^*(x, q))^2]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \phi(x, k)\psi^*(x, k)W(x, k, q)\, dx \right\} \qquad (4.6)$$

where

$$W(x, k, q) = \phi(x, k)\partial_x \psi^*(x, q) - \psi^*(x, q)\partial_x \phi(x, k) \qquad (4.7)$$

is the Wronskian of $\phi(x, k)$ and $\psi^*(x, q)$. Next, from the Schrödinger equation for these two functions it is easy to obtain the relation

$$\phi(x, k)\psi^*(x, q) = \frac{1}{k^2 - q^2}\partial_x W(x, k, q). \qquad (4.8)$$

Substituting the last equation in (4.6) we see that the integral is given entirely by boundary terms as

$$\Gamma(k, q) = \frac{t^2(k)}{4\pi i k} \left[(\phi(x, k)\psi^*(x, q))^2 + \frac{1}{k^2 - q^2} W^2(x, k, q) \right]_{-\infty}^{\infty}. \qquad (4.9)$$

In order to proceed in the clearest and simplest way, we shall make a few observations. First, observe from (1.4), (1.8) and (4.3) that the *difference* $(\phi(L, k)\psi^*(L, q))^2 - (\phi(-L, k)\psi^*(-L, q))^2$ is rapidly oscillating in the limit $L \to \infty$ for all k, q. Thus, as a distribution acting on bounded continuous functions of k and q it tends to zero. Thus, we should focus on the second term. When $k^2 - q^2 \neq 0$, the difference $W^2(L, k, q) - W^2(-L, k, q)$ oscillates rapidly, and tends to zero, in the sense of distributions, in the limit $L \to \infty$, similar to the first term. Recall that for $k^2 = q^2$, i.e., when $\phi(x, k)$ and $\psi^*(x, q)$ correspond to the same energy, $W(x, k, q)$ is a constant, and thus cannot oscillate. In that case, however, the denominator in front of this term vanishes. Thus we should study the limit $q^2 \to k^2$ carefully.

Let us concentrate then on the region $k^2 \simeq q^2$. Since we have taken the positive Fourier modes of $r(k)$ as the independent functional variables, it is enough to study the case $q \to k$. Thus, assuming $k - q = \epsilon$ with $|\frac{\epsilon}{k}| \ll 1$ and setting $k + q \simeq 2k$, we obtain from (1.4), (1.8) and (4.3) that

$$W(L, k, k - \epsilon) \simeq \frac{i}{t(k)}(2k\, e^{-i\epsilon L} - \epsilon r(k)\, e^{2ikL})$$

$$W(-L, k, k - \epsilon) \simeq \frac{i}{t(k)}\left(2k\, e^{i\epsilon L} - \epsilon t(k)\frac{r^*(k)}{t^*(k)}\, e^{2ikL}\right). \qquad (4.10)$$

Substituting (4.10) and $k^2 - q^2 \simeq 2k\epsilon$ in (4.9), and recalling the first observation made right below (4.9), we finally obtain

$$\Gamma(k, q) = \frac{\sin(2\epsilon L)}{\pi \epsilon} + \text{ROT} \qquad (4.11)$$

where the acronym ROT stands for the rapidly oscillating terms that tend to zero in the sense of distributions. The first term tends of course to $\delta(k - q)$ as $L \to \infty$, as desired. Equation (3.13) has passed the second check!

Our last consistency check concerns (3.15). The point is that for $x \to -\infty$, the integral on the right-hand side of (3.15) is the orthogonality relation

$$\int_{-\infty}^{\infty} \psi(z, q)\psi(z, k)\, dz = \frac{2\pi}{|t(k)|^2}(\delta(k + q) - r(k)\delta(k - q)). \qquad (4.12)$$

Let us sketch the proof of (4.12): in analogy with (4.8) we deduce that

$$\psi(x, k)\psi(x, q) = \frac{1}{k^2 - q^2}\partial_x \tilde{W}(x, k, q) \qquad (4.13)$$

where

$$\tilde{W}(x, k, q) = \psi(x, k)\partial_x\psi(x, q) - \psi(x, q)\partial_x\psi(x, k) \tag{4.14}$$

is the Wronskian of the functions involved. Then, after integration, we obtain

$$\int_{-L}^{L} \psi(z, q)\psi(z, k)\,\mathrm{d}z = \frac{1}{k^2 - q^2}[\tilde{W}(L, k, q) - \tilde{W}(-L, k, q)]$$

and consider this result as $L \to \infty$, using the asymptotic behaviour (1.8) and (4.3). For generic values of k, q, the difference of Wronskians is a rapidly oscillating function, which as a distribution, tends to zero as $L \to \infty$. As in the previous discussion, we observe that when $k^2 = q^2$, $\tilde{W}(x, k, q)$ is independent of x, and thus does not oscillate. By studying the limit $q \to \pm k$ carefully, we deduce (4.12).

On the left-hand side of (3.15) we have

$$\frac{\delta\psi(-L, k)}{\delta r(-q)} = \frac{\delta}{\delta r(-q)}\left(\frac{1}{t(-k)}\,\mathrm{e}^{ikL} - \frac{r(k)}{t(k)}\,\mathrm{e}^{-ikL}\right) \tag{4.15}$$

where we used (4.3). Then, from (2.3) it follows that

$$\begin{aligned}
\frac{\delta t^{-1}(k)}{\delta r(p)} &= \frac{1}{2t(k)}\frac{r^*(p)}{|t(p)|^2}\left[\delta(p - k) + \delta(p + k) + \frac{1}{i\pi}\mathrm{P.P.}\left(\frac{1}{p - k} - \frac{1}{p + k}\right)\right] \\
&= \frac{1}{2\pi it(k)}\frac{r^*(p)}{|t(p)|^2}\left(\frac{1}{p - k - i\epsilon} - \frac{1}{p + k + i\epsilon}\right).
\end{aligned} \tag{4.16}$$

Applying (4.16) to (4.15), and studying the resulting expression around $k \simeq q > 0$, we find (keeping only the singular terms) $\frac{1}{2\pi\epsilon}\frac{r(k)}{|t(k)|^2}\psi(-L, k)$, in accordance with the right-hand side of (3.15) and (4.12).

5. Summary and conclusions

In this paper we have derived explicit and relatively simple expressions for the functional derivatives of the Gelfand–Levitan–Marchenko kernel $K(x, y)$, the Schrödinger potential $V(x)$ and wavefunction $\psi(x, k)$, with respect to the reflection amplitude $r(k)$ (equations (3.12), (3.13) and (3.15), respectively). These formulae passed some simple consistency checks.

Our derivation was based on the Gelfand–Levitan–Marchenko equation (2.6) (for the case in which $K(x, y)$ connects the eigenstates of the free and the unknown Schrödinger operators) and on elementary methods of the theory of Fredholm integral equations. Our work adds to previous results in the IST for perturbations, which were obtained by somewhat different techniques [7, 9].

A possibly interesting application of the results of this paper might be the investigation of perturbations around *reflectionless* potentials with arbitrary numbers of bound states [12], which play an important role in supersymmetric quantum mechanics [13] and the theory of solitons. Reflectionless Schrödinger potentials can be constructed by purely algebraic methods, and essentially all important physical quantities in such systems can be computed explicitly. Thus, they serve as ideal models to perturb around. Our results offer the possibility of performing explicitly calculable perturbation theory around these models, with a very non-trivial (and in particular, non-local) perturbation, namely, turning on a small reflection amplitude. Finally, the present work might be useful in studying static quantum field theoretic solitons in one spatial dimension, which are subjected to external local forces.

Acknowledgments

Appendix. Miscellaneous technical details

A.1. Perturbation theory in the continuum: proof of (1.2)

Consider a perturbation $\delta V(x)$ of the Schrödinger equation (1.3). To make the problem well defined, we assume that $\delta V(x)$ is localized around some point x_0.

Under this perturbation, the solution of (1.3) will be shifted $\Psi(x) \to \Psi(x) + \delta\Psi(x)$, and our task is to compute $\delta\Psi(x)$ to first order in $\delta V(x)$. To this order, we have to solve the equation

$$(H - k^2)\delta\Psi(x, k) = -\delta V(x)\Psi(x, k). \tag{A.1}$$

The general solution is given in terms of the Green function $G(x, y; k)$ of the operator $H - k^2$ (defined with the appropriate boundary conditions) as

$$\delta\Psi(x, k) = -\int_{-\infty}^{\infty} G(x, y; k)\delta V(y)\Psi(y, k)\,\mathrm{d}y. \tag{A.2}$$

Since this expression vanishes for $\delta V(y) = 0$, there is no term which is a solution of the homogeneous equation.

The proper Green function is that which decays exponentially whenever one of its coordinate arguments tends to $\pm\infty$, when k is lifted to the upper half complex plane. There is such a unique Green function

$$G(x, y; k) = \frac{1}{w(k)}[\theta(x - y)\psi^*(x, k)\phi(y, k) + \theta(y - x)\psi^*(y, k)\phi(x, k)] \tag{A.3}$$

where

$$w(k) = -W(x, k, k) = \frac{2k}{\mathrm{i}t(k)} \tag{A.4}$$

from (4.7). Thus, in particular, for $\Psi(x, k) = \phi(x, k)$ we obtain

$$\delta\phi(x, k) = -\frac{1}{w}\left[\psi^*(x, k)\int_{-\infty}^{x}\phi(y, k)\delta V(y)\phi(y, k)\,\mathrm{d}y \right.$$
$$\left. + \phi(x, k)\int_{x}^{\infty}\psi^*(y, k)\delta V(y)\phi(y, k)\,\mathrm{d}y\right]. \tag{A.5}$$

In the limit $x \to -\infty$, we see that

$$\delta\phi(x, k) \to -\frac{\phi(x, k)}{w}\int_{-\infty}^{\infty}\psi^*(y, k)\delta V(y)\phi(y, k)\,\mathrm{d}y. \tag{A.6}$$

Thus, the function

$$\tilde{\phi}(x, k) = \frac{\phi(x, k) + \delta\phi(x, k)}{1 - \frac{1}{w}\int_{-\infty}^{\infty}\psi^*(y, k)\delta V(y)\phi(y, k)\,\mathrm{d}y} \tag{A.7}$$

tends to $\mathrm{e}^{-\mathrm{i}kx}$ as $x \to -\infty$, and should be identified with the 'ϕ-function' (1.4) of the perturbed potential $V(x) + \delta V(x)$. In (A.7) we should keep, of course, only terms up to linear order in

$\delta V(x)$. As $x \to \infty$, we see from (A.5), (1.4) and (1.8) that $\tilde{\phi}(x, k) \to \frac{1}{\tilde{t}(k)} e^{-ikx} + \frac{\tilde{r}(k)}{\tilde{t}(k)} e^{ikx}$, where $\tilde{t}(k)$ and $\tilde{r}(k)$ are the new scattering amplitudes, given by

$$\frac{1}{\tilde{t}(k)} = \frac{1}{t(k)} \left[1 + \frac{1}{w} \int_{-\infty}^{\infty} \psi^*(y, k) \delta V(y) \phi(y, k) \, dy \right]$$

$$\frac{\tilde{r}(k)}{\tilde{t}(k)} = \frac{r(k)}{t(k)} \left[1 + \frac{1}{w} \int_{-\infty}^{\infty} \left(\psi^*(y, k) - \frac{t(k)}{r(k)} \phi(y, k) \right) \delta V(y) \phi(y, k) \, dy \right] \tag{A.8}$$

from which we infer, after some simple algebra, involving (1.9) that

$$\delta r(k) = \tilde{r}(k) - r(k) = \frac{1}{2ik} \int_{-\infty}^{\infty} (t(k)\phi(y, k))^2 \delta V(y) \, dy \tag{A.9}$$

from which (1.2) follows.

A.2. Reflectionless potentials

We demonstrate in the following the positivity of the Fredholm determinant of the GLM equation (2.6) in the case of reflectionless potentials.

For reflectionless potentials, where $r(k) \equiv 0$, $N(y, z) = -\sum_{l=1}^{N} c_l^2 e^{-\kappa_l(y+z)}$ in (2.8) is a degenerate kernel of finite rank N. Thus, the integral equation degenerates into a system of linear equations, and the Fredholm determinant becomes an N-dimensional determinant. For this reason, reflectionless potentials are so easy to treat within the formalism of IST.

The Fredholm determinant (at $\lambda = 1$) is given by $(c_1 \ldots c_N)^2 \det A$, where

$$A_{mn} = \delta_{mn} + \frac{c_m c_n}{\kappa_n + \kappa_m} e^{-(\kappa_n + \kappa_m)x}. \tag{A.10}$$

This matrix is a member of a family of matrices of the general form

$$A_{mn}^{(\nu)} = \delta_{mn} + \frac{v_m v_n}{(\kappa_n + \kappa_m)^{\nu}} \tag{A.11}$$

where v_n are the components of a real vector and ν a real number. (Recall also that all $\kappa_n > 0$.) The matrix (A.10) corresponds, of course to $v_n = c_n e^{-\kappa_n x}$ and $\nu = 1$. It is easy to demonstrate that (A.11) is a positive definite matrix for any $\nu \geqslant 0$. To prove this (for $\nu > 0$, the case $\nu = 0$ being trivial), it is enough to verify that $\xi^T A \xi > 0$ for any real vector ξ. Thus, consider

$$\xi^T A \xi = \xi^T \xi + \sum_{n,m} \frac{\xi_n v_n \xi_m v_m}{(\kappa_n + \kappa_m)^{\nu}}$$

$$= \xi^T \xi + \frac{1}{\Gamma(\nu)} \int_0^{\infty} s^{\nu-1} \left(\sum_{n=1}^{N} \xi_n v_n e^{-\kappa_n s} \right)^2 ds \geqslant 0 \tag{A.12}$$

manifestly. Thus, in particular, (A.10) is positive definite and so is the corresponding Fredholm determinant.

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