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Recursive Green functions technique applied to the propagation of elastic waves in layered media

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Abstract

Guided by similarities between electronic and classical waves, a numerical code based on a formalism proven to be very effective in condensed matter physics has been developed, aiming to describe the propagation of elastic waves in stratified media (e.g. seismic signals). This so-called recursive Green function technique is frequently used to describe electronic conductance in mesoscopic systems. It follows a space-discretization of the elastic wave equation in frequency domain, leading to a direct correspondence with electronic waves travelling across atomic lattice sites. An inverse Fourier transform simulates the measured acoustic response in time domain. The method is numerically stable and computationally efficient. Moreover, the main advantage of this technique is the possibility of accounting for lateral inhomogeneities in the acoustic potentials, thereby allowing the treatment of interface roughness between layers.

Keywords: Wave propagation; Green functions; Complex media

1. Introduction

Wave propagation in stratified media is a broad topic, the applications of which are found in different fields of research. Quantum electronic waves in layered systems, seismic elastic waves propagating across the stratified subsurface, and ultrasonic waves across parallel plates, are only a few examples. In addition to the common geometry, all those examples share a number of properties, the most important being that they are all governed by wave equations, although the equations are slightly different in each case. Methods and techniques used in one field of study can in principle be applied to others, and an interdisciplinary approach has proved to be very successful in some cases.

Based on the similarities mentioned above, a technique used in Condensed Matter Physics to describe the propagation of electrons across layered structures [1] is here proposed to treat classical waves, e.g. elastic or acoustic waves. The so-called recursive Green function (RGF) technique consists of evaluating the Green function of a layered system in terms of surface Green functions which are recursively updated. To calculate the response of a layered system with an arbitrary stacking sequence, one only needs to evaluate a product of updated surface Green functions. Perfectly layered structures have in-plane translational symmetry which makes the systems equivalent to 1-dimensional structures, thereby less computationally demanding. However, when the in-plane symmetry is broken by interface roughness or lateral variations, we need to consider the full 3-dimensional structure of the system. Although we present the results for a 1-dimensional case, which corresponds to perfectly layered structures, one advantage of using the RGF technique is that it is also valid for an arbitrary number of dimensions, the only difference being that the surface Green functions updated by the recursive relations become matrices rather than scalar quantities. Finally, both time-domain and frequency-domain solutions are important when studying wave propagation. Although the RGF is formulated in the frequency domain, it can also be used for time-domain calculations when combined with an inverse Fourier transform.

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2. Method

Consider the following 1-dimensional wave equation in the frequency domain

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\omega^2}{c_0^2}\psi + \frac{\omega^2}{c_0^2}\left[\frac{c_0^2}{c^2(x)} - 1\right]\psi = 0, \quad (1)$$

where ψ is the wave-field component, ω is the angular frequency, $c(x)$ is the position-dependent wave velocity, and c_0 is a reference velocity.

By turning the continuous variable x into a discrete quantity, the original differential wave equation becomes a set of finite difference equations for ψ_j, namely the wave field ψ evaluated at the position x_j. In matrix form this set of equations can be written as

$$[\mathbf{H}][\psi] = E[\psi], \quad (2)$$

where $[\mathbf{H}]$ is a square matrix given by

$$[\mathbf{H}] = \begin{bmatrix} \ddots & & & & \\ & \epsilon_{j-1} & h & 0 & \\ & h & \epsilon_j & h & \\ & 0 & h & \epsilon_{j+1} & \\ & & & & \ddots \end{bmatrix}, \quad (3)$$

E is a scalar, and $[\psi]$ is defined as

$$[\psi] = \begin{bmatrix} \vdots \\ \psi_{j-1} \\ \psi_j \\ \psi_{j+1} \\ \vdots \end{bmatrix}. \quad (4)$$

In the equations above, $\epsilon_j = 1 + (V(x_j)\Delta^2/2)$, $h = -1/2$, $E = \omega^2\Delta^2/2c_0^2$, $V(x) = (\omega^2/c_0^2)[1 - (c_0^2/c^2(x))]$, and $\Delta = x_{j+1} - x_j$. The square matrix above is a tridiagonal matrix whose diagonal elements are associated with the position-dependent wave velocity of the medium. The similarities between Eq. (2) and the Schroedinger equation are clear. Both are eigenvalue equations whose solutions describe how waves, either classical or quantum, propagate across the medium.

The propagation of waves can be described by the associated Green functions $\mathscr{G} = (E\mathbf{I} - \mathbf{H})^{-1}$, where $\mathbf{I}$ is the identity matrix. More precisely, by the matrix element $\mathscr{G}_{j,l}$ where x_j and x_l correspond to the source and detector positions, respectively. In other words, we need to calculate the (j, l) element of the matrix $(E\mathbf{I} - \mathbf{H})^{-1}$. For the sake of simplicity, we consider the wave velocity to be homogeneous throughout the 1-dimensional space, except for a finite region where it depends on the position. The matrix to be inverted, $(E\mathbf{I} - \mathbf{H})$, corresponds to an infinite matrix in which the diagonal elements are the same ($\epsilon = 1$), except for the finite central region where the elements are determined from the velocity $c(x)$.

In the absence of scatterers, the wave velocity is homogeneous and the infinite tridiagonal matrix to be inverted consists of constant values along its diagonals. In that case, analytical solutions exist, i.e., $\mathscr{G}(x_j, x_l; \omega) = c_0 e^{i\omega|x_j - x_l|/c_0}/2i\omega$. Analytical solutions may also be found for the case of a very narrow velocity insertion, where $c(x) = c_0$ for all but one discrete value of x [2]. In that case the use of Dyson equation enables one to write the solution of the inhomogeneous system in terms of that for the homogeneous one. In both cases, the solutions could be found without the actual inversion of the matrix $(E\mathbf{I} - \mathbf{H})$.

For the general case of a disordered region the matrix inversion cannot be avoided, although it can be simplified and optimized by the so-called RGF technique, a numerical procedure already used to describe the propagation of electronic waves in mesoscopic systems. In what follows, the technique will be described and a few simple cases will be addressed.

2.1. Recursive Green function technique

We need to calculate a given off-diagonal element of the matrix

$$[\mathscr{G}] = \begin{bmatrix} E - \epsilon_{N-1} & -h & 0 \\ -h & E - \epsilon_N & -h \\ 0 & -h & E - \epsilon_{N+1} \end{bmatrix}^{-1}, \quad (5)$$

where the matrix $[\mathscr{G}]$ is infinite but here represented as a (3×3) matrix for the sake of simplicity. We start by assuming that the disordered part of the matrix is contained within the range $[1, N]$. In other words, the ranges $[-\infty, 0]$ and $[N + 1, +\infty]$ of the matrix $[\mathscr{G}]^{-1}$ correspond to the semi-infinite homogeneous parts surrounding the disordered region. Without any loss of generality, we focus on $[\mathscr{G}]_{(1,N)}$ that is, we assume that source and detector are at the boundaries of the disordered region.

We start by decoupling the disordered part of the matrix from the semi-infinite region $[N + 1, +\infty]$ and write $[\mathscr{G}]^{-1}$ as

$$[\mathscr{G}]^{-1} = \underbrace{\begin{bmatrix} E - \epsilon_{N-1} & -h & 0 \\ -h & E - \epsilon_N & 0 \\ 0 & 0 & E - \epsilon_{N+1} \end{bmatrix}}_{[\mathscr{G}_0]^{-1}} + \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -h \\ 0 & -h & 0 \end{bmatrix}}_{[-V]}. \quad (6)$$

Notice that the first matrix on the right consists of two infinite tridiagonal blocks without any coupling between them, whereas the second contains the coupling elements. Assuming that $[\mathscr{G}_0]$ corresponds to a system with two semi-infinite parts which do not interact with each other and that $[V]$ acts as a perturbation, we can rewrite the equation above as

$$[\mathscr{G}] = [\mathscr{G}_0] + [\mathscr{G}_0][V][\mathscr{G}], \quad (7)$$

which is the so-called Dyson equation.

Since the matrix $[V]$ has only two non-zero elements, the matrix equation above has a simple solution, which allows the Green function $[\mathscr{G}]_{(1,N)}$ to be written in terms of matrix elements of the Green function $[\mathscr{G}_0]$.

$$[\mathscr{G}]_{(1,N)} = [\mathscr{G}_0]_{(1,N)} + [\mathscr{G}_0]_{(1,N)} h \left\{ \left([\mathscr{G}_0]_{(N+1,N+1)} \right)^{-1} - h[\mathscr{G}_0]_{(N,N)} h \right\}^{-1} h[\mathscr{G}_0]_{(N,N)}. \quad (8)$$

At this stage, we have written the unknown quantity $[\mathscr{G}]_{(1,N)}$ in terms of other unknown elements of the matrix $[\mathscr{G}_0]$, namely $[\mathscr{G}_0]_{(1,N)}$, $[\mathscr{G}_0]_{(N,N)}$ and $[\mathscr{G}_0]_{(N+1,N+1)}$. The latter corresponds to the surface Green function of a semi-infinite homogeneous system which, as we shall see, is analytically known. The former two matrix elements correspond to the other semi-infinite half of the system which contains the disordered region. It is important to highlight that on this half of the system, only the diagonal element $[\mathscr{G}_0]_{(N,N)}$ which is the surface Green function of this part, and its off-diagonal counterpart $[\mathscr{G}_0]_{(1,N)}$ are necessary to obtain the solution. If we introduce an additional decoupling between the elements $N-1$ and N, we can once again use the Dyson equation and show that we just need to update the surface Green function and the off-diagonal matrix element of a semi-infinite half space with one less element. The updating recursive relations are given by

$$[\mathscr{G}]_{(1,N)} = [\mathscr{G}_0]_{(1,N-1)} h[\mathscr{G}]_{(N,N)} \quad (9)$$

and

$$[\mathscr{G}]_{(N,N)} = \left\{ [\mathscr{G}_0]^{-1}_{(N,N)} - h[\mathscr{G}_0]_{(N-1,N-1)} h \right\}^{-1}, \quad (10)$$

where $[\mathscr{G}]$ and $[\mathscr{G}_0]$ refer to the coupled and uncoupled systems, respectively.

By continuing this procedure up to the point where the disordered region has been totally disconnected, we end up with two semi-infinite homogeneous spaces to deal with. In that case, as previously mentioned, we can find an analytical expression for the surface Green function.

Rather than starting from the infinite system as we have done above, one can also think of this numerical procedure in reverse. Starting from two semi-infinite homogeneous half spaces, one can add lines and columns to the matrix $[\mathscr{G}]$, in which the elements are associated with the position-dependent velocity $c(x)$. We then start from the surface Green function of the homogeneous half space and update the Green functions with the recursive relations above.

2.2. Surface Green function

It is clear that the starting point in our procedure is the surface Green function of the homogeneous system, which we now show how to be obtained. Eq. (10) tells us what happens with a surface Green function associated with a given matrix $(E\mathbf{I} - \mathbf{H})$ when one additional line and column have been added to (or removed from) the matrix. We see that the only information required to obtain $[\mathscr{G}]_{(N,N)}$ is the knowledge of the previous surface Green function $[\mathscr{G}_0]_{(N-1,N-1)}$ and the matrix element $[\mathscr{G}_0]^{-1}_{(N,N)}$ which is given by $E - \epsilon_N$. By writing that the updated element is the same as the previous one, we impose convergence in the recursive relations. In other words, we obtain the surface Green function $\mathscr{S}$ of a semi-infinite homogeneous system by substituting $[\mathscr{G}_0]^{-1}_{(N,N)} = E - \epsilon_N$, and $[\mathscr{G}]_{(N,N)} = [\mathscr{G}_0]_{(N-1,N-1)}) = \mathscr{S}$ into Eq. (10). In that case, one ends up with a simple quadratic equation for $\mathscr{S}(\omega)$.

3. Results

For the sake of comparison, we start by showing results for which analytical solutions are also available. In the case of a homogeneous space ($c(x) = c_0$) the analytical expression for the frequency-domain response is given by [3]

$$\mathscr{G}(x_j, x_l; \omega) = c_0 e^{i\omega|x_j - x_l|/c_0}/2i\omega \quad (11)$$

and the time-domain solution after Fourier transform is

$$\mathscr{G}(x_j, x_l; t) = \frac{-c_0}{2}\Theta\left(t - \frac{|x_j - x_l|}{c_0}\right), \quad (12)$$

where t is time and $\Theta(z)$ is the step function. Fig. 1 shows the numerical results obtained for the free

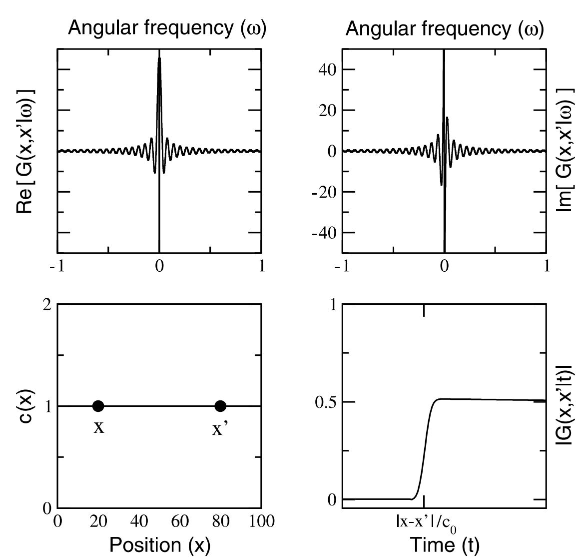

Fig. 1. Calculated response function for free propagation in 1-dimension. The top graphs show the frequency domain for the real (left) and imaginary (right) parts of the Green functions. The lower left graph shows the velocity profile and the lower right is the time-domain response function. Notice the agreeement with the analytical results (see text). The variables x and x' represent the detector and source position, respectively.

propagation case, where the top graphs show the frequency-domain response, the real part being on the left and the imaginary part on the right. The left lower graph shows the position-dependent velocity, which in this case is a constant function, and finally the lower graph on the right displays the time-domain response. As expected, both time- and frequency-domain responses agree with the expected analytical results.

Another possible comparison to be made is the simple case of a finite region of size d with a constant velocity c_1 ($c_1 \neq c_0$) embedded in the otherwise homogeneous environment. Although the full analytical solution of the response function contains an infinite number of poles in the complex frequency-plane, a good approximation [2] is to include only the lowest-order of those poles, which gives the most important contribution to the signal. Although this single-pole approximation is incapable of reproducing the multiple scattered part of the signal, it is excellent to determine the exponential decaying rate which arises in 1-dimensional structures. Fig. 2 shows three different cases. The top graphs show the velocity profile $c(x)$ and the bottom ones are the corresponding time-domain signals in logarithmic scale. The straight lines are the analytical results for the single-pole approximation. Notice that the slopes of those lines are in excellent agreement with those of the full numerical calculations (curves).

Finally, we show one set of results for which there are no analytical expressions. In Fig. 3 we consider a randomly layered system in which the velocity profile is represented by the top graph. The corresponding scattered part of the response in the time domain is shown on the bottom in a linear-log scale. The complexity of this procedure grows linearly with the size of the disordered region N, and therefore is more efficient than inverting the entire original matrix to obtain one ele-

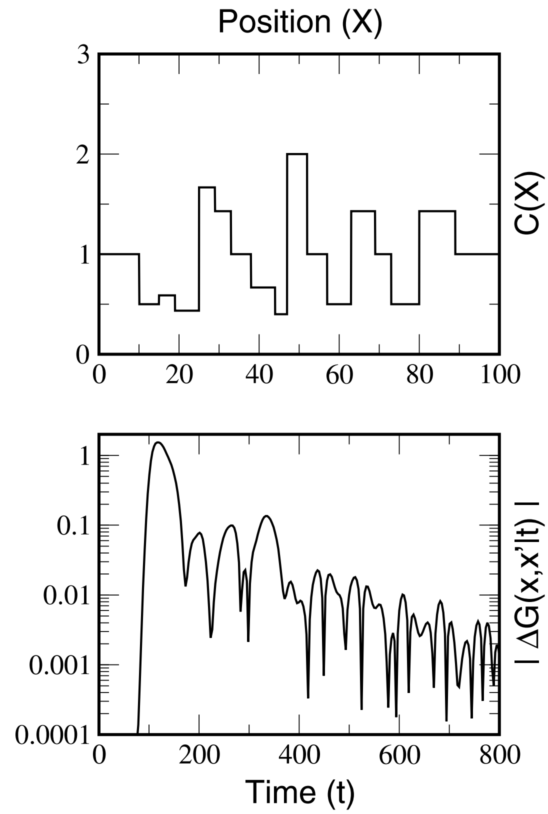

Fig. 3. Time-domain response function of a randomly layered system. The top graph shows the position-dependent velocity $c(x)$ and the lower one the corresponding response functions in a linear-log scale. The variables x and x' represent the detector and source position, respectively.

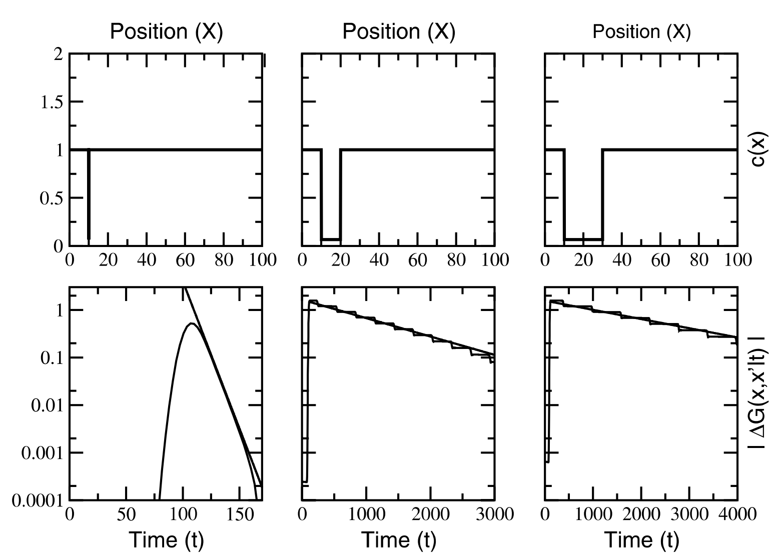

Fig. 2. Time-domain response function of a homogeneous (c_0) system separated by a finite insertion ($c_1 \neq c_0$) of different sizes. The top graphs show the position-dependent velocity $c(x)$ and the lower ones the corresponding response functions in a linear-log scale. The straight lines are analytical expressions based on the lowest-order pole approximation (see text). The variables x and x' represent the detector and source position, respectively.

ment of the propagator. It is also important to note that by considering lateral variations of the disordered region, one can use the same technique, the only difference being a matrix description for the Green functions in the recursive relations.

4. Summary and conclusions

In summary, we have applied the RGF technique to calculate the propagation of waves across a 1-dimensional system, which corresponds to perfectly layered structures. A comparison with analytical results for a few simple cases has been made. Arbitrary layering sequences have also been considered. The technique will be extended to treat lateral inhomogeneities of the scatterers.

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