The First Variation of the Scattering Matrix*

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In this paper we establish some facts about the dependence of scattering data for a perturbed wave equation on the perturbation. The results we derive hold for both acoustic and Schrödinger wave equations, but we begin by describing them in the acoustic case. Hence we consider a perturbation of the acoustic wave equation in \mathbb{R}^n ,

$$u_{tt} = Lu \equiv a(x) \nabla \cdot A(x) \nabla u - b(x)u, \quad x \in D,$$
 (I.1)

where D is the exterior of a smooth bounded obstacle in \mathbb{R}^n and u(x, t) = 0for $x \in \partial D$. All coefficients are smooth and nonnegative (A(x) is a positive definite matrix) and we assume $Lu = \Delta u$ for $|x| > \mathbb{R}$. The scattering matrix, which describes how much this equation deviates from $u_{tt} = \Delta u$, is an operator valued function S(z) defined and meromorphic on the complex plane. S(z) is a unitary operator when z is a real number and it differs from the identity by a trace class operator when z is not a pole. Thus for z real, S(z)has pure point spectrum and each of its eigenvalues has modulus 1. In scattering theory of spherically symmetric potentials the arguments of these eigenvalues are called *phase shifts*. We shall adopt this terminology for the case at hand.

In what follows we assume we have a family of equations of the form (I.1), in which the coefficients and the domain D depend smoothly on a parameter s. Our basic result is that phase shifts depend monotonically on D and the coefficients in the following sense.

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THEOREM 1. Given z > 0, let $e^{i\beta(s)}$ be a simple eigenvalue of S(z, s), not equal to 1. If $\partial a/\partial s$, $\partial A/\partial s$, and $\partial/\partial s(b/a)$ are nonnegative on D and the normal variation of ∂D with s is nonnegative, then $\partial \beta/\partial s \ge 0$.

Actually, Theorem 1 holds whenever $e^{i\beta}$ and its eigenvector are differentiable functions of *s*. When the coefficients and domain depend smoothly on *s*, the hypothesis that $e^{i\beta}$ is simple and not equal to 1 is sufficient to ensure this, since S(z, s) is a smooth function of *s* and 1 is the only possible accumulation point of its spectrum. If the dependence on *s* is analytic, one only need assume $e^{i\beta} \neq 1$. This is discussed in Section 1. Note also that β is only defined up to an additive integer multiple of 2π . However, this ambiguity obviously has no effect on the theorem.

For z > 0 the phase shifts can be chosen to be analytic functions of z, except possibly at points where they are congruent to $0 \mod 2\pi$. Thus we can differentiate the phase shift with respect to the frequency z, and in a natural way (see Section 2) Theorem 1 leads to

THEOREM 2. If D is starlike with respect to the origin and the radial derivative of each coefficient a, A, and b/a is nonpositive, then the derivative of any phase shift with respect to z will be nonnegative for z > 0.

Theorems 1 and 2 hold without modification for the Heisenberg scattering matrix for the Schrödinger equation

$$iu_t = a(x) \nabla \cdot A(x) \nabla u - b(x)u, \quad x \in D \subset \mathbb{R}^{2n-1},$$

with u(x, t) = 0 on ∂D , since it is just $S(z^{1/2})$, where S(z) is the scattering matrix of (I.1). (cf. [5 p. 220]).

A "distorted wave" formula for the derivative of S(z) with respect to s plays a key role in the proof of Theorem 1. A loose analog of this formula is used by engineers for several purposes. In fact, there is a much larger literature on scattering matrix variations in engineering than in physics or mathematics, and this topic seems to be of engineering importance. Section 3 discusses an engineering view of this subject and gives a systems theory derivation of a one-dimensional distorted wave formula.

There is a close connection between the results here and work initiated by Lax and Phillips on the purely imaginary poles of the analytic continuation of S(z). The comparison theorems on the positions of the purely imaginary poles in [1, 6, 13], and the variational results on phase shifts given here are all consequences of the monotone dependence of the "transmission coefficient" on perturbations of the coefficients a, A, and b and the region D, (see (1.5)). In a sense we have just brought the pole theorems down to the real axis. However, the phase shift results hold in cases where there are no purely imaginary poles (i.e., when n is even) and do not require hypotheses beyond the positivity of the variations in the coefficients and the domain. On the other hand this approach does not seem to yield any results for the Neumann and Robin boundary conditions considered in [6] and [1], respectively.

1. THE VARIATIONAL DERIVATIVE OF A PHASE SHIFT

We shall study $u_{tt} = Lu$ on the exterior D of a bounded region with L the differential operator (I.1). The domain of L is specified by taking the graph closure in $L^2(D)$ of L acting on smooth functions of bounded support which vanish on ∂D . The resulting operator will be self-adjoint with respect to the inner product

$$(f,g)_a = \int_D (1/a(x)) f\bar{g} dx.$$

The scattering matrix arises in the following way. There are two natural families of generalized eigenfunctions of *L*—the "iz-incoming and iz-outgoing distorted plane waves." These are parameterized by $S^{n-1} \times \mathbb{R}^1$ and denoted by $\varphi_-(x, \omega, z)$ and $\varphi_+(x, \omega, z)$. The mappings

$$\mathscr{F}_{\pm}: f \to \int f(x) \varphi_{\mp}(x, \omega, z) dx$$

extend to unitary maps of $L^2(D, 1/a \, dx)$ onto $L^2(\mathbb{R}^1, L^2(S^{n-1}))$ such that $\mathscr{F}_{\pm}^{-1}L\mathscr{F}_{\pm}$ is multiplication by z^2 . The scattering operator is defined as $\mathscr{F}_{+}\mathscr{F}_{-}^{-1}$ and one shows it has the form

$$(\mathscr{F}_{+}\mathscr{F}_{-}^{-1}f)(z,\omega) = (S(z)f(z,\cdot))(\omega),$$

where S(z) is a unitary operator on $L^2(S^{n-1})$ and S(z) is called the *scattering* matrix. This is not an especially illuminating way of introducing S(z) but it does make one property we eventually need almost obvious:

$$S(z): \varphi_{-}(x, \omega, z) \to \varphi_{+}(x, \omega, z), \qquad x \in D.$$
(1.1)

To define the distorted plane waves more precisely, one proceeds as follows. For $\sigma > 0$ and $|\xi| = 1$, let $u(x, \xi, \sigma)$ be the square integrable solution to $(L - \sigma^2) u = (L - \sigma^2) e^{\sigma x \cdot \xi}$ such that $u - e^{\sigma x \cdot \xi}$ vanishes on ∂D . The functions $u(x, \xi, \sigma)$ have analytic continuations from the positive real axis to Re $\sigma \ge 0$, $\sigma \ne 0$, as Sobolev space valued functions of σ , and are smooth on $D \times S^{n-1} \times \{\text{Re } \sigma \ge 0, \sigma \ne 0\}$ (for a sketch of the proof of this see the Appendix). For Re $\sigma \ge 0, \sigma \ne 0$, we set $\varphi(x, \xi, \sigma) = e^{\sigma x \cdot \xi} - u(x, \xi, \sigma)$. Except for a multiplicative factor depending only on x the function $\varphi(x, -\omega, iz)$ is the *iz*-outgoing distorted plane wave $\varphi_+(x, \omega, z)$. The *iz*-incoming wave φ_- is defined in an analogous way beginning with $\sigma < 0$. For $z \in \{\text{Im } z < 0\} \cup \{z > 0\}$ the scattering matrix can be written¹

$$S(z) = I + (-iz/2\pi)^{(n-1/2)} \mathscr{K}(iz),$$

where $\mathscr{K}(\sigma)$ is an integral operator on $L^2(S^{n-1})$ with kernel $k(\theta, -\omega, \sigma)$. $k(\theta, \omega, \sigma)$ is called the *transmission coefficient* associated with the scattering problem, and it satisfies

$$u(x, \theta, \sigma) = \frac{e^{-\sigma |x|}}{|x|^{(n-1)/2}} \left[k\left(\theta, \frac{x}{|x|}, \sigma\right) + O\left(\frac{1}{|x|}\right) \right]$$

for Re $\sigma \ge 0$, $\sigma \ne 0$, which can be taken as its definition. We shall use the transmission coefficient to study the scattering matrix.

As in [6, p. 744], we have for $\sigma > 0$

$$c_n k(\theta, \omega, \sigma) = \lim_{r \to \infty} \int_{|x|=r} u(\theta) \frac{\partial e^{\sigma x \cdot \omega}}{\partial r} - e^{\sigma x \cdot \omega} \frac{\partial u}{\partial r}(\theta) \, dS, \qquad (1.2)$$

where $u(\theta) = u(x, \theta, \sigma)$ and

$$c_n = \lim_{r \to \infty} \int_{S^{n-1}} \sigma(1 + \omega \cdot \omega') e^{-\sigma r(1 - \omega \cdot \omega')} r^{n-1/2} d\omega'$$

= $\sigma^{-(n-3)/2} \pi^{(n-1)/2} 2^{(n+1)/2}.$

However, an application of Green's formula shows that the function inside the limit in (1.2) is constant for |x| > R. Thus

$$c_n k(\theta, \omega, \sigma) = \int_{|x|=R} u(\theta) \frac{\partial e^{\sigma x \cdot \omega}}{\partial r} - e^{\sigma x \cdot \omega} \frac{\partial u(\theta)}{\partial r} \, dS. \tag{1.3}$$

By analytic continuation (1.3) holds for Re $\sigma \ge 0$, $\sigma \ne 0$.

Now we assume that D and the coefficients of L depend smoothly on a parameter s, where we set L(0) = L and D(0) = D. We want to differentiate (1.3) with respect to s. In the Appendix we sketch a proof that $u(x, \xi, \sigma, s)$ is a smooth function of (x, s) on $D(s) \times [-\delta, \delta]$ for any $\xi \in S^{n-1}$ and $\sigma \in \operatorname{Re} \sigma \ge 0$, $\sigma \neq 0$. Moreover, when n is odd, the functions $u(x, \xi, \sigma)$ are smooth on $D \times S^{n-1} \times {\operatorname{Re} \sigma \ge 0}$, but for n = 1 bizarrely enough $u(x, \xi, \sigma, s)$ need not be differentiable at $\sigma = 0$ (see the example in Sect. 4). Thus most of the theorems in the paper require $\sigma \neq 0$ as a hypothesis. At

¹ For a derivation of the formula see [7, Theorem 6.2]. However, a few technical remarks are in order. Our definition of $k(\theta, \omega, \sigma)$ is consistent with the notation of [6, 13]. The function s_{-} in [7] is related to k by $s_{-}(\theta, \omega, \sigma) = k(\omega, \theta, -i\sigma)$ and one must use [5, relation (5.9), p. 171] to arrive at (1.7) above. Theorem 6.2 of [7] disagrees with Theorem 5.4 of [5] by a sign, and the error seems to be in [5]. The remarks concluding Section 2 check the sign.

any rate for Re $\sigma \ge 0$, $\sigma \ne 0$ we can differentiate (1.3) and evaluate at s = 0 to obtain

$$c_{n}\frac{\partial k}{\partial s}(\theta,\omega,\sigma) = \int_{|x|=R} \frac{\partial u}{\partial s}(\theta) \frac{\partial e^{\sigma x \cdot \omega}}{\partial r} - e^{\sigma x \cdot \omega} \cdot \frac{\partial}{\partial r} \left(\frac{\partial u}{\partial s}(\theta)\right) dS$$
$$= \left(\frac{\partial u}{\partial s}(\theta), (L-\sigma^{2}) e^{\sigma x \cdot \omega}\right)_{a} - \left(e^{\sigma x \cdot \omega}, (L-\sigma^{2}) \frac{\partial u}{\partial s}(\theta)\right)_{a}$$
$$+ \int_{\partial D} \frac{\partial u}{\partial s}(\theta) \frac{\partial e^{\sigma x \cdot \omega}}{\partial \eta_{A}} - e^{\sigma x \cdot \omega} \frac{\partial}{\partial \eta_{A}} \left(\frac{\partial u}{\partial s}(\theta)\right) dS,$$

where $\eta_A = A\eta$ and η is the inner unit normal on ∂D . Thus

$$c_{n}\frac{\partial k}{\partial s} = \left(\frac{\partial u}{\partial s}\left(\theta\right), \left(L - \sigma^{2}\right)u(\omega)\right)_{a} + \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s}u(\theta)\right)_{a} - \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s}e^{\sigma x \cdot \theta}\right)_{a} + \int_{\partial D} \quad \text{(as above),}$$

where

$$\frac{\partial L}{\partial s}f = a\nabla \cdot \frac{\partial A}{\partial s}\nabla f - a\left(\frac{\partial}{\partial s}\left(\frac{b+\sigma^2}{a}\right)\right)f.$$

Now an application of Green's formula to the first term on the right yields

$$c_{n} \frac{\partial k}{\partial s} = \left((L - \sigma^{2}) \frac{\partial u}{\partial s}(\theta), u(\omega) \right)_{a} + \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s} u(\theta) \right)_{a}$$
$$- \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s} e^{\sigma x \cdot \theta} \right)_{a} + \int_{\partial D} \frac{\partial u}{\partial s}(\theta) \frac{\partial \varphi}{\partial \eta_{A}}(\omega) - \frac{\partial}{\partial \eta_{A}} \left(\frac{\partial u}{\partial s}(\theta) \right) \varphi(\omega) \, dS$$
$$= - \left(\frac{\partial L}{\partial s} u(\theta), u(\omega) \right)_{a} + \left(\frac{\partial L}{\partial s} e^{\sigma x \cdot \theta}, u(\omega) \right)_{a} + \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s} u(\theta) \right)_{a}$$
$$- \left(e^{\sigma x \cdot \omega}, \frac{\partial L}{\partial s} e^{\sigma x \cdot \theta} \right)_{a} + \int_{\partial D} \frac{\partial u}{\partial s}(\theta) \frac{\partial \varphi(\omega)}{\partial \eta_{A}} \, dS.$$

Now, integrating by parts once in each volume integral, we get no new boundary terms because $\varphi(\omega) = \varphi(\theta) = 0$ on ∂D , and arrive at the formula

$$c_n \frac{\partial k}{\partial s} = \int_D \nabla \varphi(\theta) \cdot \frac{\partial A}{\partial s} \nabla \varphi(\omega) + \varphi(\theta) \left(\frac{\partial}{\partial s} \left(\frac{\sigma^2 + b}{a} \right) \right) \varphi(\omega) \, dx$$
$$+ \int_{\partial D} \frac{\partial u}{\partial s}(\theta) \frac{\partial \varphi(\omega)}{\partial \eta_A} \, dS. \tag{1.4}$$

To eliminate $(\partial u/\partial s)(\theta)$ from the boundary integral, we choose a smooth function $\rho(x, s)$ on $\partial D \times (-\delta, \delta)$ such that

$$x \in \partial D \Leftrightarrow x + \rho(x, s) \ \eta(x) \in \partial D(s).$$

The existence of such a function may be taken as the definition of "D(s) depends smoothly on s." Then we have

$$u(x + \rho\eta, \theta, \sigma, s) = e^{\sigma(x + \rho\eta) \cdot \theta}, \quad x \in \partial D,$$

and, differentiating with respect to s,

$$\frac{\partial u}{\partial s}(x,\theta,\sigma,0) = \frac{\partial \varphi}{\partial \eta} \frac{\partial \rho}{\partial s}.$$
(1.5)

Since $\varphi(\omega) = 0$ on ∂D , the vector $\nabla \varphi$ is parallel to η on ∂D . Thus

$$\frac{\partial \varphi}{\partial \eta_A}(\omega) = (\eta \cdot A\eta) \frac{\partial \varphi}{\partial \eta}(\omega). \tag{1.6}$$

Substituting (1.5) and (1.6) into (1.4), we have the basic variational formula

$$c_{n} \frac{\partial k}{\partial s} = \int_{D} \nabla \varphi(\theta) \cdot \frac{\partial A}{\partial s} \nabla \varphi(\omega) + \varphi(\theta) \left(\frac{\partial}{\partial s} \left(\frac{\sigma^{2} + b}{a} \right) \right) \varphi(\omega) \, dx$$
$$+ \int_{\partial D} \frac{\partial \varphi}{\partial \eta} \left(\theta \right) \frac{\partial \rho}{\partial s} \frac{\partial \varphi}{\partial \eta} \left(\omega \right) \eta \cdot A \eta \, dS. \tag{1.7}$$

This is the distorted wave formula. It is valid for $\operatorname{Re} \sigma \leq 0$, $\sigma \neq 0$, and it shows $(\partial k/\partial s)$ is a smooth function of (θ, ω, σ) on $S^{n-1} \times S^{n-1} \times \{\sigma : \operatorname{Re} \sigma \leq 0, \sigma \neq 0\}$. From here on we set $\eta \cdot A\eta \, dS \equiv dS_A$. Finally we can use (1.7) and (1.2) to compute that the derivative of S(z) is

$$\frac{dS}{ds}(z) = \frac{i}{4\pi} \left(\frac{z}{2\pi}\right)^{n-2} \left(\int_{D} \nabla \varphi(\theta) \cdot \frac{\partial A}{\partial s} \nabla \varphi(-\omega) + \varphi(\theta) \frac{\partial}{\partial s} \left(\frac{-z^{2}+b}{a}\right) \varphi(-\omega) dx + \int_{\partial D} \frac{\partial \varphi}{\partial \eta}(\theta) \frac{\partial \rho}{\partial s} \frac{\partial \varphi}{\partial \eta}(-\omega) dS_{A} \right)$$
(1.8)

for Im $z \leq 0$, $z \neq 0$. When *n* is even, the analytic continuation of (1.7) to z < 0 differs from the scattering matrix by 2I (see [7, Theorem 6.4]) but, since we are computing (dS/ds), this does not affect the computation.

From this point on we will be concerned only with z > 0. When z is real, $\overline{\varphi(x, -\theta, iz)}$ and $\varphi(x, \theta, iz)$ are the *iz*-incoming and *iz*-outcoming distorted plane waves for direction $-\theta$, respectively. Moreover, these waves are normalized so that S(z) maps $\overline{\varphi(x, -\theta, iz)}$ onto $\varphi(x, \theta, iz)$, when z > 0. This follows immediately from [7, formula (6.12)] if one recalls that $S^{-1}(z) = S^*(z)$ and $k(\theta, \omega, \sigma)$ is symmetric in (θ, ω) . Thus the kernel of $S(z)(dS^*/ds(z))$ is given by

$$\frac{-i}{4\pi} \left(\frac{z}{2\pi}\right)^{n-2} \int_{D} \nabla \varphi(\theta) \frac{\partial A}{\partial s} \overline{\nabla \varphi(\omega)} + \varphi(\theta) \frac{\partial}{\partial s} \left(\frac{-z^{2}+b}{a}\right) \overline{\varphi(\omega)} \, dx \\ + \int_{\partial D} \frac{\partial \varphi}{\partial \eta} \left(\theta\right) \frac{\partial \rho}{\partial s} \frac{\overline{\partial \varphi}}{\partial \eta} \left(\omega\right) \, dS_{A} \,, \qquad (1.9)$$

for z > 0.

Next assume that $\lambda(s) = e^{i\beta(s)}$ is an eigenvalue of S(z, s), z > 0, which is differentiable at s = 0, and that a normalized eigenfunction v(s) belonging to $\lambda(s)$ may also be chosen so that it is differentiable at s = 0. If A, a, b, and ρ are analytic in s near s = 0, then an argument like the one in the Appendix shows S(z, s) is a holomorphic function of s near s = 0. Since S(z, s) is unitary for s real and differs from the identity by a compact operator, standard results from analytic perturbation theory imply $\lambda(s)$ and v(s) may be chosen differentiable at s = 0 if $\lambda(0) \neq 1$, (see [4, the reduction on pp. 368–369, and Theorem 1.10, p. 71]). Of course, differentiable choices of $\lambda(s)$ and v(s)are always possible if $\lambda(0)$ is simple and isolated. Letting (,) denote the inner product on $L^2(S^{n-1})$, we have

$$(v(s), S(z, 0) S^*(z, s) v(s)) = e^{i\beta(s)}(v(s), S(z, 0) v(s)).$$

Differentiating with respect to s and evaluating at s = 0 yields

$$\left(v(0), S(z,0) \frac{dS^*}{ds}(z,0) v(0)\right) = i \frac{d\beta}{ds}(0).$$

Combining this with the formula for the kernel of $S(z)(dS^*/ds)(z)$, we arrive at

$$\frac{d\beta}{ds}(0) = \frac{1}{4\pi} \left(\frac{z}{2\pi}\right)^{n-2} \left(\int_{D} \nabla f \cdot \frac{\partial A}{\partial s} \,\overline{\nabla f} + |f|^{2} \left(\frac{\partial}{\partial s} \left(\frac{-z^{2}+b}{a}\right) \right) dx + \int_{\partial D} \left|\frac{\partial f}{\partial \eta}\right|^{2} \frac{\partial \rho}{\partial s} \, dS_{A} \right), \tag{1.10}$$

where $f(x) = \int_{S^{n-1}} u(0, \theta) \overline{\varphi(x, \theta, iz)} d\theta$. This leads immediately to Theorem I.

2. Dependence of Phase Shifts on Frequency

One can use Eq. (1.8) for (dS/ds)(z) to compute the derivative of phase shifts with respect to z. This observation is the old one that changing the frequency of a distorted plane wave is equivalent to a radial expansion of

the spatial variable in the Hamiltonian. To be more precise define the operator

$$L_{\lambda}u = a(\lambda x) \nabla \cdot A(\lambda x) \nabla u - \lambda^2 b(\lambda x)u$$

with Dirichlet boundary conditions on ∂D_{λ} , where $x \in D \Leftrightarrow \lambda x \in D_{\lambda}$. When $\lambda = 1$ this is just the operator L of the preceding section. One can easily check that if $\varphi(x, \xi, \sigma)$ is a distorted plane wave for L, then $\varphi(\lambda x, \xi, \sigma)$ is a distorted plane wave, $\varphi_{\lambda}(x, \xi, \lambda \sigma)$, for L_{λ} at frequency $\lambda \sigma$. It follows that the scattering matrix for L at frequency σ/λ equals the scattering matrix for L_{λ} at frequency σ . Thus, the preceding work may be used to compute the behavior of the scattering matrix with change in frequency. Suppose $e^{i\beta(z)}$ is a differentiable eigenvalue of S(z) with a differentiable eigenvector. Note, that since S(z) is analytic in z for z > 0, the remarks following (1.9) apply here. Then, applying (1.10) to L_{λ} yields

$$\frac{\partial \beta}{\partial z} = \frac{-1}{4\pi} \left(\frac{z}{2\pi}\right)^{n-3} \left[\int_{D} \overline{\nabla f} \cdot rA_{r} \nabla f + |f|^{2} \left(\frac{2b}{a} + r \frac{\partial}{\partial r} \left(\frac{-z^{2} + b}{a}\right) \right) dx + \int_{\partial D} \left| \frac{\partial f}{\partial \eta} \right|^{2} (x \cdot \eta) dS \right],$$
(2.1)

which implies Theorem II.

There is a distant connection between the results of this section and the question of when S(z) has poles converging to the real axis. We mention it here mainly because it indicates that the (elusive) sign of $d\beta/ds$ in (2.1) is correct. When n is odd, $A_r = b = 0$, and a(x) is a function of |x| alone, one can show that each eigenvalue of S(z) is a Blaschke product multiplied by $e^{i\rho z}$ where $|\rho|$ is uniformly bounded for all eigenvalues. This shows that if each phase shift is monotonic increasing, the scattering matrix cannot have poles arbitrarily close to the real axis. Hence we conclude if $a_r \leq 0$ then the scattering matrix does not have poles arbitrarily close to the real axis. Actually for this case it is known that there is a pole-free band about the real axis essentially if and only if a(r)/r is monotonic decreasing as r goes from zero to ∞ (see [12]). We conclude that at least one of the signs in (2.1) is correct.

3. AN ENGINEERING VIEWPOINT

In network design and more generally in engineering "systems" design one usually associates with a given device a matrix or operator valued function called its frequency response matrix. The frequency response function is analogous to the scattering matrix and the two are in fact the same in some circumstances. There is a large engineering literature on variation of the frequency response function with systems parameters. The book [2] is a compendium of articles on the control theoretic aspects of the subject. The authors are more familiar with the network design approach to the topic and this is surveyed (as of 1971) in [11]. A popular technique for analyzing dependence of circuit response on variations of circuit elements is called the adjoint method. It was introduced in 1969 by Director and Rohrer.

We now describe the foundation of the adjoint method. A time invariant linear system consists of four linear operators A, B, C, D which in conventional engineering uses act on finite-dimensional spaces. The frequency response function for such a system is $D + C(z - A)^{-1} B \equiv F(z)$. We assume A to be dissipative and so F is analytic in the right half-plane. Suppose the operator A depends on a parameter s while B, C, and D do not. Then by the second resolvent identity,

$$\frac{dF}{ds}(z) = C(z - A(s))^{-1} \frac{dA}{ds} (z - A(s))^{-1} B.$$
(3.1)

In situations related to electrical networks the formula actually has an interpretation.² Namely, to each network N there is a network \tilde{N} (and a recipe for writing it down) with the same topology as N called the adjoint of N. Its basic property is that whereas the "state vector" $w = (zI - A)^{-1} Bu$ gives the electric flow (current, and/or voltage, depending on how you set it up) through the various paths of N when ue^{zt} is put into N, the vector $\tilde{w} = (z - A^*)^{-1} C^*u$ is the electric flow through \tilde{N} . Thus (3.1) says (u, (dF/ds)u) = $(\tilde{w}, (dA/ds)w)$. Computer algorithms can be used to find w and \tilde{w} readily, and this approach is about the easiest to use numerically for finding the sensitivity of a circuit to variations in parameters of its components.

Formula (3.1) has considerable relevance for the problem in this paper, as the following example shows. We shall work in R^1 with a relative of the equation $u_{tt} = Lu$ we have been studying. Here we investigate a first-order system and at the end of our calculations describe the connections with what we have already done. Consider

$$rac{\partial}{\partial t}inom{i}{v}=egin{pmatrix} 0&-rac{1}{l}rac{\partial}{\partial x}\ -rac{1}{c}rac{\partial}{\partial x}&0 \end{pmatrix}inom{i}{v}=\mathfrak{A}inom{i}{v}inom{i}{v},$$

which governs a transmission line (resistanceless) with capacitance c(x) and inductance l(x) at the point x; and take $c \equiv l \equiv 1$ off of the interval [-1, 1]. The energy of a vector $\binom{i}{v}$ is $\|\binom{i}{v}\|_{E}^{2} = \int_{-\infty}^{\infty} cv^{2} + h^{2} dx$. Now for x > 1, pairs $\binom{i}{v}$ giving rise to functions moving in toward the perturbation have the form

² The authors are grateful to Professor Gabor Temes, E. E. Dept. U.C.L.A., for checking the correctness of our approach to the adjoint method.

 $\binom{1}{-1} \alpha(x)$, while outgoing pairs look like $\binom{1}{1} \beta(x)$. Precisely the reverse is true for x < -1.

We shall associate a system [A, B, C, D] with this situation and do so in the spirit of the general procedure found in [14]. From this viewpoint one concentrates on the interval [-1, 1]; the operator A will act on it while B and C "communicate" information from [-1, 1] to the remainder of the transmission line. Here D = 0. We define A to be \mathfrak{A} on [-1, 1] along with boundary conditions at -1 and 1 which ensure that any electrical wave $\binom{i}{n}$ in [-1, 1] will, as time evolves, behave just as if the transmission line on [-1, 1]were embedded in the $[-\infty, \infty]$ line as described above. This means that a wave that is outgoing near x = 1 actually "goes out at 1" and the boundary condition there imposes no additional constraint which reflects any part of the wave back toward 0; thus the boundary condition at x = 1 should be v(1) = i(1). Likewise at x = -1 we require v(-1) = -i(-1). Hence we define A to be \mathfrak{A} acting on the domain $\mathscr{D} = \{\binom{t}{g} \text{ supported on } [-1, 1]:$ $\|\mathfrak{A}(g)\|_{k} < \infty, f(1) = g(1), \text{ and } f(-1) = -g(-1)$. The operator B reads incoming data into the line. It maps C² into X, a space of distributions defined in [14], and is defined for $\binom{w}{u} \in \mathbb{C}^2$ by

$$B\binom{w}{y} = \binom{1}{-1} w\delta(x-1) + \binom{1}{1} y\delta(x+1).$$

C reads off outgoing data. It maps \mathcal{D} into \mathbb{C}^2 and is defined by

$$C\binom{i}{v} = \binom{v(1) + i(1)}{v(-1) - i(-1)}.$$

We have set things up so that the solution to

$$\frac{\partial}{\partial t} \begin{pmatrix} i(x,t) \\ v(x,t) \end{pmatrix} = \mathfrak{A} \begin{pmatrix} i(x,t) \\ v(x,t) \end{pmatrix} + B \begin{pmatrix} w(t) \\ y(t) \end{pmatrix}$$
(3.2)

with boundary conditions $\binom{i}{v} \in \mathscr{D}$ is precisely the state of the transmission line on [-1, 1] when hit by incoming waves equaling $\binom{1}{-1}w(t)$ at x = 1 and $\binom{1}{1}y(t)$ at x = -1, respectively. Moreover, $C\binom{i}{v}$ gives the values at 1 and -1 of the resulting outgoing waves.

In [14], e^{At} is extended to a map from \mathscr{X} to \mathscr{X} and the solution to (3.2) is defined as

$$\int_0^t e^{A(t-s)} B\binom{w(s)}{y(s)} \, ds.$$

The frequency response function can be defined and is in fact equal to the scattering matrix for this problem.

Now let us interpret Eq. (3.1) for the variation of the response function. $(z - A)^{-1}$ maps \mathscr{X} into the space of data with finite energy and we define

$$\varphi_i(\ , z, 1) = (z - A)^{-1} B \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \varphi_i(\ , z, -1) = (z - A)^{-1} B \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Similarly we define functions $\varphi_0(z, \pm 1)$ in the space of data with finite energy by

$$\varphi_0(\ , z, 1) = (z - A)^{-1^*} C^* {l \choose 0}, \quad \varphi_0(\ , z, -1) = (z - A)^{-1^*} C^* {0 \choose 1}.$$

One could alternatively regard the φ 's as solutions to $(z - \mathfrak{A}) \varphi = 0$ satisfying boundary conditions

$$arphi_i(1, z, 1) = inom{1}{-1}, \qquad arphi_i(-1, z, -1) = inom{1}{1}, \ arphi_0(1, z, 1) = inom{1}{1}, \qquad arphi_0(-1, z, -1) = inom{1}{-1}.$$

Since $(z - A)^{-1} B_{y}^{(w)}$ [resp., $(z - A)^{-1^{*}} C^{*}(_{y}^{w})$] is a linear combination of the φ_{i} [resp., φ_{0}], Eq. (3.1) says that for each z the 2 × 2 matrix (dF/ds)(z) has entries $(dF/ds)(z)(\epsilon, \epsilon')$ with $\epsilon = \pm 1$ and $\epsilon' = \pm 1$ given by

$$\begin{split} &\left(\frac{dA}{ds}\,\varphi_i(z,\,\epsilon),\,\varphi_0(z,\,\epsilon')\right) \\ &= \int_{-1}^1 \begin{pmatrix} l & 0 \\ 0 & c \end{pmatrix} \begin{pmatrix} 0 & \frac{-\partial}{\partial s} \frac{1}{l} \frac{\partial}{\partial x} \\ \frac{-\partial}{\partial s} \frac{1}{c} \frac{\partial}{\partial x} & 0 \end{pmatrix} \varphi_i(x,\,z,\,\epsilon) \overline{\varphi_0(x,\,z,\,\epsilon')} \, dx \\ &= \int_{-1}^1 l \left[-\frac{\partial}{\partial s} \frac{1}{l} \frac{\partial}{\partial x} \varphi_i^2(z,\,\epsilon) \right] \overline{\varphi_0^{-1}(x,\,z,\,\epsilon')} \\ &+ c \left[-\frac{\partial}{\partial s} \frac{1}{c} \frac{\partial}{\partial x} \varphi_i^{-1}(z,\,\epsilon) \right] \overline{\varphi_0^{-2}(z,\,\epsilon')} \, dx, \end{split}$$

where $\varphi_j = (\varphi_j^1, \varphi_j^2)$ for j = i or 0. Since each φ satisfies $(z - \mathfrak{A}) \varphi = 0$, we have $-zl\varphi_i^1 = (\partial/\partial x) \varphi_i^2(x, z, \epsilon)$ and $-zc\varphi_i^2 = (\partial/\partial x) \varphi_i^1$ which can be substituted into our formula to give

$$\frac{dF}{ds}(z)(\epsilon,\epsilon') = -z \int_{-1}^{1} \frac{\partial l}{\partial s} \varphi_i^{-1}(z,\epsilon) \overline{\varphi_0^{-1}(z,\epsilon')} + \frac{\partial c}{\partial s} \varphi_i^{-2}(z,\epsilon) \overline{\varphi_0^{-2}(z,\epsilon')} \, dx. \quad (3.2)$$

This is a distorted plane wave formula for the "lossless" transmission line.

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Now let us compare this to the distorted wave formula (1.7) of Section 1, and check that the φ 's are in a reasonable sense distorted plane waves. The equation $\psi_t = \mathfrak{U}\psi$ is in fact a first-order system arising from the second-order equations $u_{tt} = L_j u$, where

$$L_1 = \frac{1}{c} \frac{\partial}{\partial x} \frac{1}{l} \frac{\partial}{\partial x}$$
 and $L_2 = \frac{1}{l} \frac{\partial}{\partial x} \frac{1}{c} \frac{\partial}{\partial x}$.

Thus φ_0 and φ_i satisfy $(z^2 - L_1) \varphi^1 = 0$ and $(z^2 - L_2) \varphi^2 = 0$. The boundary values of φ_0 satisfy

$$\varphi_0^{1}(1, z, +1) = \varphi_0^{2}(1, z, +1) = \frac{1}{z} \frac{\partial}{\partial x} \varphi_0^{1}(1, z, +1)$$

and so at the point x = 1 the boundary values of φ_0^{-1} and $(\partial/\partial x) \varphi_0^{-1}$ equal the functions (e^{zx}/e^z) and $(1/e^z)(de^{zx}/dx)$. Consequently up to a multiplicative factor depending only on z the function φ_0^{-1} is the outgoing distorted plane wave from Section 1. The other φ 's can be treated similarly. Thus Eq. (3.2) derived here is the same as the distorted wave formula (1.7) for the differential operator L_1 (the z's here differ from those in Section 2 by a factor of *i*).

4. REMARKS

(I)
$$\partial A/\partial s \ge 0$$
, $\partial a/\partial s \ge 0$, $(\partial/\partial s)(b/a) \ge 0$, and $\partial \rho/\partial s \ge 0$,

one has

(II) $(\partial\beta/\partial s)(s, 0) \ge 0$ on R_+ for any phase shift β meeting the differentiability requirements.

We call perturbations satisfying (I) "positive." It is far from true that any perturbation for which (II) holds must be positive. As an example, consider the operator $L(s) = (d^2/dx^2) - b(x, s)$ on R^1 with $L(0) = (d^2/dx^2)$. In this case (1.9) shows the kernel of $iS(z, 0)(dS^*/ds)(z, 0)$ is simply

$$\frac{1}{2z}\int e^{iz\theta x}\frac{\partial b}{\partial s}\,e^{-iz\omega x}\,dx,$$

where θ and ω range over $\{1, -1\}$. Hence (II) holds if

$$\int \frac{\partial b}{\partial s}(x,0)\,dx \geqslant \left|\int \frac{\partial b}{\partial s}(x,0)\,e^{i\varepsilon x}\,dx\right| \qquad \varepsilon > 0.$$

This condition is clearly weaker than (I).

We have not been able to find a reasonable strengthening of (II) that implies (I) or even anything much in that direction. Such a strengthening would be useful in inverse scattering problems. The only work in this direction that has come to our attention is the paper of Newton [10], where the variation of a spherically symmetric potential with respect to phase shifts is computed.

2. For *n* odd, we can look at the sum of all the phase shifts. To do this note that for *n* odd, (1.9) holds for $z \in \mathbb{R}/0$. Moreover, for *n* odd, S(z) is holomorphic in $\text{Im } z \leq 0$ and differs from the identity by a trace class operator. Hence, S(z) has a determinant in the sense of [3]. Det S(z) is a holomorphic scalar function in $\text{Im } z \leq 0$ which has modulus 1 on Im z = 0 and may be extended to a meromorphic function in Im z > 0 by Schwartz reflection. Its poles are just the poles of the scattering matrix. For z real, log det S(z) is congruent mod $2\pi i$ to

$$i\sum_k \beta_k(z),$$

where the phase shifts β_k are chosen so that $-\pi/2 < \beta_k < \pi/2$ for all but finitely many k. Hence we call $\delta(z) \equiv (1/i) \log \det S(z)$ the "total phase shift." As we have seen, S(z, s) is a smooth function of s for any smooth variation of (I.1), except possibly at z = 0. Moreover, (1.8) and Schwartz reflection show (dS/ds)(z) is a holomorphic trace class operator valued function away from the poles of S(z). In [3, Chap. IV, Sect. 1 (1.14)], it is shown that

$$\frac{d}{ds}\log \det S(z) = -\operatorname{tr}\Big(S(z)\frac{dS^*}{ds}(z)\Big). \tag{4.1}$$

Since the trace of an integral operator with kernel $k(\theta, \omega)$ is $\int k(\theta, \theta) d\theta$, combining (1.9) and (4.1) we have for real z

$$\frac{d\delta}{ds}(z) = \frac{1}{4\pi} \left(\frac{z}{2\pi}\right)^{n-2} \left[\int_{S^{n-1}} d\theta \left[\int_{D} \nabla \varphi(\theta) \cdot \frac{\partial A}{\partial s} \overline{\nabla \varphi(\theta)} + |\varphi(\theta)|^2 \frac{\partial}{\partial s} \left(\frac{-z^2 + b}{a}\right) dx + \int_{\partial D} \left| \frac{\partial \varphi}{\partial \eta}(\theta) \right|^2 \frac{\partial \rho}{\partial s} dS_A \right] \right]. \quad (4.2)$$

Since both sides of (3.2) have analytic continuations to $\mathbf{C} - (\{z: z \text{ or } \overline{z} \text{ is a pole of } S(z)\} \cup \{0\})$, we have

$$egin{aligned} rac{d\delta}{ds}(z) &= rac{1}{4\pi} \left(rac{z}{2\pi}
ight)^{n-2} \Big[\int_{S^{n-1}} d heta \int_{D}
abla arphi(x, heta,iz) \cdot rac{\partial A}{\partial s} \, \overline{
abla arphi(x, heta,iar{z})} \, dx \ &+ \int_{S^{n-1}} d heta \left[\int_{D} arphi(x, heta,iz) \, rac{\partial}{\partial s} \left(rac{-z^2+b}{a}
ight) \, \overline{arphi(x, heta,iar{z})} \, dx \ &+ \int_{\partial D} rac{\partial arphi}{\partial \eta} \left(x, heta,iz
ight) rac{\partial
ho}{\partial s} \, rac{\partial arphi}{\partial \eta} \left(x, heta,iar{z}
ight) \, dS_A \Big] \Big]. \end{aligned}$$

This formula looks interesting, but we have not found a good use for it.

3. Given S(z, s) has a pole at $z = \lambda(s)$, one can begin with (1.7) and compute $d\lambda/ds$. A computation of this type is given in [13, Proposition 4.1]. However, in the odd-dimensional case, it is possible to compute $d\lambda/ds$ without introducing the transmission coefficient at all. This approach was taken by J. La Vita in his New York University thesis (1969).

Let B(s) be a one-parameter family of (unbounded) operators with common domain \mathcal{D} for which $B(s)\psi$ is differentiable when $\psi \in \mathcal{D}$. Suppose that \mathcal{D}^* is a domain for $B(s)^*$ with the same property. Let $\lambda(s)$, $\psi(s)$ be eigenvalues and eigenvectors for B, i.e., $B(s)\psi(s) = \lambda(s)\psi(s)$, which vary differentiably. We can take a very weak derivative of $B(s)\psi(s)$ to obtain

$$(B'(s) \psi(s), \varphi) + (\psi'(s), B(s)^* \varphi) = \lambda'(s)(\psi(s), \varphi) + \lambda(s)(\psi'(s), \varphi)$$

for a φ in \mathscr{D}^* . If φ is taken to be an eigenvector of $B(s)^*$ with eigenvalue $\overline{\lambda}(s)$, then

 $(B'(s) \psi(s), \varphi(s)) + \lambda(s)(\psi'(s), \varphi(s)) = \lambda'(s)(\psi(s), \varphi(s)) + \lambda(s)(\psi'(s), \varphi(s))$

from which we get

$$\lambda'(s) = \frac{1}{(\psi(s), \varphi(s))} \left(B'(s) \, \psi(s), \varphi(s) \right). \tag{4.3}$$

From here on our proof requires familiarity with [8]. To a scattering problem with coefficients perturbed inside a ball of radius ρ , Lax and Phillips associate (see [8, Sect. 4]) a maximal dissipative operator *B* defined on a Hilbert space *K* having eigenvalues precisely at the poles of the scattering matrix (under weak hypothesis; see [8, Theorem 5.5]). To the λ eigenvector *b* for *B* there corresponds an outgoing eigenvector *f* (in an extended space) for the perturbed Hamiltonian *A* with the property that its natural "projection" $P_+{}^a f$ onto K^a equals *b* (see [8, Eq. (5.3)]). Under the assumptions of [7] the operator B^* has a $\bar{\lambda}$ eigenfunction b^+ and similar statements hold for *g*, the corresponding incoming $\bar{\lambda}$ eigenfunction (extended space) for A^* . From [8, Eq. (4.6)] one gets $B(s) P_+{}^a f = P_+{}^a A(s) f$ and so

$$\lambda'(s) = (1/(b, b^{+}))(P_{+}^{a}A'(s)f, g)_{\kappa a}$$
(4.4)

for the case where the Hamiltonian A(s) depends on a parameter s.

Everything so far was within the framework of abstract Lax-Phillips scattering theory. Concrete scattering theory uses Hamiltonians which are in fact differential operators. For such A(s) we have that A'(s) is for each s a differential operator with coefficients supported in the interior of the ρ -ball of \mathbb{R}^{2n-1} . It is easy to see from the definition of K^a that all functions supported in the ρ -ball are in K^a ; consequently $P_+{}^aA'(s) = A'(s)$ and we finally obtain

$$\lambda'(s) = \frac{1}{(b, b^+)} \int_{|x| < \rho} \langle A'(s)f, g \rangle, \qquad (4.5)$$

where \langle , \rangle denotes the pointwise energy inner product appropriate to the problem. This formula describes how poles move when A is changed.

In energy dissipative scattering, zeros as well as poles are possible in the Im z > 0 half-plane. By [8, Theorem 5.6] and its prelude, each such zero of s(z) occurs at an eigenvalue λ of A. If $\overline{\lambda}$ is an eigenvalue of A^* , then (4.3) implies (4.5), where f, g are λ , $\overline{\lambda}$ eigenvectors for A, A^* , and b, b^+ can be taken equal to f, g. Thus (4.5) also describes how zeroes move when A changes.

Appendix

Under our assumptions the functions $u(x, \xi, \sigma, s)$ are smooth functions of (x, ξ, σ, s) for Re $\sigma \ge 0$, $\sigma \ne 0$. This is a standard result for Re $\sigma > 0$, since then u can be represented as $(L(s) - \sigma^2)^{-1}g + h$, where g and h are smooth and have bounded support in x. However, the following technique due to Lax and Phillips (employed in the proof of [7, Theorem 5.2] and by Majda, [9]) enables us to get a good representation for u when σ is near $i\mu_0$, $\mu_0 \in \mathbb{R}/0$.

We begin by making a smooth s-dependent change of coordinates $x = \Phi(s, y)$ which is the identity for |y| > R and which maps D onto D(s). This transforms L(s) into another second-order elliptic operator M(s). Let β be a smooth function such that $\beta = 1$ for |x| < R, $1 > \beta > 0$ for R < |x| < 2R, and $\beta = 0$ for |x| > 2R. Given $g \in L^2(D)$ such that g = 0 for |x| > R, and σ near $i\mu_0$, we will attempt to construct a solution to $(M(s) - \sigma^2) u = g$ with u = 0 on ∂D of the form

$$u = \beta v + (1 - \beta)w. \tag{(*)}$$

Here v is the solution to $(M(s) - \sigma^2 + i)v = f$ with v = 0 on $\partial D \cup |x| = 2R$ and f is a function supported in $D \cap |x| \leq 2R$, which is to be determined. Since M(s) has real spectrum, v is well defined for σ near $i\mu_0$. $w = G_{\sigma}f$, where, for Re $\sigma > 0$, G_{σ} is the inverse of $\Delta - \sigma^2$ acting in $L^2(\mathbb{R}^n)$, and it is defined by analytic continuation in a neighborhood of Re $\sigma \ge 0$, $\sigma \neq 0$. G_{σ} can be given explicitly, but the only property we require is that G_{σ} is a holomorphic function of σ whose values are bounded operators from $\{f \in H^m(\mathbb{R}^n) : f = 0 \text{ for } |x| > 2R\}$ to $H^{m+2}(\mathbb{R}^n)$.

Given u in the form (*), the equation $(M(s) - \sigma^2) u = g$ becomes

$$g = f + [(M(s) - \sigma^2)(\beta v + (1 - \beta)w) - f] \equiv f + T(s, \sigma)f$$

 $T(s, \sigma)f$ is a sum of first-order differential operators applied to v and w. Hence by standard elliptic theory $T(s, \sigma)$ is a bounded operator from $\{f \in H^m(D) : f = 0 \mid x \mid > 2R\}$ to $H^{m+1}(D \cap \mid x \mid < 2R)$, when σ is near $i\mu_0$. Moreover, easy arguments also show $T(s, \sigma)$ is a smooth function of (s, σ) and all of its derivatives with respect to s are holomorphic in σ . Since $T(s, \sigma)$ considered as an operator on $L^2(D \cap |x| < 2R)$ is compact, $(T(s, i\mu_0) + I)^{-1}$ exists unless $(T(s, i\mu_0) + I)f = 0$ for some nonzero $f \in L^2(D \cap |x| < 2R)$. In this case u defined by (*) is an $i\mu_0$ -incoming solution to the homogeneous equation and standard arguments show $u \equiv 0$. Thus v = 0 for |x| < R which implies f = 0 for |x| < R. Also w = 0 for |x| > 2R and $v - w = (-1/\beta)w$ for |x| < 2R. Thus $z = (1/\beta)w$ is a solution to

$$(\Delta + \mu_0^2 + i(1 - \beta)) z = 0.$$
 (**)

z belongs to $H^2(|x| \leq 2R)$ and vanishes on |x| = 2R. Multiplication by \overline{z} and an integration by parts in (**) shows z = 0 for R < |x| < 2R. Thus $f \equiv 0$ and we conclude $(T(s, \sigma) + I)^{-1}$ exists for σ in a neighborhood of $i\mu_0$. Hence it is possible to represent a solution to our original problem in the form (*) with $f = (T(s, \sigma) + I)^{-1}g$. For σ near $i\mu_0$ there is a unique σ -incoming solution and it is the one given by (*). In particular, when σ is near $i\mu_0$, we can represent $u(\varphi(s, y), \xi, \sigma, s)$ as the sum of a smooth function and a solution in the form (*) to $(M(s) - \sigma^2) u = g$, where g is a smooth function of (x, ξ, σ, s) vanishing for |x| > R. This leads directly to the desired smoothness of $u(x, \xi, \sigma, s)$.

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