

UPPER AND LOWER VARIATIONAL BOUNDS IN EM SCATTERING

K. Kalikstein
Hunter College of the City University
New York, N. Y.

C. J. Kleinman
Long Island University
Brooklyn Center
Brooklyn, N.Y.

Leonard Rosenberg and Larry Spruch
New York University
New York, N.Y.

Abstract

A formulation of the variational bound method is presented which together with some previous work can provide both upper and lower bounds on the phase shifts or equivalent network elements of obstacles located in single and multimode waveguides. As an illustration numerical results are obtained for a rectangular parallel epiped obstacle. The upper and lower bounds on the phase shifts are quite close to one another.

Introduction

A variational bound principle called (VBI) originally developed for quantum mechanical scattering¹, was subsequently extended and applied to the scattering of electromagnetic waves by isotropic obstacles in single and multimode waveguides². The method described in Ref. 2 provides only one bound on the scattering parameters. Here we present a formulation designated as (VBII) for obtaining the opposite bound. Unlike the usual stationary variational principle of Schwinger and others³ which in general gives neither upper nor lower bounds, the VBI and VBII formulation yield bounds which converge to the correct values from above and below. As an illustration, a numerical example is presented for a rectangular parallelepiped obstacle.

Lower Variational Bound

The variational bound principle (VBI) provides a lower bound on the normalized R' matrix in multimode scattering, or on the phase shift in the case of a single mode. We define two dyadic projection operators P and Q , such that for any vector function $J(x,y,z)$

$$PJ(x,y,z) = \int e(x,y) \cdot J(x',y',z) dx'dy' \\ \div \int e(x,y) \cdot \dot{e}(x,y) dx'dy'$$

and

$$Q = 1 - P ;$$

that is, P projects onto the propagating mode and Q projects onto the higher (evanescent) modes. The extension to many propagating modes is immediate.

Using these projection operators it can be shown^{2,4} that Maxwell's wave equation

$$-\nabla \times (\nabla \times \vec{E}) + \epsilon (\omega/c)^2 \vec{E} = 0, \quad (1)$$

reduces to the following expression

$$P(H + HQGQH - W)P\vec{E} = 0 \quad (2)$$

where E is the electric field, ϵ the dielectric constant, ω the angular frequency, and c the velocity of light. We also have

$$H = T + V \\ W = (\omega/c)^2,$$

where

$$-T = \nabla^2 \\ V = \nabla \cdot \nabla + (1-\epsilon)(\omega/c)^2.$$

With H , W , T , and V symbolically identified with the Hamiltonian and with the total, the kinetic, and the potential energies, respectively, we have a connection with the Schroedinger equation.

Equation (2) cannot be solved since the Green's function G^0 is generally not known. G^0 is defined by

$$G^0 \equiv Q[Q(W-H)Q]^{-1}Q. \quad (3)$$

When, as is generally the case, the inequality

$$Q(W-H)Q < 0 \quad (4)$$

is satisfied, it follows that

$$G^0 < 0 \quad (5)$$

The phase shift η_i^P of the i -th mode obtained from the static (single mode) or close coupling (multimode) equations

$$P(H-W)P\vec{E}^P = 0 \quad (6)$$

provides a bound on the phase shift η_i of the original problem corresponding to (2). This bound is a consequence of the monotonicity theorem which states that if the potential $V_1 \geq V_2$ then $\eta_1 \leq \eta_2$.

A formulation which is in principle much superior, in that it supplies a variational upper bound, as opposed to just a bound, on the phase shift or the \vec{R}' matrix is described in Ref. 2. The VBI principle takes the form

$$2k[\cot(\eta-\theta) - \cot(\eta^P-\theta)] \leq S \quad (7)$$

for single mode and

$$-(\vec{A} \cdot \vec{R}' \vec{A} - \vec{A} \cdot \vec{R}'^P \vec{A}) \leq S \quad (8)$$

for multimode, where

$$S = 2 \int \vec{P}\vec{E}^P \cdot \vec{W}Q\vec{E}_t \, d\tau + \int \vec{Q}\vec{E}_t \cdot [H+HPG^P PH-W] \vec{Q}\vec{E}_t \, d\tau, \quad (9)$$

and where \vec{E}_t is a trial function in Q space and

$$G^P \equiv P[P(W-H)P]^{-1}P.$$

Variational bounds contain variational parameters which enable one to approach monotonically the exact value of some quantity of interest, while a bound gives just a number without a means of improvement.

The Opposite Bound

It is possible to obtain the opposite bound by obtaining a simple numerical lower bound G^Q on G^Q . Thus, let us assume that we can find an energy W^Q such that

$$QHQ \geq W^Q > W. \quad (10)$$

This may be possible when (4) is valid. We then have

$$G^Q \geq Q(W-W^Q)^{-1}Q \equiv G_L^Q. \quad (11)$$

The solution of the equation

$$P[H+(W-W^Q)^{-1}HQH-W]P\vec{E}_L = 0 \quad (12)$$

then provides the other bound, the upper bound on the η_i .

A variational upper bound (VBII) on the η_i is available⁴. If the inequality (10) is satisfied it is shown that

$$G^Q \geq (W-W^Q)^{-1} \left\{ 1 + F \int \vec{E}_t \cdot \vec{E}_t \, d\tau \right\}^{-1} \times \left[\int \vec{E}_t F (1-F) \vec{E}_t \, d\tau \right]^{-1} \times \int \vec{E}_t F \, d\tau = G_\sigma^Q, \quad (13)$$

where

$$F = Q(H-W^Q)^{-1}Q/(W-W^Q). \quad (14)$$

The solution of the equation obtained by replacing G^Q in (2) by the known operator G_σ^Q .

$$P[(H-W)+HQG_\sigma^Q QH]P\vec{E}_\sigma = 0 \quad (15)$$

provides variational upper bounds on the phase shift. [Note that the term $\int \vec{E}_t F d\tau$ in (13) integrates over $QHPE_\sigma$ which occurs in (15)].

Inequalities on trigonometric functions of phase shifts are normally more useful than inequalities on the phase shifts themselves. By bounding the modified Green's function⁴ G^Q defined by

$$Q[H+HG^P H-W]QG^Q = -Q, \quad (16)$$

one obtains the opposite bound on the left hand side of (7) and (8).

Numerical Example

Lower variational bounds on the even and odd phase shifts η_e and η_o for a specific case of scattering by a dielectric obstacle were obtained previously² by means of (7). For the same case we determined the (non-variational) upper bounds on η_e and η_o using (12). We have

$$34^\circ 54' \leq \eta_e \leq 35^\circ 39'$$

$$19^\circ 18' \leq \eta_o \leq 20^\circ 34'.$$

The upper bounds can be improved by using the more involved variational expression (15).

Using (6) and (12), (non-variational) rough bounds were obtained on the normalized matrix elements R'_{ij} for an obstacle located in a multimode waveguide propagating only the TE_{10} and TE_{30} modes.

$$R' = \begin{bmatrix} R'_{11} & R'_{13} \\ R'_{31} & R'_{33} \end{bmatrix}$$

with $R'_{13} = R'_{31}$,

corresponds to the even standing waves of the above modes.

The bounds are

$$-0.583 \leq R'_{11} \leq -0.496$$

$$-0.999 \leq R'_{13} \leq -0.627$$

$$-0.223 \leq R'_{33} \leq -0.147$$

Conclusion

Formulations for determining upper and lower bounds, and variational upper and lower bounds on the network elements that characterize electromagnetic scattering by obstacles in waveguides are described. Numerical results for certain specific case are given.

Acknowledgment

Work supported by the U.S. Army Research Office, Durham, Grant No. DA-ARO-D-31-124-72-G92 and by the Office of Naval Research, Grant No. N00014-67-A-0467-0007.

References

1. Y. Hahn, T.F. O'Malley, and L. Spruch, "Improved minimum principle for single-channel scattering," Phys. Rev., vol. 130, pp. 381-394, April 1963 and "Improved minimum principle for multichannel scattering," Phys. Rev., vol. 134, pp. B911-B919, May 1964.
2. Aronson, K. Kalikstein, C.J. Kleinman, and L. Spruch, "Variational bound principle for scattering of electromagnetic waves by obstacles in a waveguide", IEEE Trans. Microwave Tech., vol. MTT-18, Oct. 1970, pp. 725-731. "Variational bound principle for multimode waveguide scattering," IEEE Trans. Microwave Theory Tech., vol. MTT-19, Aug. 1971, pp. 673-677.
3. J. Schwinger and D.S. Saxon, Discontinuities in Waveguides. New York; Gordon and Breach, 1968; N. Marcuvitz, Waveguide Handbook (M.I.T. Radiation Laboratory Series, vol. 10). New York: McGraw-Hill, 1951; R. E. Collins, Field Theory of Guided Waves. New York: McGraw-Hill, 1960.
4. Y. Hahn and L. Spruch, "Remarks on variational bounds in scattering," Phys. Rev. vol. 153, pp. 1159-1164, January 1967.