

## Operators, Eigen Functions, Green's Functions, Variational Methods

Many problems in widely scattered fields of mathematical analysis exhibit a striking similarity (isomorphism) when clothed in the picturesque geometrical language of abstract linear spaces. The latter are generalizations of the conventional three-dimensional Euclidean space that serve as the analytical background for phenomena of common experience. An abstract space is a set (usually infinite) of elements subject to prescribed combinatorial rules (axiomatic algebra) from which relations between the elements are deducible. Such spaces become of practical importance when the elements and their combinatorial rules provide an algorithmic means for calculation of the properties of physical quantities and their laws of behavior.

The importance of the abstract point of view arises not so much because a geometrical background is imparted to problems of mathematical analysis but rather because an "invariant" procedure is set up for solving such problems. Invariance implies an independence of the technique of solution both on the dimensionality of the space as well as the particular representation (coordinate system) within the given space. To delimit more clearly the underlying point of view let us consider some linear problems for the determination of functions of a continuous variable and also for functions of a discrete variable.

The mathematical problems of electrophysics interest are phrased in general either as partial differential equations or as integral equations. These two classes frequently are not unrelated. For example,

$$\left[ -\nabla^2 - \lambda V(r) - \mu \right] f(r) = g(r) \quad (1.1)$$

with

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \dots, \quad r = (x, y, \dots)$$

represents an inhomogeneous partial differential equation with  $V(r)$ ,  $\mu$ ,  $\lambda$  and the source function  $g(r)$  known and with  $f(r)$  the desired unknown function. Boundary conditions that characterize the domain of admissible functions  $f(r)$  are necessary for uniqueness but need not be specified at this point.

A Green's function  $G(r, r')$  defined by the simpler equation:

$$\left[ -\nabla^2 - \mu \right] G(r, r') = \delta(r - r') \quad (1.2)$$

for a delta-function source  $\delta(r - r')$  (zero for  $r \neq r'$  and with unit integral over  $r'$ ), permits the problem posed by Eq.(1.1) to be rephrased as an integral equation

$$f(r) - \lambda \int G(r, r') V(r') f(r') dr' = h(r) \quad (1.3a)$$

where

$$h(r) = \int G(r, r') g(r') dr'$$

Since  $G(r, r')$ , the Green's function inverse to the operator  $-(\nabla^2 + \mu)$ , represents the field of a point source, the integral equations (1.3a) represents the desired solution  $f(r)$  as a linear superposition of fields of source distributions  $g(r)$  and  $\lambda V(r) f(r)$ . Equation (1.3a) may be expressed more symmetrically as

$$\hat{f}(r) - \lambda \int K(r, r') \hat{f}(r') dr' = \hat{h}(r) \quad (1.3b)$$

$$\text{where} \quad \hat{f}(r) = \sqrt{V(r)} f(r)$$

$$\hat{h}(r) = \sqrt{V(r)} h(r)$$

$$K(r, r') = \sqrt{V(r)} G(r, r') \sqrt{V(r')}$$

The explicit determination of the  $f(r)$ , defined equivalently either by the partial differential equation (1.1) or the integral equations (1.3), may be attempted in various ways. Since solutions usually are expressed in series form, the relative desirability of various solutions will be judged by their rapidity of convergence. For example, using the method of iteration (Liouville, Neumann, Picard method) one finds

$$\hat{f}(r) = \hat{h}(r) + \lambda \int K(r, r') \hat{h}(r') dr' + \lambda^2 \iint K(r, r') K(r', r'') \hat{h}(r'') dr' dr'' + \dots \quad (1.4)$$

$\hat{f}(r)$

as a power series in  $\lambda$ , the  $\lambda$  radius of convergence of which is usually finite. Alternatively using the Fredholm method, one can rewrite the solution  $\hat{f}(r)$  as:

$$\hat{f}(r) = \hat{h}(r) + \lambda \int \frac{D(r, r'; \lambda)}{\Delta(\lambda)} \hat{h}(r') dr' \quad (1.5)$$

where

$$D(r, r'; \lambda) = D_0(r, r') - \lambda D_1(r, r') + \frac{\lambda^2}{2!} D_2(r, r') - \dots$$

$$\Delta(\lambda) = \Delta_0 - \lambda \Delta_1 + \frac{\lambda^2}{2!} \Delta_2 - \dots$$

are known in terms of  $K(r, r')$  etc., the power series in  $\lambda$  being convergent for all  $\lambda$  in this case.

Alternatively, in the eigenfunction method (Hilbert-Schmidt method), the solution is represented as

$$f(r) = f_0(r)\Phi_0(r) + f_1(r)\Phi_1(r) + f_2(r)\Phi_2(r) + \dots \quad (1.6)$$

where  $\Phi_i(r)$  ( $i = 0, 1, 2, \dots$ ), which form a complete set of orthogonal eigenfunctions, are determined so as to permit a simple evaluation of the amplitudes  $f_i$ . For example, the homogeneous partial differential equations

$$\left[ -\nabla^2 - \lambda V(r) - \mu_i \right] \Phi_i(r) = 0 \quad (1.7)$$

subject to specified boundary conditions, yields a simple set of eigenfunctions  $\Phi_i(r)$  and eigenvalues  $\mu_i$ . The so determined  $\Phi_i(r)$  with properties:

$$\int_{-\infty}^{+\infty} \Phi_i(r) \Phi_j(r) dr = \delta_{ij}$$

provide a set of functions in terms of which not only  $f(r)$  but also any (physical) function can be represented.

Thus if

$$g(r) = \sum_i g_i \Phi_i(r)$$

then in Eq(1.1), the amplitudes  $f_i$  are found to be

$$f_i = \frac{g_i}{\mu_i - \mu} \quad (1.8)$$

whence  $f(r)$  follows by (1.6). This eigenfunction procedure is extremely powerful and will be discussed it length below.

In many practical applications it is unnecessary to obtain the complete solution of (1.1) or (1.3) for  $f(r)$  at every value of  $r$ . Some more modest measure of  $f(r)$  such as  $\int h(r) V(r) f(r) dr = S$  suffices. One readily finds from (1.3) that

$$\frac{1}{S} = \frac{\int V(r) [f(r)]^2 dr - \lambda \iint V(r) f(r) G(r, r') V(r') f(r') dr dr'}{\left[ \int h(r) V(r) f(r) dr \right]^2} \quad (1.9)$$

The expression (1.9) is a functional of  $f(r)$  such that, if the correct  $f(r)$  is inserted, the correct value of  $I/S$  will be obtained. However, if a trial  $f(r)$  incorrect to the first order in say  $\lambda$  is inserted into (1.9), it can be shown that (if  $G(r,r') = G(r',r)$ ) the resulting value of  $I/S$  will be incorrect only to second order. This stationary property of  $I/S$  about the correct  $f(r)$  implies that (1.9) is a so called variational expression for  $I/S$ . Any reasonable choice of a trial  $f(r)$  in (1.9) will result in a good approximation to  $I/S$ . An approximate solution of the defining Eq(1.1) or Eq(1-3) for  $f(r)$  is a particularly good choice. Other choices are embodied in the Rayleigh Ritz procedure for the determination of a trial  $f(r)$ . It should be noted that only the form of  $f(r)$  is relevant since Eq(1.9) remains unchanged on multiplication of  $f(r)$  by a constant factor.

It is fruitful, for computational algorithms, to consider the analogue of the above functional deliberations for simpler and more familiar problems involving a set of simultaneous linear equations in  $N$  unknowns. In this case the basic problem is to find the  $f_i$  ( $i = 1, \dots, N$ ) given implicitly by the equations

$$\sum_{j=1}^N (a_{ij} - \lambda v_{ij} + \mu \delta_{ij}) f_j = g_i \quad i = 1, \dots, N \quad (1.10)$$

where the matrices  $(a_{ij})$ ,  $(v_{ij})$ , (assumed symmetric for simplicity) as well as  $g_i$ ,  $\lambda$  and  $\mu$  are known. The problem can be rephrased by the introduction of a symmetric inverse Green's matrix  $(g_{kj})$  defined by

$$\sum_k (a_{ik} + \mu \delta_{ik}) g_{kj} = \delta_{ij} \quad (1.11)$$

$$\text{with} \quad \delta_{ij} = 0 \quad \text{if } i \neq j \\ = 1 \quad \text{if } i = j$$

The Eqs(1.10) for the  $f_i$  then may be transformed on using Eq(1.11) into

$$\hat{f}_i - \lambda \sum_j k_{ij} \hat{f}_j = \hat{h}_i \quad , \quad i = 1, \dots, N \quad (1.12)$$

$$\text{where} \quad \hat{f}_i = \sum_j \sqrt{v_{ij}} f_j$$

$$\hat{h}_i = \sum_j \sqrt{v_{ij}} h_j, \quad h_j = \sum_k g_{jk} g_k$$

$$k_{ij} = \sum_{m,n} \sqrt{v_{im}} g_{mn} \sqrt{v_{nj}}$$

As in the functional case the explicit solution for the  $f_i$  can be obtained in a variety of ways. By the iteration procedure one finds

$$\hat{f}_i = \hat{h}_i + \lambda \sum_j k_{ij} \hat{h}_j + \lambda^2 \sum_{j,k} k_{ij} k_{jk} \hat{h}_k + \dots \quad (1.13)$$

By the Fredholm method, which in this case represents the application of Cramer's rule to (1.12), one obtains the  $f_i$  in the form:

$$\hat{f}_i = \hat{h}_i + \lambda \sum_j \frac{d_{ij}}{\Delta} \hat{h}_j \quad (1.14)$$

$$\text{where } d_{ij} = d_{ij}^{(0)} + \lambda d_{ij}^{(1)} + \frac{\lambda^2}{2!} d_{ij}^{(2)} + \dots$$

$$\Delta = \Delta_0 + \lambda \Delta_1 + \frac{\lambda^2}{2!} \Delta_2 + \dots$$

In the eigenmethod one seeks to find the  $f_i$  in the form

$$f_i = f^{(0)} \Phi_i^{(0)} + f^{(1)} \Phi_i^{(1)} + f^{(2)} \Phi_i^{(2)} + \dots, \quad i = 1, \dots, N \quad (1.15)$$

with the N element vectors  $\Phi_i^{(k)}$  so defined as to simplify the determination of the  $f^{(k)}$ . The homogeneous equations

$$\sum_{j=1}^N (a_{ij} - \lambda v_{ij} + \mu^{(k)} \delta_{ij}) \Phi_j^{(k)} = 0, \quad i = 1, \dots, N \quad (1.16)$$

provide a set of N "eigenvectors"  $\Phi_i^{(k)}$  and "eigenvalues"  $\mu^{(k)}$  which insure a simple determination of the  $f^{(k)}$ . If it is possible to represent

$$g_i = \sum_{k=1}^N g^{(k)} \Phi_i^{(k)}$$

then

$$f^{(k)} = - \frac{g^{(k)}}{\mu^{(k)} - \mu} \quad (1.17)$$

whence the  $f_i$  follow from (1.15). If the N unknowns  $f_i$  are not desired but rather a measure of them such as

$$\sum_{i=1}^N \hat{h}_i \hat{f}_i = S$$

one can deduce from (1.12) the following expression for  $I/S$ :

$$\frac{1}{S} = \frac{\sum_i \hat{f}_i^2 - \lambda \sum_{i,j} \hat{f}_i k_{ij} \hat{f}_j}{\left[ \sum_i \hat{f}_i \hat{h}_i \right]^2} \quad (1.18)$$

This expression can be shown to be stationary for variations of the  $\hat{f}_i$  about their correct values. Hence it furnishes a basis for a variational calculation of  $I/S$  by use either of guessed or approximate choices for the  $f_i$ .

The foregoing presentation of problems involving a set of unknown elements  $f_i$  or an unknown function  $f(r)$  has been sketchy and for simplicity limited to special classes of such problems. However, it should be evident that if the  $f_i$ ,  $i = 1, \dots, N$ , are regarded as defining an element (vector) in an N dimensional space, then it is suggestive to regard  $f(r)$ , for all  $r$  in a given interval, as defining an element in a (continuously) infinite dimensional space. It would then appear that many algebraic problems and their technique of solution in an N dimensional space are significant in the limit  $N \rightarrow \infty$ . Although this is in a large measure true, several difficulties arise in carrying out the limiting process. Chief among these from a pragmatic point of view is that

the conventional determinant technique, so basic to the solution of linear problems in an  $N$  dimensional space, becomes prohibitive as  $N$  approaches infinity. Nevertheless, the isomorphic geometrical character of the aforementioned spaces suggests the existence of a technique for solution of many inversion problems that is applicable equally to the finite dimensional and to the infinite dimensional (function) space. This invariant technique is perhaps best discussed by consideration of linear abstract spaces.

Abstract spaces are distinguished by the nature of the associated combinatorial algebra. Since the algebra of many abstract linear spaces is similar in a number of respects, it is possible to develop first a linear algebra of quite general applicability and then introduce the specialization peculiar to the various spaces at a later stage. In subsequent updates, however, we shall treat primarily and separately the theories of two abstract linear spaces: the finite dimensional complex Euclidean space and the infinitely dimensional Hilbert space, and in so doing attempt to point out basic similarities and differences. As noted in the introduction, the former arises in the theory of linear simultaneous equations in a finite number of unknowns, the latter in the theory of partial differential and integral equations.

For [literature](#) :

