Generalized optical theorem for scattering in inhomogeneous media

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The scattering of scalar waves by objects embedded in an inhomogeneous medium contained by a bounded volume is discussed using the method of pseudopotentials. The scattering amplitude for the object in an extended uniform medium is assumed known and used as input. The scattering process is described by using an expansion of the scattering amplitude in terms of spherical harmonics. An appropriate multipole decomposition of the Green function in the bounded medium is developed and the effective scattering amplitude in this environment is defined. The generalized optical theorem obeyed by this effective scattering amplitude is obtained and analyzed. The scattering problem is formulated entirely and explicitly in terms of the bounded medium's Green functions. This approach is thus very flexible in regards to the choice of incident field. In the case of waveguides the connection between propagation and scattering is explicit. At the same time it still allows for independent computation of the propagation and scattering aspects of the problem. This is the main advantage of using as input the scattering amplitude in an extended uniform medium.

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I. INTRODUCTION

The problem of interest here consists in describing the scattering of scalar waves by an object imbedded in a heterogeneous medium and obtaining the generalized optical theorem satisfied by the effective scattering amplitudes in the medium. The heterogeneity may originate from nonuniform properties of the medium, such as position-dependent wave propagation speeds, the presence of boundaries and interfaces or a combination of all these factors. The difficulty in solving this problem arises from the fact that one has to enforce boundary conditions both on the surface of the scattering object as well as on the interfaces and boundaries. For non-uniform media additional difficulties are encountered since, typically, only numerical solutions are available for describing wave propagation in such media.

A promising way of tackling those problems is to assume that the single object scattering problem in an extended uniform medium can be solved independently and then formulate the scattering problem in the inhomogeneous medium in such a way as to incorporate this result into the full solution of the problem. The pseudopotential introduced by Huang and Yang [1] offers a convenient approach to this problem since from the start it separates the implementation of both sets of boundary conditions. The scattering properties of the object are subsumed in a series of field-dependent source terms added to the Helmholtz equation, the solution of this equation must then satisfy proper boundary conditions on the medium's boundaries. The pseudopotential of Huang and Yang makes use of the expansion of the scattering amplitude into partial spherical waves. One might think that this restricts the method to spherically symmetric scattering objects but this approach can be generalized to the case of arbitrary scattering objects [2].

Once the effective scattering amplitude in the inhomogeneous medium is defined the generalized optical theorem for scattering of an arbitrary incident field by the embedded object can be obtained by an application of Green's theorem. This approach to the optical theorem via Green's theorem was used by Feenberg in a seminal paper on atom-electron scattering [3], where the optical theorem was introduced in a quantum-mechanical context. Van de Hulst in 1949 developed a physically intuitive method for relating extinction of a scattered scalar wave to the forward scattering amplitude [4]. An interesting application of the optical theorem is found in an article by Carney *et al.* [5], where it is generalized to scatterers whose properties are known only in a statistical sense. The optical theorem is there shown to be a powerful tool for inverse scattering applications. This is an important application that appears in a variety of situations, for example, from nondestructive probing of materials to medical applications and also in atmospheric physics and underwater acoustics.

The practical importance of the optical theorem provides the impetus to extend it to physical situations not addressed in the pioneering works on this subject. In the case of classical waves, such as sound and light for example, one often has to address both propagation in a substrate (which may be bounded by interfaces and other boundaries) and scattering by an object embedded in such substrate. A lucid discussion of energy fluxes in the context of acoustic scattering by an object in a stratified medium typical of oceanic acoustic waveguides is presented in an article by Ratilal and Makris [6] who derived the optical theorem based on an approximate description of the scattering process in a stratified medium. A more recent article by Carney *et al.* [7] derives and discusses the generalized optical theorem for scalar waves scattered by an object embedded in an inhomogeneous medium. The work presented here complements these two previous works and is not restricted to stratified media. In particular the formulation presented here allows for insights in the multiple scattering of the incident field by both the scattering object and boundaries and inhomogeneities in the embedding medium. These physical effects were neglected in Ref. [6] and although included in the scattering formulation used in Ref. [7] they were not explicitly discussed there.

The basic formulation of the approach adopted in this work was presented in Ref. [2]. The general formulation is presented in Sec. II. In Sec. III the generalized optical theorem is obtained and discussed. Finally, in Sec. IV the results are summarized and compared to those in other works on similar problems.

II. SCATTERING IN AN INHOMOGENEOUS MEDIUM

The scattering of time-harmonic scalar waves with angular frequency ω in an extended and uniform medium by an arbitrary scattering object is characterized by a scattering matrix T given by the following projection of the scattering amplitude into spherical harmonics [2]:

$$T_{lm,l'm'}(k) = \frac{i^{l-l'}}{4\pi} \int d\hat{\mathbf{p}} Y^{*}_{lm}(\hat{\mathbf{p}}) \int d\hat{\mathbf{q}} Y_{l'm'}(\hat{\mathbf{q}}) f(\hat{\mathbf{p}},\hat{\mathbf{q}}). \quad (1)$$

In Eq. (1) $f(\hat{\mathbf{p}},\hat{\mathbf{q}})$ is the scattering amplitude defined in the usual way in terms of the asymptotic limit for $r \to \infty$ of the full wave field created by the scattering of an incident plane wave by the object [8]. Note that the expression in Eq. (1) differs from the one used in Ref. [2] by a factor $k=\omega/c$ where c is the wave phase speed in the medium.

The procedure developed in Ref. [2] can be used to obtain equations describing scattering in a general case and it can be formulated without a specific expression for the Green function of the Helmholtz equation. This Green function obeys the Helmholtz equation plus appropriate boundary conditions:

$$\nabla^2 G_0(\mathbf{r},\mathbf{r}_0) + k(\mathbf{r})^2 G_0(\mathbf{r},\mathbf{r}_0) = \delta(\mathbf{r}-\mathbf{r}_0). \quad (2)$$

In order to use the operator T as an input in the computation of scattering in an arbitrary medium one must assume that in a neighborhood fully containing the object in the arbitrary medium the wave number, $k(\mathbf{r})$, can be assumed to be locally uniform. Thus for $\mathbf{r}$ and $\mathbf{r}_0$ in this region, that is for $d+\varepsilon > |\mathbf{r}-\mathbf{r}_T| > d$ and $d+\varepsilon > |\mathbf{r}_0-\mathbf{r}_T| > d$ where d is the largest linear dimension of the object, $\mathbf{r}_T$ is the position vector of the object and ε is positive (perhaps very small) one has $k(\mathbf{r}) \approx k(\mathbf{r}_0) \approx k(\mathbf{r}_T)$ and $G_0(\mathbf{r},\mathbf{r}_0)$ can be written as

$$G_0(\mathbf{r},\mathbf{r}_0) = g_T(\mathbf{r},\mathbf{r}_0) + G_0^{NS}(\mathbf{r},\mathbf{r}_0),$$

$$g_T(\mathbf{r}) = -\frac{e^{ik_T r}}{4\pi r}, \quad k_T = k(\mathbf{r}_T). \quad (3)$$

That is, the Green function inside this region can be split into two parts, a singular one, which is just the Green function in the equivalent unbounded medium, and a nonsingular part that enforces the boundary conditions and accounts for the inhomogeneous medium.

In the presence of an scattering object the Green function obeys a wave equation with pseudopotentials and satisfies the same boundary conditions as $G_0(\mathbf{r},\mathbf{r}_0)$:

$$\nabla^2 G(\mathbf{r},\mathbf{r}_0) + k(\mathbf{r})^2 G(\mathbf{r},\mathbf{r}_0) = \delta(\mathbf{r}-\mathbf{r}_0) - \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \times \left\{ \frac{(2l+1)!!}{k_T^l} \left[Y_{lm}(\hat{\mathbf{s}}) \frac{\delta(s)}{s^{l+2}} \left(T \frac{I}{I+ik_T T} A \right)_{lm} \right]_{\mathbf{s}=\mathbf{r}-\mathbf{r}_T} \right\}. \quad (4)$$

In the above equation $\mathbf{r}$ is the observation point, $\mathbf{r}_0$ is the position of the point source, and $\mathbf{r}_T$ is the position of the scattering object. The coefficients A_{lm} are given by

$$A_{lm} = \frac{(2l+1)!!}{k_T^l (2l+1)!} \partial_s^{2l+1} \left[s^{l+1} \int d\hat{\mathbf{t}} Y_{lm}(\hat{\mathbf{t}})^* G(\mathbf{r}_T + s\hat{\mathbf{t}},\mathbf{r}_0) \right]_{s=0}. \quad (5)$$

The Green function of the Helmholtz equation, $G_0(\mathbf{r},\mathbf{r}_0)$, is now used to obtain an integral equation:

$$G(\mathbf{r},\mathbf{r}_0) = G_0(\mathbf{r},\mathbf{r}_0) - \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{(2l+1)!!}{k_T^l} \int d\mathbf{r}' G_0(\mathbf{r},\mathbf{r}') \times \left\{ Y_{lm}(\hat{\mathbf{s}}) \frac{\delta(s)}{s^{l+2}} \left(T \frac{I}{I+ik_T T} A \right)_{lm} \right\}_{\mathbf{s}=\mathbf{r}'-\mathbf{r}_T}. \quad (6)$$

The pseudopotential reduces this integral equation to a set of coupled linear algebraic equations by expressing the scattered field in terms of the A_{lm}. The full Green function is expressed in terms of the A_{lm} as follows:

$$G(\mathbf{r},\mathbf{r}_0) = G_0(\mathbf{r},\mathbf{r}_0) - \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{(2l+1)!!}{k_T^l} \left(T \frac{I}{I+ik_T T} A \right)_{lm} \times \left\{ \lim_{t\to 0} \left[\frac{1}{t^l} \int d\hat{\mathbf{t}} Y_{lm}(\hat{\mathbf{t}}) G_0(\mathbf{r},\mathbf{r}_T + \mathbf{t}) \right] \right\}. \quad (7)$$

The linear algebraic equations for the scattering coefficients A_{lm} are obtained by inserting the expression for $G(\mathbf{r},\mathbf{r}_0)$ from Eq. (7) into Eq. (5).

In order to obtain explicit expressions for these scattering equations one must compute the following quantities:

$$G_{lm}^{inc}(\mathbf{r}_T,\mathbf{r}_0) = \frac{(2l+1)!!}{k_T^l (2l+1)!} \times \left\{ \lim_{s\to 0} \partial_s^{2l+1} \left[s^{l+1} \int d\hat{\mathbf{s}} Y_{lm}(\hat{\mathbf{s}})^* G_0(\mathbf{r}_T + \mathbf{s},\mathbf{r}_0) \right] \right\}, \quad (8)$$

$$G_{lm}^{out}(\mathbf{r},\mathbf{r}_T) = \frac{(2l+1)!!}{k_T^l} \left\{ \lim_{t\to 0} \left[\frac{1}{t^l} \int d\hat{\mathbf{t}} Y_{lm}(\hat{\mathbf{t}}) G_0(\mathbf{r},\mathbf{r}_T + \mathbf{t}) \right] \right\}, \quad (9)$$

$$K_{lm,l'm'}(\mathbf{r}_T) = \frac{(2l+1)!!}{k_T^l(2l+1)!}\frac{(2l'+1)!!}{k_T^{l'}}\lim_{s\to 0}\partial_s^{2l+1}\left(s^{l+1}\int d\hat{\mathbf{s}}Y_{lm}(\hat{\mathbf{s}})^*\left\{\lim_{t\to 0}\left[\frac{1}{t^{l'}}\int d\hat{\mathbf{t}}Y_{l'm'}(\hat{\mathbf{t}})G_0^{NS}(\mathbf{r}_T+\mathbf{s},\mathbf{r}_T+\mathbf{t})\right]\right\}\right). \tag{10}$$

The quantity $G_{lm}^{inc}(\mathbf{r}_T,\mathbf{r}_0)$, defined in Eq. (8), is the appropriate multipole decomposition of the incident field on the scatterer located at $\mathbf{r}_T$ due to a point source positioned at $\mathbf{r}_0$. The $G_{lm}^{out}(\mathbf{r},\mathbf{r}_T)$ are the appropriate partial wave components of the scattered field observed at point $\mathbf{r}$. The quantity $K_{lm,l'm'}(\mathbf{r}_T)$ is a matrix coupling the partial waves. This matrix originates from the inhomogeneities of the embedding medium and carries information about multiple scattering processes in the medium between the scatterer and boundaries and other inhomogeneities [such as position dependence of the wave number in Eq. (2)].

One should also notice that the singular part of $G_0(\mathbf{r},\mathbf{r}_0)$, namely $g_T(\mathbf{r}-\mathbf{r}_0)$, the Green function of the Helmholtz equation in an unbounded and uniform medium, yields the following result [2]:

$$\lim_{s\to 0}\partial_s^{2l+1}\left\{s^{l+1}\int d\hat{\mathbf{s}}Y_{lm}(\hat{\mathbf{s}})^*\lim_{t\to 0}\left[\frac{1}{t^{l'}}\int d\hat{\mathbf{t}}Y_{l'm'}(\hat{\mathbf{t}})g_T(\mathbf{r}_T+\mathbf{s}-\mathbf{r}_T-\mathbf{t})\right]\right\} = \frac{k_T^{2l+1}(2l+1)!}{\mathrm{i}[(2l+1)!!]^2}\delta_{ll'}\delta_{mm'}. \tag{11}$$

The above equation is obtained by using the well-known partial wave expansion of the free space Green function.

In terms of a new set of scattering coefficients, namely,

$$a_{lm} = [(I+ik_TT)^{-1}A]_{lm}, \tag{12}$$

the following equations for the scattering coefficients are obtained [2]:

$$a_{lm} = G_{lm}^{inc} - \sum_{l'm'}\sum_{l''m''}K_{lm,l'm'}(\mathbf{r}_T)T_{l'm',l''m''}a_{l''m''}. \tag{13}$$

The expression for the Green function can now be written as

$$G(\mathbf{r},\mathbf{r}_0) = G_0(\mathbf{r},\mathbf{r}_0) - \sum_{lm}\sum_{l'm'}G_{lm}^{out}(\mathbf{r},\mathbf{r}_T)T_{lm,l'm'}a_{l'm'}. \tag{14}$$

The resulting equation for the scattering coefficients a_{lm}, Eq. (13), show that, in the presence of boundaries and/or a heterogeneous medium, there is a coupling among the scattered partial waves. One should also notice that the only quantity related to the scatterer that appears in the coupling matrix, Eq. (10), is its position. This indicates that no matter what the nature of the scatterer is, the coupling matrix given by Eq. (10) determines the coupling amongst the scattered partial waves induced by the inhomogeneities of the medium.

The limits in Eqs. (8)–(10) can be explicitly computed in terms of partial derivatives of the Green functions that appear in the right-hand side of those equations. This is so because none of those Green functions is being evaluated at a singular point since the physics of scattering requires that $\mathbf{r}\neq\mathbf{r}_0$ and $\mathbf{r}\neq\mathbf{r}_T$ and $G_0^{NS}(\mathbf{r},\mathbf{r}')$ is nonsingular by definition. At this point it is convenient to define the following operator:

$$D_{lm}(\boldsymbol{\nabla}) = \frac{(2l+1)!!}{k_T^l}\frac{1}{l!}\int d\hat{\mathbf{s}}\,Y_{lm}(\hat{\mathbf{s}})^*(\hat{\mathbf{s}}\cdot\boldsymbol{\nabla})^l. \tag{15}$$

This operator is simply a polynomial of degree l in the partial derivative operators ∂_x, ∂_y, and ∂_z. In fact one can show that for $m\geqslant 0$

$$\begin{aligned} D_{lm}(\boldsymbol{\nabla}) &= \frac{4\pi i^l}{k_T^l}p^lY_{lm}(\hat{\mathbf{p}})^* \\ &= \frac{4\pi i^l}{k_T^l}\frac{(-1)^m}{2^l l!}N_{lm}(p_x-ip_y)^m\partial_u^{l+m}(u^2-p^2)^l\Big|_{u=p_z}, \end{aligned} \tag{16}$$

where $\mathbf{p}=-i\boldsymbol{\nabla}$, $p^2=-\nabla^2$ and N_{lm} is the normalization factor for the spherical harmonics. For $m<0$ one uses $Y_{l,-|m|}(\hat{\mathbf{q}})^*=(-1)^{|m|}Y_{l|m|}(\hat{\mathbf{q}})$ and an expression analogous to the one in Eq. (16) is obtained. It is straightforward, albeit tedious, to show that the quantities defined in Eqs. (8) and (9) can be reduced to

$$G_{lm}^{inc}(\mathbf{r}_T,\mathbf{r}_0) = D_{lm}(\boldsymbol{\nabla})G_0(\mathbf{r},\mathbf{r}_0)|_{\mathbf{r}=\mathbf{r}_T} \quad \text{for } \mathbf{r}_0\neq\mathbf{r}_T, \tag{17}$$

$$G_{lm}^{out}(\mathbf{r},\mathbf{r}_T) = D_{lm}^*(\boldsymbol{\nabla}')G_0(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_T} \quad \text{for } \mathbf{r}\neq\mathbf{r}_T, \tag{18}$$

and the coupling matrix defined in Eq. (10) is equivalent to

$$K_{lm,l'm'}(\mathbf{r}_T) = D_{lm}(\boldsymbol{\nabla})D_{l'm'}^*(\boldsymbol{\nabla}')G_0^{NS}(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'=\mathbf{r}_T}. \tag{19}$$

The equation for the Green function including scattering by an object at $\mathbf{r}=\mathbf{r}_T$ can now be written as

$$\begin{aligned} G(\mathbf{r},\mathbf{r}_0) = G_0(\mathbf{r},\mathbf{r}_0) - \sum_{lm}\sum_{l'm'}D_{lm}^*(\boldsymbol{\nabla}') \\ G_0(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_T}\mathbf{T}_{lm,l'm'}(\mathbf{r}_T)D_{l'm'}(\boldsymbol{\nabla}'') \\ G_0(\mathbf{r}'',\mathbf{r}_0)|_{\mathbf{r}''=\mathbf{r}_T}, \end{aligned} \tag{20}$$

where the effective scattering operator, $\mathbf{T}$, is given by

$$\begin{aligned} \mathbf{T}(\mathbf{r}_T) = T(k_T) - \mathbf{T}(\mathbf{r}_T)K(\mathbf{r}_T)T(k_T), \text{ or } \mathbf{T}(\mathbf{r}_T) \\ = T(k_T)[I+K(\mathbf{r}_T)T(k_T)]^{-1}. \end{aligned} \tag{21}$$

In the case of a layered medium this result, apart from differences in notation, is similar to that obtained by Sammelmann and Hackman [9]. The scattering term in Eq. (20) can be interpreted as stating that a multipole decomposition of the incident field, $G_{lm}^{inc}(\mathbf{r}_T,\mathbf{r}_0)$ in Eq. (17), is scattered into a similar multipole decomposition of the outgoing scattered field, $G_{lm}^{out}(\mathbf{r},\mathbf{r}_T)$ in Eq. (18).

As an example to illustrate the structure of the above equations let us consider the case where the wavelength of the incident field on the object is much larger than a typical dimension of the object. In this case it is reasonable to consider the object as an isotropic scatterer where only the terms with $l=0$ contribute to the scattered field. One obtains in this case the following expression for the Green function including the scattered field:

$$G(\mathbf{r},\mathbf{r}_0) = G_0(\mathbf{r},\mathbf{r}_0) - \frac{4\pi f}{1+4\pi f G_0^{NS}(\mathbf{r}_T,\mathbf{r}_T)} G_0(\mathbf{r},\mathbf{r}_T) G_0(\mathbf{r}_T,\mathbf{r}_0), \tag{22}$$

where $f=T(k_T)_{00,00}$ is the isotropic scattering amplitude. Thus one sees that in the inhomogeneous medium the effective scattering amplitude is

$$f_{eff} = \frac{f}{1+4\pi f G_0^{NS}(\mathbf{r}_T,\mathbf{r}_T)}. \tag{23}$$

This is similar to a result obtained by Kunze and Lenk in a study of the effect of boundaries on scattering in a quantum wire [10]. It also similar to a result obtained by Ye and Feuillade for acoustic scattering by bubbles near surfaces [11]. The most obvious consequence of Eq. (23) is that the effective scattering amplitude varies with the position of the scattering object. The closer the object is to a boundary or interface the stronger this variation will be. Another consequence is that even if the scattering amplitude in the extended and uniform medium is not resonant it is possible for the effective scattering amplitude to be resonant. If f is resonant then the resonant frequency will be shifted in f_{eff}. For example, the implications of this resonance shift for bubbles near a pressure release surface are discussed in the above mentioned Ref. [11].

III. THE GENERALIZED OPTICAL THEOREM

An important relation satisfied by the effective scattering operator defined in Eq. (21) can be obtained by examining the energy flux across a surface that encloses the scattering object. Let us consider the case of a non-energy-absorbing medium and an object that also does not absorb energy. Then the total energy flux across a closed surface that surrounds the scattering object but excludes the point source is zero since all the incident energy eventually leaves the volume enclosed by the surface. Part of this energy is carried by the incident field and part of it is in the scattered field but none is dissipated into heat or other forms of energy. The total energy flux across the closed surface is

$$F_T = \frac{1}{2i\omega} \oint d\mathbf{S} \cdot [G(\mathbf{r},\mathbf{r}_0)^* \,\boldsymbol{\nabla}\, G(\mathbf{r},\mathbf{r}_0) - G(\mathbf{r},\mathbf{r}_0)\,\boldsymbol{\nabla}\, G(\mathbf{r},\mathbf{r}_0)^*]. \tag{24}$$

The divergence theorem then yields

$$F_T = \frac{1}{2i\omega} \int dV_S [G(\mathbf{r},\mathbf{r}_0)^* \nabla^2 G(\mathbf{r},\mathbf{r}_0) - G(\mathbf{r},\mathbf{r}_0) \nabla^2 G(\mathbf{r},\mathbf{r}_0)^*]. \tag{25}$$

Now, from Eqs. (2) and (20)

$$\nabla^2 G(\mathbf{r},\mathbf{r}_0) = -k(\mathbf{r})^2 G(\mathbf{r},\mathbf{r}_0) + \delta(\mathbf{r}-\mathbf{r}_0) - H(\boldsymbol{\nabla}')\,\delta(\mathbf{r}-\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}_T}, \tag{26}$$

where

$$H(\boldsymbol{\nabla}') = \sum_{lm} \left\lfloor \sum_{l'm'} \mathbf{T}_{lm,l'm'}(\mathbf{r}_T) D_{l'm'}(\boldsymbol{\nabla}'') \, G_0(\mathbf{r}'',\mathbf{r}_0)\big|_{\mathbf{r}''=\mathbf{r}_T} \right\rfloor D^*_{lm}(\boldsymbol{\nabla}'). \tag{27}$$

Thus one obtains

$$F_T = \frac{1}{2i\omega} [H(\boldsymbol{\nabla}')^* G(\mathbf{r}',\mathbf{r}_0) - H(\boldsymbol{\nabla}') G(\mathbf{r}',\mathbf{r}_0)^*]_{\mathbf{r}'=\mathbf{r}_T}. \tag{28}$$

Notice that, according to Eq. (23), $G(\mathbf{r},\mathbf{r}_0)=G_0(\mathbf{r},\mathbf{r}_0) - H(\boldsymbol{\nabla}')G_0(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}_T}$; thus

$$F_T = \frac{1}{2i\omega} \{H(\boldsymbol{\nabla}')^* G_0(\mathbf{r}',\mathbf{r}_0) - H(\boldsymbol{\nabla}') G_0(\mathbf{r}',\mathbf{r}_0)^* + H(\boldsymbol{\nabla}')H(\boldsymbol{\nabla}'')^*[G_0(\mathbf{r}',\mathbf{r}'')^* - G_0(\mathbf{r}'',\mathbf{r}')]\}_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}_T}. \tag{29}$$

The expression involving two H operators can be evaluated by using Eq. (3), the expansion of g_T in spherical harmonics and the definition of the K operator in Eq. (19). If one considers $G^{inc}_{lm}(\mathbf{r}_T,\mathbf{r}_0)$, defined in Eq. (21), as components (labeled by the partial wave indexes lm) of a vector G_{inc}, then the total energy flux can be written as

$$F_T = \frac{1}{2i\omega} G_{inc}{}^{\dagger} [\mathbf{T}^{\dagger} - \mathbf{T} + 2ik_T \mathbf{T}^{\dagger}\mathbf{T} + \mathbf{T}^{\dagger}(K^{\dagger} - K)\mathbf{T}] G_{inc}. \tag{30}$$

In Eq. (30) $\mathbf{T}^{\dagger}$ is the Hermitian conjugate of $\mathbf{T}$, that is $(\mathbf{T}^{\dagger})_{lm,l'm'} = (\mathbf{T}_{l'm',lm})^*$. Since G_{inc} is arbitrary (the source position is arbitrary) in order for the total flux to be equal to zero the expression between square brackets in the right-hand side of Eq. (30) must also be equal to zero. Thus the generalized optical theorem for the effective scattering operator can be stated as the following relationship between the components of $\mathbf{T}$:

$$2ik_T \mathbf{T}^{\dagger}\mathbf{T} = \mathbf{T} - \mathbf{T}^{\dagger} + \mathbf{T}^{\dagger}(K - K^{\dagger})\mathbf{T}. \tag{31}$$

In a similar way it can be shown that for a non-energy-absorbing scattering object the scattering operator T obeys a similar generalized optical theorem [8]:

$$2ik_T T^{\dagger} T = T - T^{\dagger}. \tag{32}$$

The generalized optical theorem formulated in terms of the scattering amplitudes for classical waves in the case of a scatterer embedded in an extend homogeneous medium is discussed in detail in Ref. [12], the excellent and exhaustive treatise on optics by Born and Wolf. The generalized optical theorem, Eq. (32), for a nonabsorbing scatterer can also be interpreted as implying the unitarity of the S matrix. For the scalar wave problem discussed in this work and using the definition of the T matrix in Eq. (1), the S matrix has a simple relationship to the T matrix, namely $S=I+2ik_T T$. From Eq. (32) and its Hermitian conjugate it follows that $S^\dagger S = SS^\dagger = I$, that is, the S matrix is unitary. A good discussion of the S matrix in classical wave scattering and its relationship to the T matrix can be found in Ref. [13].

Comparing Eqs. (31) and (32) one sees that the formal difference between them is related to the operator K that accounts for multiple interactions between the scattering object and the boundaries, interfaces and inhomogeneities of the medium where the scatterer is embedded. Thus it is clear that if one were to define an effective S matrix for scattering in the bounded and/or inhomogeneous medium, with the same relationship to the effective T-matrix $\mathbf{T}$ as the relationship between the usual S matrix and T, this effective S matrix would not be unitary due to the term on Eq. (31) that depends on the coupling matrix K. The multiple bounces between the object and a boundary are simple and intuitive to visualize but a position dependence of the wave phase speed will have similar effects. For example, suppose the object is in a region like a sound channel in the ocean for example, corresponding to a minimum of the sound speed as a function of depth. Some of the energy scattered off the object will be redirected towards the object by refraction and rescattered by the object, cumulative repetition of this process leads to the presence of the operator K in the expression for the effective scattering operator. The explicit presence of K in Eq. (31) indicates that those multiple scattering processes trap a fraction of the energy incident on the object. If the object is assumed to be in a homogeneous layer then the quantitative importance of K depends on the ratio between a typical dimension of the object and its distance from the layer boundaries, the greater this ratio the larger the impact of the multiple scattering processes that K incorporates. This is related to the phenomena of trapped modes and complex resonances in waveguides containing a scattering obstacle; see Ref. [14] for details and further references on this matter.

Assuming Eq. (32) to be true one can prove that Eq. (31) is also true by simply using Eq. (21) to write T in terms of $\mathbf{T}$ in Eq. (32). In particular, if one expresses $\mathbf{T}$ in terms of T then Eq. (30) can be written as

$$F_T = \frac{1}{2i\omega}\left(\frac{I}{I+KT}G_{inc}\right)^\dagger [2ik_T T^\dagger T + T^\dagger - T]\left(\frac{I}{I+KT}G_{inc}\right). \tag{33}$$

Obviously when Eq. (32) is satisfied Eq. (33) yields zero total flux which is correct since the source was assumed to be outside the volume bounded by the closed surface through which the total flux was computed. If the scattering object were energy absorbing then the right-hand side of Eq. (33) would be the negative of the power absorbed by the object since in this case Eq. (32) does not hold [8,12]. The discussion in Sec. 13.3 of Ref. [12] of the case of an absorbing scatterer is particularly relevant here as it is formulated in terms of classical scalar waves.

Now let us introduce the quantities $\Phi_{inc}(\mathbf{r}) = G_0(\mathbf{r},\mathbf{r}_0)$ and $\Phi_{sct}(\mathbf{r}) = -H(\boldsymbol{\nabla}')G_0(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_T}$, where $\Phi_{inc}(\mathbf{r})$ is the incident field, $\Phi_{sct}(\mathbf{r})$ is the scattered field, and the total field is $\Phi_T(\mathbf{r}) = \Phi_{inc}(\mathbf{r}) + \Phi_{sct}(\mathbf{r})$. The velocity vectors associated with those fields are defined as $\mathbf{V}_\alpha = [1/i\omega\rho(\mathbf{r})]\boldsymbol{\nabla}\Phi_\alpha(\mathbf{r})$. The total flux can be written as [6] $F_T = \mathrm{Re}\{\oint d\mathbf{S}\cdot\mathbf{V}_T^*\Phi_T\} = F_{inc} - E + W_{sct}$. The incident flux, F_{inc}, is zero since the source is outside the volume delimited by the closed surface, W_{sct} is the scattered energy flux involving only $\Phi_{sct}(\mathbf{r})$ and E is the extinction term that involves the negative of the contribution to the total flux due to the interference of the incident and scattered fields:

$$W_{sct} = \mathrm{Re}\left\{\oint d\mathbf{S}\cdot\mathbf{V}_{sct}^\star\Phi_{sct}\right\},$$

$$E = -\mathrm{Re}\left\{\oint d\mathbf{S}\cdot[\mathbf{V}_{sct}^\star\Phi_{inc} + \mathbf{V}_{inc}^\star\Phi_{sct}]\right\}. \tag{34}$$

Procedures similar to the ones that lead to Eq. (30) yield

$$W_{sct} = \frac{1}{2i\omega}G_{inc}{}^\dagger[2ik_T\mathbf{T}^\dagger\mathbf{T} + \mathbf{T}^\dagger(K^\dagger - K)\mathbf{T}]G_{inc},$$

$$E = \frac{1}{2i\omega}G_{inc}{}^\dagger[\mathbf{T} - \mathbf{T}^\dagger]G_{inc}. \tag{35}$$

Thus the generalized optical theorem states that, in the absence of energy absorption by the object and the medium, the scattered power is equal to the power subtracted from the incident field by its interference with the scattered field. As pointed out above, in the case of an energy-absorbing object equations such as (30) and (35) still hold but (31) does not as Eq. (32) is no longer true since a term due to energy-absorption by the scattering object is missing [12]. In this case the expression for the power extinguished from the incident field is still given by the corresponding equation in Eq. (35). In the case of an energy-absorbing medium the procedures that yielded Eqs. (30) and (35) generate extra terms that have to do with the power absorbed by the medium in the volume enclosed by the closed surface across which the fluxes were computed. It is clear that it is not empirically possible to separate extinction effects due to scattering and absorption by the scattering object from the effects of energy absorption in the medium when both processes are present.

IV. SUMMARY AND DISCUSSION

In this article the theory of scattering of scalar waves by an object in a bounded/inhomogeneous medium such as a layered waveguide was formulated in such a way as to use as inputs the scattering amplitude computed in an unbounded, homogeneous medium. In the case of a layered medium the scattering formulation presented here is similar to that developed by Sammelmann and Hackman [9].

The scattering problem is formulated entirely and explicitly in terms of the bounded and/or inhomogeneous medium's Green functions. This approach is thus very flexible in regards to the choice of incident field. In the case of waveguides the connection between propagation and scattering is explicit. In particular the Green function approach avoids the need to discuss propagating and evanescent waves separately, in this context compare with the discussion of the optical theorem for incident fields containing evanescent waves in Ref. [15]. The use of the T matrix, Eq. (1), and the wave equation with pseudopotentials for the Green function avoids having to discuss the analytic extensions of the scattering amplitudes for imaginary angles as done in Ref. [15].

This new scattering formulation allowed for the derivation of the generalized optical theorem which provides significant insights in the physics of scattering in a bounded and/or inhomogeneous medium. It was shown that the boundary interactions alter the balance between scattered and incident energy in comparison with scattering in an unbounded medium and its relation to the phenomena of trapped modes and complex resonances in waveguides [14] was postulated. The circumstances where one expects the greatest impact of those interactions on observable quantities were discussed.

The scattering formulation presented in this work is applicable only to scalar waves. It is possible to generalize the pseudopotential approach to the case of vector waves. This would be necessary to discuss elastic and electromagnetic waves for example. The generalized optical theorem for electromagnetic fields, including the case of a scatterer contained in a dielectric half-space, was obtained in a recent publication [16] by some of the authors of Ref. [7]; it would be very interesting to extend this result to more general inhomogeneous media.

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