CONSTRAINED VARIATIONAL SOLUTION OF FIELD PROBLEMS

A Thesis

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Doctor of Philosophy

by

Bruce Henry McDonald

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ABSTRACT

Scalar field problems are solved variationally, with a guarantee of energy convergence. Static and time-harmonic fields are obtained directly by solution of a partial differential equation using finite-element segmentation of the physical region which may be inhomogeneous or anisotropic. Fields in free-space regions are obtained by seeking layer source distributions in solution to a Fredholm integral equation of the first kind, using only the simple free-space Green's functions with finite-element segmentation of the source layer. Unbounded field problems where there are local inhomogeneities are solved by combining these field and source methods: the inhomogeneities are enclosed in picture-frames and field is sought; and the remaining free-space region is represented by a layer source distribution on the picture-frame boundaries. Field and source finite elements are mutually constrained to solve the picture-frame problem. The Green's function singularities are treated by removing them from general integrals and dealing with them analytically. This addition-subtraction technique is also found useful in handling special singular source distributions which are introduced to improve convergence. The Green's function behaves regularly in one picture-frame method presented: the integral equation is used to relate potential at the picture-frame boundaries to that on a contour within the picture-frames, and the separation between the boundaries and the contour permits numerical methods to be applied directly. The methods are general purpose in nature, and there is no restriction on the shape of inhomogeneous objects.

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CHAPTER I

INTRODUCTION

In his quest to understand the world about him, man has devised theories, based often on empirical evidence, which have helped him to explain natural phenomena. With the rapid growth of scientific knowledge in the past century, it was only to be expected that different theories would arise to explain the same phenomenon and that each theory would have its own advocates today.

Hammond [1] has identified this situation in electromagnetism: "... The history of electromagnetic investigation is the history of the interplay of two fundamentally different modes of thought. The first of these, the method of electromagnetic fields which ascribes the action to a continuum, is associated with such thinkers as Gilbert, Faraday and Maxwell. The second, the method of electromagnetic sources, concentrates attention on the forces between electric and magnetic bodies and is associated with Franklin, Cavendish and Ampere .... field problems are conveniently handled by differential equations and sources by integral equations .... the rigid distinction between field and source methods can be discarded only when it is seen that there is a freedom of choice ...".

The purpose of the work reported here has been to study the use of both methods, separately and simultaneously, in solving static and time-harmonic scalar problems in a region of space Ω. The static problem

requires solution of Poisson's equation

$$-\nabla\cdot(\varepsilon\nabla\phi) = \rho \tag{1.1}$$

and the time-harmonic or propagation problem requires solution of the deterministic Helmholtz equation

$$-\nabla\cdot(\varepsilon\nabla\phi) - W\phi = \rho \quad . \tag{1.2}$$

Here, ϕ is the unknown scalar potential to be determined and ρ is a given source distribution. The permittivity ε is a scalar function of position unless the material in Ω is anisotropic (properties dependent upon direction) in which case ε is a tensor. The propagation function W is a known scalar function which will be specified shortly in terms of the material properties of Ω and the frequency of propagation.

While equations (1.1) or (1.2) prescribe the field behaviour at any point in Ω , it is usually necessary, for complete problem definition, to have ϕ satisfy certain conditions on S, the boundary of Ω . The Dirichlet boundary condition is

$$\phi(\underline{r}) = g(\underline{r}) \; ; \; \underline{r} \text{ on } S_1 \quad . \tag{1.3a}$$

The Neumam boundary condition is

$$\hat{n}\cdot(\varepsilon(\underline{r})\nabla\phi(\underline{r})) = h(\underline{r}) \; ; \; \underline{r} \text{ on } S_2 \tag{1.3b}$$

and the mixed boundary condition is

$$\hat{n}\cdot(\varepsilon(\underline{r})\,\nabla\phi(\underline{r})) + \alpha(\underline{r})\phi(\underline{r}) = h(\underline{r}) \; ; \; \underline{r} \text{ on } S_3 \quad . \tag{1.3c}$$

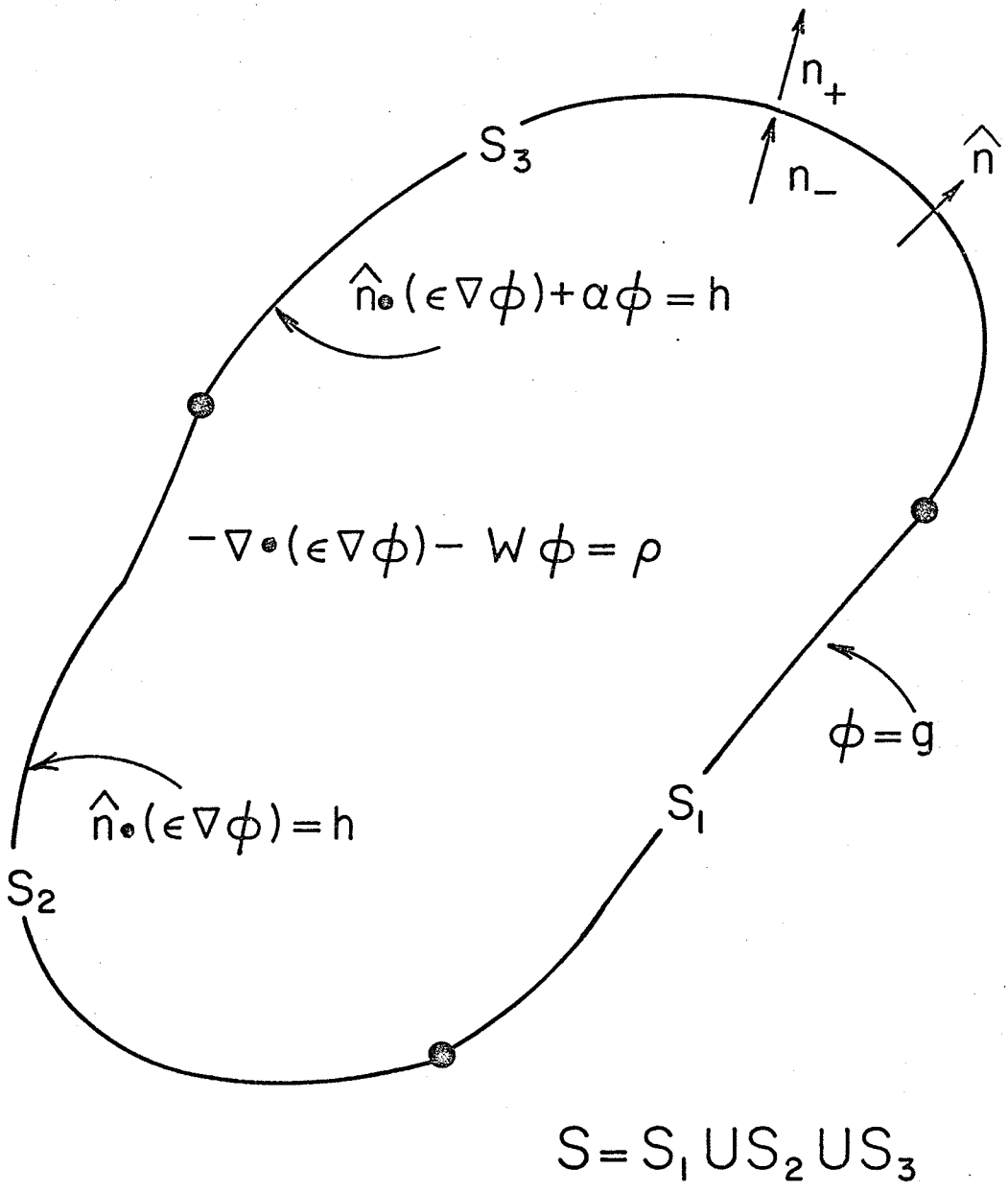


Fig. 1.1 The Boundary Value Problem

The unit vector $\hat{n}$ is taken pointing out of Ω and the boundary of Ω is $S = S_1+S_2+S_3$, as shown in Fig. 1.1. Part or all of S may be at infinity, in which case Ω is an unbounded region.

If the region Ω is anisotropic (i.e. with tensor ε) there is no difficulty in the static case; the scalar potential is adequate. Propagation in such material normally requires a vector formulation if electromagnetic phenomena are to be handled correctly [2, p. 104-109]; the scalar potential ϕ is inadequate. As the work here deals with scalar potential, only isotropic material is considered in the case of propagation. Nevertheless the mathematical treatment is general, with W taken to be a known scalar function.

When the region Ω is isotropic, the propagation function W in (1.2) is simply

$$W = \omega^2\mu\varepsilon^2 \tag{1.4}$$

where ω is the frequency (radians/second) and μ is the permeability of the material in Ω. If the region is homogeneous free space (i.e. $\varepsilon=\varepsilon_o = 8.85 \times 10^{-12}$ farads/meter and $\mu=\mu_o = 4\pi \times 10^{-7}$ henrys/meter), the Helmholtz equation (1.2) assumes the more familiar form

$$- \nabla^2\phi - k^2\phi = \frac{\rho}{\varepsilon_o} \tag{1.5}$$

where the propagation constant k is defined by

$$k^2 = \omega^2\mu_o\varepsilon_o \quad . \tag{1.6}$$

Throughout this work the permeability is taken to be μ_o. (As a matter of interest, note that if the material were anisotropic, with tensor ε, and one attempted to use (1.4), a tensor propogation function W would result. In this case (1.2) would not make sense unless the potential were a vector function.)

Equation (1.5) has an analytical solution in free space which is given by:

$$\phi(\underline{r}) = \frac{1}{\varepsilon_o} \int_{\Omega} \rho(\underline{r}') \, G(\underline{r}|\underline{r}') \, d\Omega' \quad . \tag{1.7}$$

The Green's function for this problem is [3, p. 55]:

$$G(\underline{r}|\underline{r}') = \frac{e^{jk|\underline{r}-\underline{r}'|}}{4\pi|\underline{r}-\underline{r}'|} \quad . \tag{1.8}$$

This is an"action-at-a-distance" function with an integrable singularity at $\underline{r}'=\underline{r}$. It is the solution of the PDE [2]

$$-\nabla^2 G(\underline{r}|\underline{r}') - k^2 G(\underline{r}|\underline{r}') = \delta(\underline{r}-\underline{r}') \tag{1.9}$$

where δ is the Dirac delta function [4, p. 340] and where G satisfies the radiation condition at infinity [5]. If k=0, Poisson's equation is solved with vanishing potential at infinity.

An addition and a subtraction allow (1.8) to be written

$$G(\underline{r}|\underline{r}') = \frac{1}{4\pi|\underline{r}-\underline{r}'|} + \frac{e^{jk|\underline{r}-\underline{r}'|}-1}{4\pi|\underline{r}-\underline{r}'|} \quad . \tag{1.10}$$

The second term of this expression is not singular at $\underline{r}=\underline{r}'$, as

$$\lim_{d\to 0} \frac{e^{jkd}-1}{4\pi d} = \lim_{d\to 0} \frac{1}{4\pi} \{ jk + \frac{(jk)^2 d}{2!} + + \} = \frac{jk}{4\pi} \tag{1.11}$$

and it vanishes at k=0. The first term of (1.10) is the Green's function for Poisson's equation, and contains the integrable singularity. It is important to note that consideration of the singularity for the static case suffices for the propagation case as well.

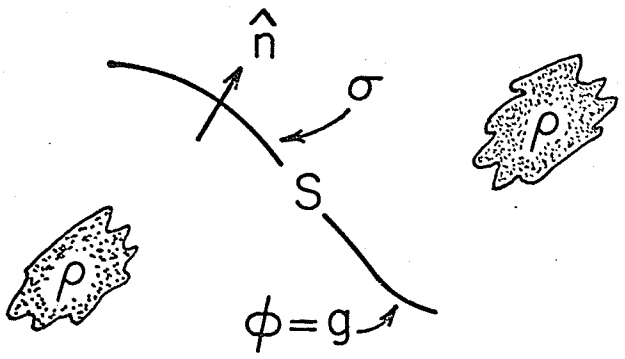
Suppose now that a Dirichlet condition is specified on some surface S in free space. If it should happen that (1.7) generates a potential satisfying $\phi=g$ on S, the problem is solved. If not, it is convenient to place a simple layer of source σ on S, as in Fig. 1.2 and adjust it until the Dirichlet condition is satisfied. Then, throughout free space,

$$\phi(\underline{r}) = \frac{1}{\varepsilon_o} \int_S \sigma(\underline{r}') \, G(\underline{r}|\underline{r}')ds' + \frac{1}{\varepsilon_o} \int_\Omega \rho(\underline{r}') \, G(\underline{r}|\underline{r}')d\Omega' \, . \tag{1.12}$$

To find σ, one must solve a Fredholm integral equation (IE) of the first kind [3, pp.48-49]:

$$\frac{1}{\varepsilon_o} \int_S \sigma(\underline{r}') \, G(\underline{r}|\underline{r}')ds' = g(\underline{r}) - \frac{1}{\varepsilon_o} \int_\Omega \rho(\underline{r}') \, G(\underline{r}|\underline{r}')d\Omega' \; ; \; \underline{r} \text{ on S} \, . \tag{1.13}$$

The right-hand side of (1.13) is completely known, and the unknown source distribution σ appears within an integral. This problem has a unique solution if S is piecewise continuous [6, pp.277-315; 7, pp.180-186] and k is not an eigenvalue of equation (1.13) [5]. One benefit of this approach is that ϕ generated by (1.12) satisfies the PDE (1.5) exactly at any point not on S.



$$\phi = \frac{1}{\epsilon_o}\int_S \sigma G\, ds + \frac{1}{\epsilon_o}\int_\Omega \rho G\, d\Omega$$

Fig. 1.2. The Integral Equation Dirichlet Problem.

The PDE and IE methods may now be compared. The first method requires finding ϕ in Ω which satisfies not only boundary conditions at S but also the PDE in Ω. Inhomogeneities are handled fairly easily: one substitutes (1.2) for (1.5) as the PDE to be satisfied. Approximate solutions often require a number of unknowns proportional to the size of Ω [8, pp.11-14], so that large regions may be less easily accomodated. On the other hand, the IE method requires finding σ on S to satisfy the Dirichlet condition at S, with the result that ϕ may be obtained anywhere in the infinite region Ω by an integration. If the region is not homogeneous the simple free-space Green's function (1.8) is not by itself applicable; dyadic Green's functions [9, pp.1769-1772;

10, p.46-66], or other modified Green's functions [11-12] are often required, complicating the IE procedure. Futhermore, computation is made difficult by the presence of the Green's function singularity; it must be taken into account in any computation [13, p.422-436]. If the region Ω is infinitely large and inhomogeneous, neither method is easily applied: the PDE approach suffers due to the size of the region, and the IE method, due to the presence of the inhomogeneities.

Consider the case where the region is infinitely large with localized inhomogeneities, as shown in Fig. 1.3. Transformation and other analytic techniques [14, pp.72-120] are not easily applied. One may enclose the inhomogeneities in small regions Ω_i called picture-frames, and in each of these the PDE method is applicable, given appropriate conditions on the Ω_i boundaries. The remaining region $\Omega_e = \Omega - \Sigma\Omega_i$ is homogeneous, and the IE method is applicable

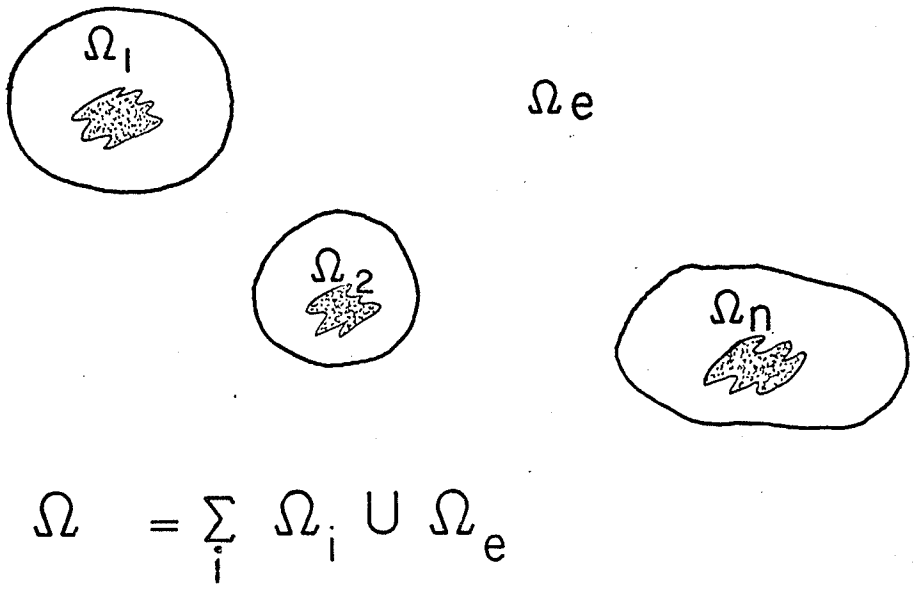


Fig. 1.3. Picture-frame Segmentation of Ω .

with a suitable Dirichlet condition on the Ω_i boundaries. Forcing ϕ to be smooth and continuous at the Ω_i boundaries permits the two methods to be used together, simultaneously, in production of the solution over the entire infinite region. There have been several recent reports of such techniques [15-21], and here, in Chapter III a method is presented whereby the PDE picture-frame solutions, constrained by an IE expression for Ω_e, are obtained variationally using finite elements [22].

In Chapter IV methods are described which permit IE problems to be solved variationally [23-24] and in Chapter VI, variational methods for both the PDE and the IE portions of the picture-frame problem are mutually constrained to produce the solution. In Chapter V a somewhat different approach is presented: when the inhomogeneity is uniform (for example a homogeneous dielectric with relative permittivity ε_r), purely IE variational methods may be mutually constrained to produce the solution [24].

In each example the approximate solution is obtained by solving a system of linear equations:

$$[A]\ \underline{x} = \underline{b} \quad . \tag{1.14}$$

The variational methods described here are used to construct the matrix $[A]$ and the vector $\underline{b}$. While less emphasis has been placed on techniques for solving (1.14) than on techniques for constructing it, certain useful approaches for handling systems of equations are described in Chapter VII.

The presentation begins by describing the application of variational methods to the PDE, using finite-element techniques.

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CHAPTER II

BASIC VARIATIONAL METHODS

In this chapter functional minimization is presented as a means of obtaining energy convergent approximate solutions to PDE problems. A proof of convergence for certain applications of Galerkin's Method, given by Mikhlin [1] permits energy convergent solutions to be obtained for propagation problems by seeking functions which make the functional stationary.

The variational approach involves use of the Fundamental Lemma of the calculus of variations [2, p.39] which may be stated as follows: if $\eta(\underline{r})$ is an arbitrary piecewise continuous function in R, the only function u which satisfies

$$I = \int_R \eta(\underline{r})\, u(\underline{r})\, dR = 0 \tag{2.1}$$

is the function $u=0$. If $u>0$ in some elementary region R', it is only necessary to set $\eta=1$ in R' and $\eta=0$ in R-R' to have

$$I = \int_{R'} u(\underline{r})\, dR > 0 \quad . \tag{2.2}$$

Therefore contradictions result unless

$$u = 0 \quad . \tag{2.3}$$

2.1 Linear Operators

Consider the linear operator equation

$$Lu = f \tag{2.4}$$

where the function u, in the domain of the operator (D_L), is sought to make (2.4) true at all points in a region R. The PDE (1.2) and the IE (1.13) of Chapter I are both linear operator equations. In the case of a PDE it is assumed for the moment that u satisfies any given boundary conditions.

An inner product over R may be defined by [3]

$$\langle u,v \rangle = \int_R w(\underline{r})\ u(\underline{r})\ v^*(\underline{r})\ dR \tag{2.5}$$

where w is a weighting function (here taken to be unity) and where, for real variables, the complex conjugate v^* equals v. If u and v are vectors, two inner products may be defined; the scalar form:

$$\langle \underline{u}^T, \underline{v} \rangle = \sum_{i=1}^{N} \langle u_i, v_i \rangle \tag{2.6}$$

and the dyadic form:

$$\langle \underline{u}, \underline{v}^T \rangle = \begin{bmatrix} \langle u_1, v_1 \rangle & \cdots & \langle u_1, v_N \rangle \\ \vdots & & \vdots \\ \langle u_N, v_1 \rangle & \cdots & \langle u_N, v_N \rangle \end{bmatrix} . \tag{2.7}$$

The vector conventions used are described in Appendix A.

The operator L is self-adjoint [1, p.26] if

$$\langle Lu, v \rangle = \langle u, Lv \rangle \tag{2.8}$$

and it is positive-definite [1, p.31] if

$$\langle Lu,u\rangle \begin{cases} > 0 & u\neq 0 \\ = 0 & u=0 \end{cases} \quad . \tag{2.9}$$

The norm of u over R [1, p.15] is given by

$$|| u || = \langle u,u\rangle^{\frac{1}{2}} \tag{2.10}$$

and the energy norm of u over R [1, p.52], by

$$\| u \| = \langle Lu,u\rangle^{\frac{1}{2}} \quad . \tag{2.11}$$

It is clear that the energy norm is real-valued only if L is a positive-definite operator. The operator is positive-bounded-below [1, p.36] if

$$\| u \| \geq \gamma || u|| \quad ; \quad \gamma>0 \tag{2.12}$$

where γ is a real-valued constant.

One useful result of positive-definiteness is that the solution to (2.4), if it exists, is unique [1, p.74] . Suppose that there are 2 solutions, u_1 and u_2. Let $v = u_1-u_2$ and consider

$$Lu_1 - Lu_2 = Lv = 0 \quad ; \tag{2.13}$$

one may then write

$$\langle Lv, v\rangle = 0 \quad . \tag{2.14}$$

But L is positive-definite and therefore $v=0$. Hence

$$u_1 = u_2 \tag{2.15}$$

and the solution is unique. It follows as well that the only solution to $Lv = 0$ is the trivial solution, $v=0$.

The Laplacian operator, $-\nabla^2$, is self-adjoint and positive-definite with homogeneous Dirichlet boundary conditions. Using Green's first identity [1, p.12] and real-valued ϕ:

$$\begin{aligned} \langle -\nabla^2\phi \ \phi \rangle &= \int_\Omega \nabla\phi \cdot \nabla\phi \ d\Omega - \int_S \phi \frac{\partial\phi}{\partial n} ds \\ &= \int_\Omega \nabla\phi \cdot \nabla\phi \ d\Omega \quad . \end{aligned} \tag{2.16}$$

This is proportional to the electrostatic energy U, and for this reason, $\langle Lu,u \rangle$ is called the energy of u in L over R. Mikhlin has established that the Laplacian is positive-bounded-below for finite regions with homogeneous mixed or Dirichlet boundary conditions [1, pp.138-151].

2.2 The Quadratic Functional and Energy Convergence

The Minimal Functional Theorem [1, p.318] states that if L is a positive-definite, self-adjoint operator, the function u which minimizes the functional

$$F(u) = \langle Lu,u\rangle - \langle u,f\rangle - \langle f,u\rangle \tag{2.17}$$

also satisfies the equation Lu=f. Consider the first variation of F(u):

$$\delta F(u) = \langle L\delta u,u\rangle + \langle Lu,\delta u\rangle - \langle \delta u,f\rangle - \langle f,\delta u\rangle \quad . \tag{2.18}$$

The self-adjointness of L allows this to be written as

$$\delta F(u) = \langle \delta u,Lu\rangle + \langle Lu,\delta u\rangle - \langle \delta u,f\rangle - \langle f,\delta u\rangle \quad . \tag{2.19}$$

The stationary point is obtained by setting the first variation to zero:

$$\begin{aligned}\delta F(u) &= \langle \delta u,Lu-f\rangle + \langle Lu-f,\delta u\rangle \\ &= 2\ \mathrm{Re}\colon \langle Lu-f,\delta u\rangle = 0 \quad .\end{aligned} \tag{2.20}$$

Since δu is arbitrary, Lu=f by the Fundamental Lemma. (See the discussion at (2.1).) The second variation of F at the solution point is

$$\delta^2 F(u) = 2\langle L\delta u,\delta u\rangle \quad . \tag{2.21}$$

Since L is positive-definite, this is non-negative (2.9), and the stationary point of F is a minimum. Note that self-adjointness is required to obtain a stationary point, and that positive-definiteness is required to show that this point is a minimum.

Suppose that the solution is to be approximated by a linear combination of real-valued functions with possibly complex coefficients:

$$u_N(\underline{r}) = \sum_{i=1}^{N} c_i v_i(\underline{r}) = \underline{c}^T \underline{v} = \underline{v}^T \underline{c} \quad . \tag{2.22}$$

The error of this approximation is defined by

$$e_N = u - u_N \quad . \tag{2.23}$$

The set of functions $\{v_i\}$ is said to be complete [1, p.65] if

$$\lim_{N\to\infty} ||e_N|| = 0 \tag{2.24}$$

and it is energy complete [1, p.68] if

$$\lim_{N\to\infty} \|e_N\| = 0 \quad . \tag{2.25}$$

If L is positive-bounded-below as well, from equation (2.12)

$$\lim_{N\to\infty} \|e_N\| \geq \lim_{N\to\infty} \gamma ||e_N|| \neq 0 \quad ; \quad \gamma > 0 \tag{2.26}$$

and u_N converges to u in the mean (i.e. in the rms sense). Convergence is said to be in the energy of u_N in L, and the sequence of approximations, u_N, is called a minimizing sequence [1, p.83].

Completeness in energy may be used to derive the quadratic functional (2.17) as follows: from (2.11) and (2.25)

$$\lim_{N\to\infty} \| e_N \| = \lim_{N\to\infty} \langle Le_N, e_N \rangle^{\frac{1}{2}} = 0 \quad . \tag{2.27}$$

Then, using (2.23) and (2.4)

$$\begin{aligned} \langle Le_N, e_N \rangle &= \langle L(u-u_N),\ u-u_N \rangle \\ &= \langle f,u \rangle - \langle Lu_N, u \rangle - \langle f, u_N \rangle + \langle Lu_N, u_N \rangle \geq 0 \ . \end{aligned} \tag{2.28}$$

The inequality follows from the definition of a positive-definite operator (2.9). Now, if L is self-adjoint

$$\langle Lu_N, u \rangle = \langle u_N, Lu \rangle = \langle u_N, f \rangle \tag{2.29}$$

and

$$\langle Le_N, e_N \rangle = \langle Lu_N, u_N \rangle - \langle u_N, f \rangle - \langle f, u_N \rangle + \langle f, u \rangle \geq 0 \quad . \tag{2.30}$$

This may be written as

$$F(u_N) = \langle Lu_N, u_N \rangle - \langle f, u_N \rangle - \langle u_N, f \rangle \geq - \langle f, u \rangle \tag{2.31}$$

and is seen, in comparison with (2.17), to be a statement of the Minimal Functional Theorem. The minimum value of F is $-\langle f,u\rangle$, achieved in the limit as $N\to\infty$. That is

$$\lim_{N\to\infty} F(u_N) = F(u) = -\langle f,u\rangle \quad . \tag{2.32}$$

From this derivation it is evident that minimization of the functional is equivalent to minimization of the energy norm of the error e_N.