A variational principle for resonances

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A stationary variational principle for calculation of the complex poles of Green functions is given.

1. INTRODUCTION

Consider the problem

$$(-\nabla^2 - k^2)u = 0 \text{ in } \Omega, \quad u|_\Gamma = 0, \tag{1}$$

where Ω is an exterior domain, Γ is its closed smooth boundary, $D = \mathbb{R}^3 \setminus \Omega$ is bounded. Problem (1) has nontrivial solution iff ($\equiv$ if and only if) k is a complex pole k_q of the Green function of the exterior Dirichlet problem. The nontrivial solution has the following asymptotic near infinity

$$u = r^{-1}\exp(ikr)\sum_{j=0}^{\infty} f_j(n,k)r^{-j}, \tag{2}$$

$$n = x/|x|, \quad r = |x|, f_0 \not\equiv 0.$$

If u and v are of the form (2) with $k = k_1$ and $k = k_2$, respectively, $\text{Re}(k_1 + k_2) \neq 0$, $\pi < \arg k_j < 2\pi$, $j = 1,2$, then the following limit exists

$$\langle u,v\rangle = \lim_{\epsilon \to +0}\int \exp(-\epsilon r \ln r)u(x)v(x)\,dx, \quad \int = \int_\Omega. \tag{3}$$

This will be proved in Sec. 2. From (1) and (3) it follows that

$$\text{st}K(u) = \text{st}\{\langle\nabla u,\nabla u\rangle/\langle u,u\rangle\} = k^2, \tag{4}$$

where st means the stationary value and the admissible functions vanish on Γ and are of the form (2) near infinity. The stationary principle (4) looks like Rayleigh–Ritz quotient but is actually different in the following respects: (i) the functional (4) is complex-valued, the variational principle is a stationary one and not an extremal as for the usual Rayleigh–Ritz functionals; (ii) the functions which give stationary values to K are growing exponentially at infinity.

The variational principle (4) can be used for calculations as follows:

(1) Take a test function of the form

$$u_N = r^{-1}\exp(ikr)\sum_{j=0}^{N}\sum_{|m|\leqslant j} r^{-j}Y_{jm}(n)c_{jm}(k)\cdot g(x), \tag{5}$$

where $Y_{jm}(n)$ are the spherical harmonics, $Y_{jm}(n) = P_{j,m}(\cos\theta)\cdot\exp(im\phi)$, $n = (\theta,\phi)$; $P_{j,m}(\cos\theta)$ are the associated Legendre polynomials; $c_{jm}(k)$ do not depend on r,n; N is a fixed number; $g(x) \geqslant 0$ is a fixed smooth function which is equal to 1 outside of a ball which contains D and which is equal to zero on Γ.

(2) Put (5) in (4) and use the necessary conditions for K to be stationary: $\partial K/\partial c_{jm} = 0$.

Because the numerator and denominator in (4) are quadratic forms in c_{jm} we can write the above condition as

$$\sum_{q=0}^{Q}[a_{sq}(k) - k^2 b_{sq}]\,c_q(k) = 0, \quad 0 \leqslant s \leqslant Q, \tag{6}$$

where for brevity we denote by one index q the double index jm and by Q the maximal value of q which is defined by N. We took into account also that the Lagrange multiplier is equal to k^2 according to (4). The elements $a_{sq}(k)$ and $b_{sq}(k)$ can be explicitly expressed in the form

$$a_{sq}(k) = \langle\nabla\{b(x,k)F_s(r,n)\}, \nabla\{b(x,k)F_q(r,n)\}\rangle, \tag{7}$$

$$b_{sq}(k) = \langle b(x,k)F_s(r,n), b(x,k)F_q(r,n)\rangle, \tag{8}$$

where

$$b(x,k) = g(x)r^{-1}\exp(ikr), \quad F_q(r,n) = r^{-j}Y_{jm}(n). \tag{9}$$

The elements (7), (8) are entire functions of k of exponential type, i.e., the inequalities $|a_{sq}(k)| \leqslant c\exp[A|k|]$ hold, where $c = \text{const} > 0$ and $A = \text{const}$ which depends on D but does not depend on N. The system (6) has a nontrivial solution iff

$$\det\{a_{sq}(k) - k^2 b_{sq}(k)\} = 0. \tag{10}$$

This equation has infinitely many roots $k_l^{(Q)}$, $l = 1,2,\cdots$, generally speaking, since its left-hand side is an entire function of k.

(3) The mathematical question related to this numerical scheme can be formulated as follows: is it true that $k_l^{(Q)} \to k_l$ as $Q \to \infty$, where k_l are the complex poles of the Green function?

2. EXISTENCE OF THE LIMIT (3)

First let us note that it is enough to prove that for sufficiently large $R > 0$ the following limit exists

$$\lim_{\epsilon \to +0}\int_{|x|\geqslant R}\exp(-\epsilon r\ln r)u(x)v(x)\,dx.$$

For $|x| \geqslant R$ we can use series (2) representing u and v. These series converge absolutely and uniformly in n and r, $r \geqslant R$. Therefore it is enough to prove existence of the limit

$$\lim_{\epsilon \to +0}\int_R^\infty \exp(-\epsilon r\ln r)r^{-j}\exp(br + iar)\,dr,$$

where

$$j \geqslant -2,$$

$$b = -\text{Im}(k_1 + k_2) > 0, \quad a = \text{Re}(k_1 + k_2) \neq 0.$$

Suppose that $a > 0$. Let

$$C_N = \{z:|z - R| = N, \quad 0 \leqslant \arg(z - R) \leqslant \theta\},$$

$$C_{\theta N} = \{z:\arg(z - R) = \theta, \quad 0 \leqslant |z - R| \leqslant N\},$$

$$C_R = \{z:R \leqslant z \leqslant R + N\}, \quad C_\theta = C_{\theta\infty}, \quad C = C_N \cup C_{\theta N} \cup C_R.$$

It is clear that

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$$\int_{C_N} \exp(-\epsilon r \ln r) r^{-j} \exp(br + iar)\, dr \to 0$$

as $N \to \infty$, $\forall \epsilon > 0$. Thus

$$\int_R^\infty \exp(-\epsilon r \ln r) r^{-j} \exp(br + iar)\, dr$$

$$= \int_{C_\theta} \exp(-\epsilon r \ln r) r^{-j} \exp(br + iar)\, dr.$$

Let us take $0 < \theta \leqslant \pi/2$ such that a $\sin\theta > n \cos\theta$. Then the integral over C_θ converges absolute for $\epsilon > 0$ and its limit as $\epsilon \to +0$ exists.

The case $a < 0$ can be considered similarly, with $-\theta$ instead of θ. This completes the proof.

Remark 1: The limit (3) was used by B. Vainberg[1] in connection with the orthogonality of the generalized eigen and root functions, corresponding to different complex poles of the Green function, but our argument differs from the argument in Ref. 1. In Ref. 2 the Green function of the Schrödinger operator with a compactly supported potential was considered and the limit with the weight function $\exp(-\epsilon r^2)$ instead of $\exp(-\epsilon r \ln r)$ was considered. There is a mistake in calculation in Ref. 1: the authors claim that the limit $\lim_{\epsilon \to +0} \int_\Omega \exp(-\epsilon r^2)\, uv\, dx$ exists for any k_1, k_2, but this limit does not exist for $5\pi/4 < \arg(k_1 + k_2) < 7\pi/4$. In Refs. 3 and 6 a method for calculation of the complex poles of the Green functions in diffraction problems and in the potential scattering problem was given and justified. This method used Galerkin-type procedure. In Refs. 4, 5, and 7 some facts about the location and properties of the complex poles are given.

Remark 2: Justification of the numerical approach suggested in Sec. 1 is an open mathematical problem. For some other variation principles in nonselfadjoint problems the importance of the mathematical analysis of the situation was mentioned in Ref. 9. In Refs. 3 and 6 the mathematical justification of the numerical approach described in Refs. 3 and 6 was based on the compactness of the integral operators in the equations to which the problem of calculation of the complex poles was reduced in Refs. 3 and 6. In the situation described in this paper the operator is essentially $-\nabla^2 - k^2$ with Dirichlet boundary condition and it is noncompact.

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