7 December 1998

PHYSICS LETTERS A

Physics Letters A 249 (1998) 243–247

Remarks on boundary conditions for scalar scattering

T.D. Visser [1], P.S. Carney, E. Wolf

Department of Physics and Astronomy and Rochester Theory Center for Optical Science and Engineering, University of Rochester, Rochester, NY 14627, USA

Received 6 August 1998; accepted for publication 8 September 1998
Communicated by P.R. Holland

Abstract

The question is discussed whether potential scattering problems can be treated as boundary value problems associated with differential equations, as is sometimes suggested in the literature. We show that, except in some very special cases, this is not possible. The values of the wave function and its normal derivative on the boundary of a finite-range potential cannot be prescribed arbitrarily but are implicit in the integral equation of potential scattering. We derive two coupled singular integral equations for the boundary values for the case when the scattering potential is homogeneous. © 1998 Published by Elsevier Science B.V.

PACS: 03.65.Nk; 03.80.+r; 41.20.Cv; 42.25.Fx
Keywords: Potential scattering; Nonrelativistic scattering; Boundary values in scattering; Surface integral equations in scattering

1. Introduction

Potential scattering problems, whether in quantum mechanics, optics, acoustics or in other fields are generally treated by means of integral equations. For relatively simple situations, such as for scattering of a plane wave by a homogeneous sphere, alternative methods are available, e.g. expanding the solution formally both inside and outside the scatterer in terms of modes and determining the coefficients of the modes by matching the two expansions at the boundary, making use of the (assumed) continuity of the wave function and of its normal derivative.

In contrast to these well-known standard approaches, several problems have been treated in the literature as true boundary value problems of differential equations. Such problems are basically limited to scattering by a hard sphere and a soft sphere in acoustics. The hard sphere can be regarded as the limiting case of an infinitely strong scattering potential. For the soft sphere, however, it is not clear whether there exists an equivalent scattering potential. Perhaps because of the success of the boundary value approach in these two special cases, the impression has been given in the literature that more general scattering problems can also be treated in this way [1,2]. However, it is well known that the values of the wavefunction on the boundary of a finite-range potential are implicitly contained in the integral equation of potential scattering and they cannot, therefore, be specified a priori.

In this Letter we show that for the case of scattering from a homogeneous finite-range potential, the values of the wavefunction and of its normal derivative on

[1] On leave from Department of Physics and Astronomy, Free University, Amsterdam, The Netherlands.

0375-9601/98/$ – see front matter © 1998 Published by Elsevier Science B.V. All rights reserved.
PII S0375-9601(98)00705-1

the boundary of the scatterer satisfy a coupled pair of singular integral equations, indicating more explicitly than is apparent from the integral equation that the boundary values cannot be prescribed arbitrarily.

2. Potential scattering of scalar waves

Let us consider a monochromatic plane wave of unit amplitude and frequency ω, propagating in the direction specified by a unit vector $\boldsymbol{s}_0$,

$$V^{(i)}(\boldsymbol{r},t) = U^{(i)}(\boldsymbol{r})\exp(-\mathrm{i}\omega t), \tag{2.1}$$

$$U^{(i)}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}k\boldsymbol{s}_0\cdot\boldsymbol{r}}, \tag{2.2}$$

incident on a scattering medium occupying a volume V, bounded by a closed surface S in free space (see Fig. 1). In Eq. (2.2) $k = \omega/c = 2\pi/\lambda_0$ is the wavenumber, c being the speed of light in vacuum and λ_0 the vacuum wavelength. We assume that the macroscopic physical properties of the scatterer are independent of time. We denote by $n(\boldsymbol{r})$ the refractive index of the medium at frequency ω. In general it is a function of position, specified by the position vector $\boldsymbol{r}$. The total field (i.e. the sum of the incident and the scattered field) generated by the interaction of the incident field with the scatterer satisfies the basic equation of potential theory [3,4]

$$(\nabla^2 + k^2)U(\boldsymbol{r}) = -4\pi F(\boldsymbol{r})U(\boldsymbol{r}), \tag{2.3}$$

where

$$F(\boldsymbol{r}) \equiv \frac{k^2}{4\pi}[n^2(\boldsymbol{r}) - 1] \tag{2.4}$$

is the so-called scattering potential. The solution of Eq. (2.3) for the total field must behave far away from the scatterer as the sum of the incident plane wave and an outgoing spherical wave, i.e. it must have the asymptotic behavior

$$U(r\boldsymbol{s}) \sim \mathrm{e}^{\mathrm{i}k\boldsymbol{s}_0\cdot\boldsymbol{r}} + f(\boldsymbol{s},\boldsymbol{s}_0)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \tag{2.5}$$

as $kr \to \infty$, with the direction of scattering, characterized by the unit vector $\boldsymbol{s}$, kept fixed, f being the scattering amplitude.

The solution of Eq. (2.3), subject to the usual assumption that $U(\boldsymbol{r})$ and its normal derivative $\partial U/\partial n \equiv \boldsymbol{n}\cdot\boldsymbol{\nabla}U$ at the boundary S of the scattering volume are continuous and subject to the asymptotic condition (2.5) represents the total field $U(\boldsymbol{r})$ generated by scattering. (A generalization of the theory which takes into account possible discontinuities at the boundaries has recently been discussed in Ref. [5]. It indicates that under certain circumstances such discontinuities can have significant effects on the far field.)

As is well known, Eq. (2.3) subject to the continuity conditions, may be recast into the integral equation [4,6]

$$U(\boldsymbol{r}) = U^{(i)}(\boldsymbol{r}) + \int_V F(\boldsymbol{r}')U(\boldsymbol{r}')\frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}', \tag{2.6}$$

where

$$G(\boldsymbol{r}-\boldsymbol{r}') = \frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{2.7}$$

is the outgoing free space Green's function of the Helmholtz operator $\mathcal{L} \equiv \nabla^2 + k^2$.

There is a different class of scattering problems which is sometimes discussed in the literature (see, for example, Ref. [1]). For such problems one *prescribes* boundary conditions on the surface S of the scatterer and one seeks a solution which behaves as an outgoing spherical wave at infinity. Problems of this kind are treated most frequently for a "hard" and a "soft" sphere [7]. In the former case one imposes the Dirichlet boundary condition $U(\boldsymbol{r}) = 0$ on S; in the latter case one imposes the Neumann boundary condition $\partial U(\boldsymbol{r})/\partial n = 0$ on S [8]. It is sometimes suggested that many more problems of scattering from a bounded medium may also be treated as boundary value problems [2,7]. However, the physical significance and

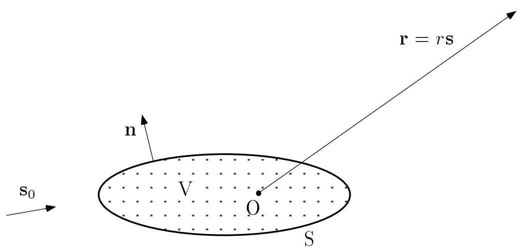

Fig. 1. A plane wave, propagating along the direction of the unit vector $\boldsymbol{s}_0$, is incident on a scattering volume V. The volume is bounded by a closed surface S, with outward unit normal $\boldsymbol{n}$. The direction of scattering is denoted by $\boldsymbol{s}$.

even the possibility of such an approach is obscure at best.

The solutions to the potential scattering problem and to a boundary value problem have certain features in common such as the asymptotic behavior expressed by relation (2.5) and results such as certain reciprocity theorems and the optical cross-section theorem. However, the boundary value formulation does not explicitly take into account the nature of the medium, characterized by the scattering potential. Although, in principle, boundary values are, of course, associated with any potential scattering problem, knowledge of them can only be obtained by solving them first by other methods, e.g. by the use of the integral equation of potential scattering or by solving a pair of singular integral equations for the boundary values and their normal derivatives as we will now show.

3. Boundary values for the field and its normal derivative

In this section we derive integral equations for the values of the field and its normal derivative on the boundary of the scatterer. Our starting point is the scalar version of the so-called Ewald–Oseen extinction theorem (see, for instance, Refs. [9,10]).

We consider a homogeneous scattering volume V with constant refractive index n. The scalar version of the extinction theorem is expressed by the formula (see Ref. [11] or Eq. (A.4) of Appendix A of this Letter)

$$U^{(i)}(\boldsymbol{r}_<) = -\frac{1}{4\pi}\int_S \left(U(\boldsymbol{r}')\frac{\partial G(\boldsymbol{r}_< - \boldsymbol{r}')}{\partial n'} - G(\boldsymbol{r}_< - \boldsymbol{r}')\frac{\partial U(\boldsymbol{r}')}{\partial n'}\right) \mathrm{d}S. \tag{3.1}$$

Here $\boldsymbol{r}_<$ is any point inside the scatterer, and G is the outgoing free space Green's function, given by Eq (2.7). As the point $\boldsymbol{r}_<$ approaches the boundary S, with $\boldsymbol{r}_s$ denoting a point on the surface S, the first term of the integrand of Eq. (3.1) becomes singular when $\boldsymbol{r}' = \boldsymbol{r}_s$. A similar expression occurs also in potential theory. The result is [12,13]

$$U^{(i)}(\boldsymbol{r}_s) = \tfrac{1}{2}U(\boldsymbol{r}_s) - \frac{1}{4\pi}\mathrm{P}\int_S \left(U(\boldsymbol{r}')\frac{\partial G(\boldsymbol{r}_s - \boldsymbol{r}')}{\partial n'} - G(\boldsymbol{r}_s - \boldsymbol{r}')\frac{\partial U(\boldsymbol{r}')}{\partial n'}\right) \mathrm{d}S, \tag{3.2}$$

where P denotes the Cauchy principal value taken at $\boldsymbol{r}' = \boldsymbol{r}_s$.

The field inside the scatterer satisfies the equation

$$(\nabla^2 + k_1^2)U(\boldsymbol{r}) = 0, \tag{3.3}$$

where $k_1 = 2\pi n/\lambda_0$ (with λ_0 denoting the wavelength in vacuo) is the wave number of the field inside the scatterer. Let G_1 be a Green's function of the operator $\mathcal{L}_1 \equiv \nabla^2 + k_1^2$. It satisfies the differential equation

$$(\nabla^2 + k_1^2)G_1(\boldsymbol{r} - \boldsymbol{r}') = -4\pi\delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}'). \tag{3.4}$$

By a trivial generalization of the Helmholtz–Kirchhoff integral theorem for free space (see Section 8.3 of Ref. [4]) to a homogeneous material medium we obtain the formula

$$U(\boldsymbol{r}_<) = -\frac{1}{4\pi}\int_S \left(U(\boldsymbol{r}')\frac{\partial G_1(\boldsymbol{r}_< - \boldsymbol{r}')}{\partial n'} - G_1(\boldsymbol{r}_< - \boldsymbol{r}')\frac{\partial U(\boldsymbol{r}')}{\partial n'}\right) \mathrm{d}S. \tag{3.5}$$

As the point $\boldsymbol{r}_<$ approaches the boundary surface S, one obtains in a similar manner as in connection with Eq. (3.2)

$$U(\boldsymbol{r}_s) = \tfrac{1}{2}U(\boldsymbol{r}_s) - \frac{1}{4\pi}\mathrm{P}\int_S \left(U(\boldsymbol{r}')\frac{\partial G_1(\boldsymbol{r}_s - \boldsymbol{r}')}{\partial n'} - G_1(\boldsymbol{r}_s - \boldsymbol{r}')\frac{\partial U(\boldsymbol{r}')}{\partial n'}\right) \mathrm{d}S. \tag{3.6}$$

Eqs. (3.2) and (3.6) are two coupled singular integral equations for the field U and its normal derivative $\partial U/\partial n$ on the boundary of the scatterer. We note that these equations imply, if we recall that the scattered field $U^{(s)} = U - U^{(i)}$, that at any point $\boldsymbol{r}_s$ on the boundary of the scatterer,

$$U^{(s)}(\boldsymbol{r}_s) = \frac{1}{4\pi}\mathrm{P}\int_S \left(U(\boldsymbol{r}')\frac{\partial \mathcal{G}(\boldsymbol{r}_s - \boldsymbol{r}')}{\partial n'} - \mathcal{G}(\boldsymbol{r}_s - \boldsymbol{r}')\frac{\partial U(\boldsymbol{r}')}{\partial n'}\right) \mathrm{d}S, \tag{3.7}$$

where

$$\mathcal{G}(\boldsymbol{r}-\boldsymbol{r}') = G(\boldsymbol{r}-\boldsymbol{r}') - G_1(\boldsymbol{r}-\boldsymbol{r}'). \tag{3.8}$$

This is a necessary condition which the scattered field on the boundary must satisfy.

From Eq. (3.6) or (3.7) it is seen that neither the field nor its normal derivative can be prescribed arbitrarily at the boundary of the scatterer.

Finally, we mention that a pair of singular integral equations for the value of an electromagnetic field and of its normal derivative at the boundary, rather than for a scalar field, was derived by Pattanayak [14].

4. Conclusions

We have shown that, contrary to suggestions often made in the literature, potential scattering problems involving finite-range potentials cannot be formulated as boundary value problems of differential equations, except in some very special cases. In fact, to determine the boundary values which the field and its normal derivative take on the boundary of the scatterer, one must first solve the scattering problem by other methods (e.g. by using the integral equation of potential scattering) which yields the boundary values as a byproduct. We have derived a coupled pair of singular integral equations (Eqs. (3.2) and (3.6)) which the field and its normal derivative must satisfy on the boundary of a homogeneous scatterer.

Acknowledgement

This research was supported by the National Science Foundation and the New York State Foundation for Science and Technology.

Appendix A. The extinction theorem for scalar fields

In this appendix we present a simple derivation of the scalar version of the extinction theorem in the form originally derived by Pattanayak and Wolf [11]. We recall Eq. (2.3),

$$(\nabla^2 + k^2)U(\boldsymbol{r}) = -4\pi F(\boldsymbol{r})U(\boldsymbol{r}), \tag{A.1}$$

and the fact that the outgoing free-space Green's function G satisfies the equation

$$(\nabla^2 + k^2)G(\boldsymbol{r}-\boldsymbol{r}') = -4\pi\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}'). \tag{A.2}$$

We interchange the role of $\boldsymbol{r}$ and $\boldsymbol{r}'$, multiply Eq. (A.1) by G, Eq. (A.2) by U, subtract the resulting equations, integrate over the scattering volume V and use Green's theorem. We then find that if the point $\boldsymbol{r}$ is within the scattering volume (in which case we again write $\boldsymbol{r}_<$ rather than $\boldsymbol{r}$)

$$\int_S \left(U(\boldsymbol{r}') \frac{\partial G(\boldsymbol{r}_< - \boldsymbol{r}')}{\partial n'} - G(\boldsymbol{r}_< - \boldsymbol{r}') \frac{\partial U(\boldsymbol{r}')}{\partial n'} \right) \mathrm{d}S = -4\pi U(\boldsymbol{r}_<) + 4\pi \int_V F(\boldsymbol{r}')U(\boldsymbol{r}') \frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}_< - \boldsymbol{r}'|}}{|\boldsymbol{r}_< - \boldsymbol{r}'|} \mathrm{d}^3\boldsymbol{r}'. \tag{A.3}$$

The volume integral on the right of Eq. (A.3) represents $U^{(s)}(\boldsymbol{r}_<) = U(\boldsymbol{r}_<) - U^{(i)}(\boldsymbol{r}_<)$, where $U^{(s)}(\boldsymbol{r}_<)$ is the scattered field (cf. Eq. (2.6)). Hence Eq. (A.3) may be expressed in the form

$$U^{(i)}(\boldsymbol{r}_<) = -\frac{1}{4\pi} \int_S \left(U(\boldsymbol{r}') \frac{\partial G(\boldsymbol{r}_< - \boldsymbol{r}')}{\partial n'} - G(\boldsymbol{r}_< - \boldsymbol{r}') \frac{\partial U(\boldsymbol{r}')}{\partial n'} \right) \mathrm{d}S, \tag{A.4}$$

which is the extinction theorem, Eq. (3.1). It shows that the values which U and $\partial U/\partial n$ take on the boundary are such that the incident field is extinguished at every point $\boldsymbol{r}_<$ inside the scattering volume.

References

[1] P.M. Morse, K.U. Ingard, Theoretical Acoustics (Princeton Univ. Press, Princeton, 1968) pp. 410, 419.

[2] M. Kerker, The Scattering of Light and other Electromagnetic Radiation (Academic Press, New York, 1969) p. 430.

[3] P. Roman, Advanced Quantum Theory, Ch. 3 (Addison-Wesley, Reading, 1965).

[4] M. Born, E. Wolf, Principles of Optics, 7th Ed., Section 13.1 (Cambridge Univ. Press, Cambridge), in press.

[5] T.D. Visser, E. Wolf, Phys. Lett. A 234 (1997) 1; 237 (1998) 389 (E).

[6] A. Sommerfeld, Wave Mechanics (Dutton, New York, 1929) pp. 43, 195.

[7] H.W. Wyld, Mathematical Methods for Physics (Addison-Wesley, Reading, 1976) pp. 197–203.
[8] E. Butkov, Mathematical Physics (Addison-Wesley, Reading, 1968) p. 323.
[9] E. Wolf, in: Coherence and Quantum Optics, Proc. of the Third Rochester Conference on Coherence and Quantum Optics, eds. L. Mandel, E. Wolf (Plenum Press, New York, 1973) p. 339.
[10] H. Fearn, D.V.F. James, P.W. Milonni, Am. J. Phys. 64 (1996) 986.
[11] D.N. Pattanayak, E. Wolf, Phys. Rev. D 13 (1976) 913.
[12] O.D. Kellogg, Foundations of Potential Theory (Springer, Berlin, 1967) pp. 215, 160–172.
[13] H. Hönl, A.W. Maue, K. Westpfahl, in: Handbuch der Physik, Band XXV/1 (Springer, Berlin, 1961) pp. 233–236.
[14] D.N. Pattanayak, Opt. Comm. 15 (1975) 335.