

ELASTIC WAVE SCATTERING CALCULATIONS AND THE
MATRIX VARIATIONAL PADÉ APPROXIMANT METHOD

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ABSTRACT

The matrix variational Padé approximant and its generalization to elastic wave scattering are discussed. Predictions of the method for the scattering of a longitudinal plane wave are compared with the exact scattering from spherical voids and inclusions. Its predictions are also compared to those of the first and second Born approximations and to the standard matrix Padé approximant based on these Born approximations.

INTRODUCTION

This is a preliminary report on the application of the Lippmann-Schwinger variational principle to the scattering of elastic waves from voids and inclusions.¹ This particular variational principle has the advantage of being formulated in terms of the scattering matrix and hence directly giving the physical quantities of experimental interest. The trial functions used in this application of the variational principle allow the stationary value of the variational form to be expressed in a compact block-matrix form with the block-matrix elements corresponding to terms in the Born-Neumann series solution to the integral equation of scattering.

Our principal motivation for using the variational approach is to develop a method for treating the scattering of elastic waves from complexly-shaped defects when the wavelength of the incident wave is comparable to the size of the defect and from collections of defects. Present methods, like the eigenfunction expansion methods,²⁻⁵ are for practical reasons limited to axially-symmetric defects and are awkward to apply to a collection of defects.

Below we summarize some exact results from the integral equation approach to scattering theory. Then we discuss four approximations: the first and second Born approximations, the [1/1] matrix Padé approximant, and the variational approach, formally called the variational matrix Padé approximant. The first two approximations are necessary components to our application of the fourth approximation. We include the third method as a way to bridge the variational method and the two perturbation approximations.

EXACT RESULTS

The integral equation describing the scattering of an elastic wave from voids and inclusions is⁶

$$u_i(\vec{r}) = u_i^0(\vec{r}) + \int d\vec{r}' g_{ij}(\vec{r}, \vec{r}') v_{jk}(\vec{r}') u_k(\vec{r}') \quad (1)$$

where $u_i^0(\vec{r})$ is the incident wave. $g_{ij}(\vec{r}, \vec{r}')$ is the Green's function, and $v_{jk}(\vec{r}')$ describes the void or

inclusion. If the void or inclusion is embedded in an unbounded, isotropic medium, then

$$g_{ij}(\vec{r}, \vec{r}') = \frac{1}{4\pi\rho\omega^2} \left[\beta^2 \delta_{ij} \frac{e^{i\beta R}}{R} + \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left(\frac{e^{i\alpha R}}{R} - \frac{e^{i\beta R}}{R} \right) \right] \quad (2)$$

with

$$R = |\vec{r} - \vec{r}'|$$

and α and β equal to the longitudinal and transverse wavenumbers. We also have that

$$v_{ij}(\vec{r}) = \delta\rho\omega^2\theta(\vec{r})\delta_{ij} + \delta C_{ikjl} \frac{\partial}{\partial x_k} \theta(\vec{r}) \frac{\partial}{\partial x_l} \quad (3)$$

with $\delta\rho$ and δC_{ijkl} equal to the density and stiffness differences between the flaw and host material and with

$$\theta(\vec{r}) = \begin{cases} 1, & \text{for } \vec{r} \text{ inside the defect} \\ 0, & \text{otherwise} \end{cases} \quad (4)$$

The parameter ρ is the density of the host material, and ω is the circular frequency of the incident wave.

In the far-field the solution to (1) has the form

$$u_i \sim u_i^0 + A_i \frac{e^{i\alpha R}}{r} + B_i \frac{e^{i\beta r}}{r}$$

with the scattered amplitudes given by

$$A_i = \hat{r}_i \hat{r}_j f_j(\vec{\alpha}) \quad (5a)$$

$$B_i = (\delta_{ij} - \hat{r}_i \hat{r}_j) f_j(\vec{\beta}) \quad (5b)$$

and the f-vector defined by

$$f_i(\vec{k}) = \frac{k^2}{4\pi\rho\omega^2} \int d\vec{r} e^{-i\vec{k}\cdot\vec{r}} v_{ij}(\vec{r}) u_j(\vec{r}) \quad (6)$$

where $\vec{k} = k\hat{r}$ and \hat{r} is the direction of scattering.

The quantity of experimental interest is the differential cross-section. If the incident wave is a plane wave of the form

$$u_i^0 = d_i e^{i\vec{k}^0 \cdot \vec{r}} \quad (7)$$

then the differential cross-section for the longitudinal component of the scattering is

$$\frac{dP}{d\Omega} = \left| \frac{A}{d} \right|^2 \quad (8)$$

There is an alternate integral equation approach to the scattering that is formulated in terms of the scattered amplitudes. If both sides of (1) were operated on by $\exp(-i\vec{k} \cdot \vec{r})v_{ij}(\vec{r})$ and then integrated over \vec{r} , it follows from (6) that (1) is now equivalent to

$$f_i(\vec{k}) = \frac{k^2}{4\pi\rho\omega^2} \left[\int d\vec{r}' e^{-i\vec{k} \cdot \vec{r}'} v_{ij}(\vec{r}') u_{je}^{i\vec{k}^0 \cdot \vec{r}'} + \int d\vec{r}' \int d\vec{r}'' e^{-i\vec{k} \cdot \vec{r}'} v_{ij}(\vec{r}') g_{jk}(\vec{r}', \vec{r}'') v_{jk}(\vec{r}'') u_k(\vec{r}'') \right] \quad (9)$$

so with the definitions

$$f_i(\vec{k}) \equiv \frac{k^2}{4\pi\rho\omega^2} T_{ij}(\vec{k}, \vec{k}^0) d_j \quad (10)$$

$$V_{ij}(\vec{k}, \vec{k}^0) \equiv \int d\vec{r}' e^{-i\vec{k} \cdot \vec{r}'} v_{ij}(\vec{r}') e^{i\vec{k}^0 \cdot \vec{r}'} \quad (11)$$

and the use of the Fourier transform of (2),

$$G_{ij}(\vec{q}) = \int d\vec{q}' e^{-i\vec{q} \cdot \vec{r}'} g_{ij}(\vec{r} - \vec{r}') e^{i\vec{q}' \cdot \vec{r}'}$$

the equation (9) becomes

$$T_{ij}(\vec{k}, \vec{k}^0) = V_{ij}(\vec{k}, \vec{k}^0) + \int d\vec{q} v_{ik}(\vec{k}, \vec{q}) G_{kl}(\vec{q}) T_{lj}(\vec{q}, \vec{k}^0) \quad (12)$$

The matrix function $T_{ij}(\vec{k}, \vec{k}^0)$ has the following simple relation to the scattered amplitudes

$$A_i = \hat{r}_i \hat{r}_j T_{jk}(\vec{\alpha}, \vec{k}^0) d_k / 4\pi(\lambda + 2\mu) \quad (13a)$$

$$B_i = (\delta_{ij} - \hat{r}_i \hat{r}_j) T_{jk}(\vec{\beta}, \vec{k}^0) d_k / 4\pi\mu \quad (13b)$$

where λ and μ are the Lamé parameters. The other matrix function $V_{ij}(\vec{k}, \vec{k}^0)$ equals

$$V_{ij}(\vec{k}, \vec{k}^0) = t_{ij}(\vec{k}, \vec{k}^0) S(\vec{k}, \vec{k}^0) \quad (14)$$

where

$$t_{ij}(\vec{k}, \vec{k}^0) = [\delta_{ij} \rho\omega^2 - \delta_{ij}(\vec{k} \cdot \vec{k}^0)] \delta_{ij} - \delta_{ik} k_j k_j^0 - \delta_{jk} k_i k_i^0 \quad (15)$$

and the shape factor

$$S(\vec{k}, \vec{k}^0) = \int d\vec{r}' \Theta(\vec{r}') e^{i(\vec{k}^0 - \vec{k}) \cdot \vec{r}'} \quad (16)$$

Several additional definitions and equations will prove useful. First, if we use (9) for incident wave and if we define $U_{ij}(\vec{r})$ by

$$u_i(\vec{r}) = U_{ij}(\vec{r}) d_j \quad (17)$$

then we can rewrite (1) as

$$U_{i\ell}(\vec{r}) = U_{i\ell}^0(\vec{r}) + \int d\vec{r}' g_{ij}(\vec{r}, \vec{r}') v_{jk}(\vec{r}') U_{k\ell}(\vec{r}') \quad (18)$$

where

$$U_{i\ell}^0(\vec{r}) = \delta_{i\ell} e^{i\vec{k}^0 \cdot \vec{r}} \quad (19)$$

Also, we note that the specific formula for the scattering matrix is now

$$T_{ik}(\vec{k}, \vec{k}^0) = \int d\vec{r}' e^{-i\vec{k} \cdot \vec{r}'} v_{ij}(\vec{r}') U_{jk}(\vec{r}') \quad (20)$$

APPROXIMATIONS

The First and Second Born Approximations - A formal solution to the integral equation for the scattering matrix can be obtained by iterating the equation to produce what is often called the Born-Neumann series. If only the first term in this series is used (i.e., no iterations are performed), then the resulting approximation is called the first Born approximation. The first Born approximation to (12) corresponds to

$$T_{ij}(\vec{k}, \vec{k}^0) \approx V_{ij}(\vec{k}, \vec{k}^0) \quad (21)$$

If the first two terms of the Born-Neumann series are kept (i.e., one iteration is performed), then the approximation is called the second Born approximation. For (12) the second Born approximation corresponds to

$$T_{ij}(\vec{k}, \vec{k}^0) \approx T_{ij}^{(1)}(\vec{k}, \vec{k}^0) + T_{ij}^{(2)}(\vec{k}, \vec{k}^0) \quad (22)$$

where

$$T_{ij}^{(1)}(\vec{k}, \vec{k}^0) = V_{ij}(\vec{k}, \vec{k}^0) \quad (23a)$$

$$T_{ij}^{(2)}(\vec{k}, \vec{k}^0) = \int d\vec{q} t_{ik}(\vec{k}, \vec{q}) S(\vec{k}, \vec{q}) G_{kl}(\vec{q}) \cdot S(\vec{q}, \vec{k}^0) t_{lj}(\vec{q}, \vec{k}^0) \quad (23b)$$

The matrix functions $T_{ij}^{(1)}$ and $T_{ij}^{(2)}$ are called the first and second Born terms.

The evaluation of the second Born term is not a trivial numerical task. Normally, the second Born term is a 6-dimensional integral with a singular integrand. In our particular case, because the defect volume is assumed to be finite, the integral is finite. The way we chose to express the second Born term has reduced the dimensionality of the integration to 3; the integrand is still singular, but the integral is now infinite. A possible advantage to the present approach is the isolation of the shape dependence of problem in the shape factor (16). How the second Born term is integrated numerically is essentially independent of the flaw shape. The shape factor is just some subroutine, usually a simple one since (16) can often be evaluated analytically or else reduced to a one or two-dimensional numerical integration.

Through the shape factor it is also easy to study multiple defect problems. For example, for N identical defects whose centroids are located by \vec{R}_i , the shape factor gets replaced by

$$S(\vec{k}, \vec{k}^0) \sum_{i=1}^N e^{i\vec{k}_i \cdot (\vec{k}^0 - \vec{k})}$$

where $S(\vec{k}, \vec{k}^0)$ is the shape factor for one of the defects. The summation in the above is called the structure factor.

The [1/1] Matrix Padé Approximation - If $\underline{F}(x)$ is a matrix function of x and if

$$\underline{F}(x) = \underline{F}^{(0)} + \underline{F}^{(1)}x + \underline{F}^{(2)}x^2 + \dots$$

then the $[M/N]$ matrix Padé approximant to $\underline{F}(x)$ is defined by⁸

$$\underline{F}^{[M/N]}(x) = \underline{P}_M(x) \underline{Q}_N(x)^{-1} \quad (25a)$$

where

$$\underline{Q}_N(x) \underline{F}(x) - \underline{P}_M(x) = \mathcal{O}(x^{M+N+1}). \quad (25b)$$

(For compactness, we now denote matrices by underlined, capital Roman letters. Below, all matrices representing physical quantities are 3×3 .)

Specifically, from (18) and (20),

$$\begin{aligned} \underline{I}^{[1/1]}(\vec{k}, \vec{k}^0) &= \underline{I}^{(1)}(\vec{k}, \vec{k}^0) [\underline{I}^{(1)}(\vec{k}, \vec{k}^0) \\ &- \underline{I}^{(2)}(\vec{k}, \vec{k}^0)]^{-1} \underline{I}^{(1)}(\vec{k}, \vec{k}^0). \end{aligned} \quad (26)$$

Hence, if the first two terms of the Born series are known, it is a trivial procedure to evaluate the $[1/1]$ matrix Padé approximant. The result may be a better approximation than given by the second Born approximation.

Technically, the definition (21) is of a left-handed matrix Padé approximant. If $\underline{P}_M(x)$ is inverted instead of the $\underline{Q}_N(x)$, then a right-handed matrix Padé approximant is defined. The different definitions can be shown to give equivalent answers.

The Variational Matrix Padé Approximant - First, we identify $\underline{W}(\vec{r})$ as the matrix function satisfying the adjoint equation of (18)

$$\underline{W}(\vec{r}) = \underline{W}^0(\vec{r}) + \int d\vec{r}' \underline{g}^*(\vec{r}, \vec{r}') \underline{v}(\vec{r}') \underline{W}(\vec{r}') \quad (27a)$$

where

$$\underline{W}^0(\vec{r}) = \underline{I} e^{i\vec{k} \cdot \vec{r}}. \quad (27b)$$

Next, we operate on both sides of (18) with $\underline{W}^*(\vec{r}) \underline{v}(\vec{r})$, integrate over \vec{r} , and subtract (20) from the result to find

$$\begin{aligned} \underline{I}(\vec{k}, \vec{k}^0) &= \int d\vec{r} e^{-i\vec{k} \cdot \vec{r}} \underline{v}(\vec{r}) \underline{U}(\vec{r}) \\ &+ \int d\vec{r} \underline{W}^*(\vec{r}) \underline{v}(\vec{r}) e^{i\vec{k}^0 \cdot \vec{r}} \\ &+ \int d\vec{r} \underline{W}^*(\vec{r}) \underline{v}(\vec{r}) \left[e^{i\vec{k}^0 \cdot \vec{r}} - \int d\vec{r}' \underline{g}(\vec{r}, \vec{r}') \underline{v}(\vec{r}') \underline{U}(\vec{r}') \right]. \end{aligned} \quad (28)$$

Clearly, if $\underline{W}(\vec{r})$ and $\underline{U}(\vec{r})$ are exact, the above is an exact expression for the scattering matrix. The expression also has the feature that considered as a functional of $\underline{W}(\vec{r})$ and $\underline{U}(\vec{r})$ it is stationary with respect to independent and arbitrary variations of $\underline{W}(\vec{r})$ and $\underline{U}(\vec{r})$ about their exact values. When used as a variational form, the expression is a generalization to elastic wave scattering of the Lippmann-Schwinger variational principle.⁹⁻¹²

There are many ways to choose the trial functions $\underline{W}(\vec{r})$ and $\underline{U}(\vec{r})$. We chose

$$\begin{aligned} \underline{U}(\vec{r}) &= \sum_{i=1}^N \underline{a}^{(i)} e^{i\vec{k}^{(i)} \cdot \vec{r}} \\ \underline{W}(\vec{r}) &= \sum_{i=1}^N \underline{b}^{(i)} e^{i\vec{k}^{(i)} \cdot \vec{r}}. \end{aligned} \quad (29)$$

When (28) is made stationary with respect to these choices,

$$\underline{a}^{(i)} = \underline{b}^{(i)}$$

and (28) can be expressed in the following compact form

$$\begin{aligned} \underline{I}(\vec{k}, \vec{k}^0) &= \begin{bmatrix} \underline{I}^{(1)}(\vec{k}, \vec{k}^{(1)}) \\ \vdots \\ \underline{I}^{(1)}(\vec{k}, \vec{k}^{(N)}) \end{bmatrix}^T \\ &\times \begin{bmatrix} \underline{X}_{11} & \cdots & \underline{X}_{N1} \\ \vdots & & \vdots \\ \underline{X}_{1N} & \cdots & \underline{X}_{NN} \end{bmatrix}^{-1} \begin{bmatrix} \underline{I}^{(1)}(\vec{k}^{(1)}, \vec{k}^0) \\ \vdots \\ \underline{I}^{(1)}(\vec{k}^{(N)}, \vec{k}^0) \end{bmatrix} \end{aligned} \quad (30a)$$

where we have defined

$$\underline{X}_{ij} = \underline{I}^{(1)}(\vec{k}^{(i)}, \vec{k}^{(j)}) - \underline{I}^{(2)}(\vec{k}^{(i)}, \vec{k}^{(j)}). \quad (30b)$$

Equation (30) is a block-matrix equation: Matrix multiplication is done by the rule of block-matrix multiplication. The transpose operation is on block elements and not on the individual matrices comprising those elements. In (30) the need to calculate the first and second Born approximations is evident. The reader should compare (30) with (26).

RESULTS

For an incident longitudinal plane wave we computed the longitudinal backscattering from spherical defects predicted by each of the four approximations and compared the results to the exact scattering from spherical voids and inclusions.¹³ We studied the breakdown of the approximations as ka is increased and as the density and stiffness of an inclusion is incrementally decreased from that of the host material to that of a void. (k is the scattered wave number, and a is the radius of the sphere.)

For the variational part of the calculation

our trial function was

$$\underline{U}(\underline{r}) = \underline{a}^{(1)} e^{i\vec{k}^0 \cdot \underline{r}} + \underline{a}^{(2)} e^{i\vec{k} \cdot \underline{r}} \quad (31)$$

not a serious choice. It was, however, an effective and convenient choice to study the internal behavior of our computer program. (If (31) were used to calculate the forward scattering, then the two wave vectors in (31) become equal, and the square matrix in (31) becomes singular and non-invertible. With (31) and the second Born term, only two additional second Born terms are needed for a non-trivial variational calculation.)

ational calculation, when (31) is used, is never better than the first Born approximation. In Fig. 1 we plotted our results only for the second Born approximation. Including the results of the other calculations clutters the figure without revealing more information than what was just said. Presently we are trying to find a more reasonable choice of trial functions. We will report our results elsewhere, accompanied by a more expansive treatment of the theoretical methods.

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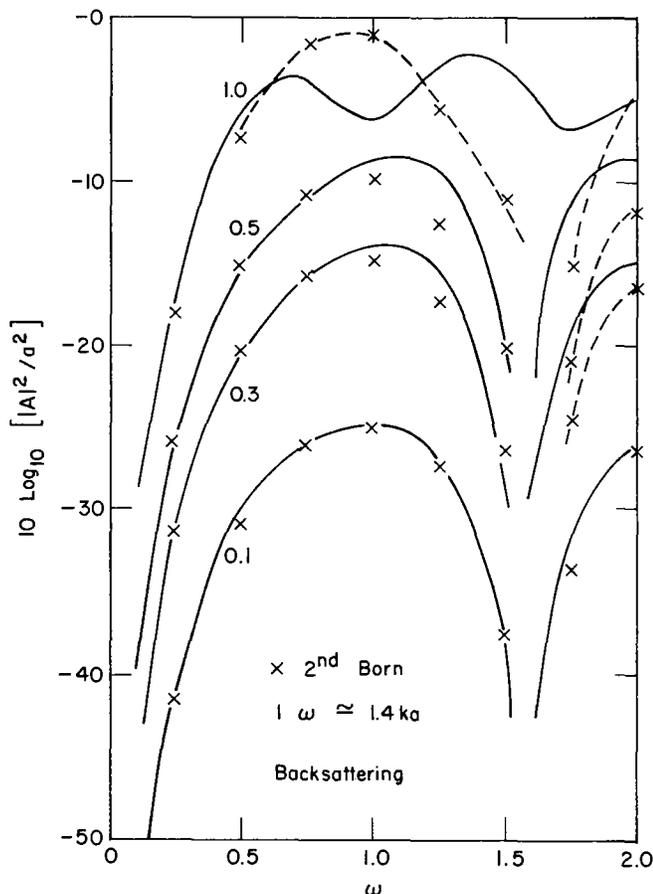


Fig. 1 The longitudinal backscattering from a spherical void and inclusions that is predicted by the second Born approximation plotted as a function of ka . Each line is for an inclusion whose density and Lamé parameters are reduced by a factor of 0.1, 0.3, 0.5, and 1.0 relative to the host medium. The reduction of 1.0 corresponds to a void.

We were uncertain how well the variational calculation would work, but believed that the second Born approximation would have larger ranges of validity than the first Born approximation and that the [1/1] matrix Padé approximant would be at least valid as the second Born approximation. This is what we found. Additionally, we found the vari-

SUMMARY DISCUSSION

Bruce Thompson, Chairman (Rockwell Science Center [now Ames Laboratory]): We have, perhaps, time for one question.

Jim Rose (Ames Laboratory): What's included in the scattering? Any double scattering? What have you left in and what have you left out?

Jim Gubernatis (Los Alamos Scientific Laboratory): With respect to variational principle, that's not always a reasonable question. What I am doing can not be described as a perturbation approach. Variational principles in general are non-perturbative. With this particular choice of variational form, it's simply that along with computing the variational results, I also compute the perturbations. I am not identifying something in a small parameter. What I am attempting is to choose a trial wave function which to some extent has an approximate relationship to the physical answer, so what has to be put into the calculation is intuition.

Jim Rose: What's your perturbation to the pade?

Jim Gubernatis: The pade I'm not interested in. I am unclear of the full significance of the word "pade" in the matrix. Variational pade approximant method other than the results are expressible in what is called in the pade literature as the nutall compact form. So the method is really a variational principle. At least I don't see, with respect to pade approximants what it's doing for you other than it does preserve the symmetry (reciprocity) of your matrices. I don't think of the method in terms of perturbations.

Unidentified Speaker: Where is the literature on the method?

Jim Gubernatis: For a start, there were several papers which appeared two years ago in Physical Review. By Bessis and some co-workers.

Bruce Thompson, Chairman: Thank you, Jim. I think perhaps we had better go on.