

SECOND ORDER DIFFERENTIAL OPERATORS ON GRAPHS

Vadnere S. M.

Department of Mathematics, Shivneri Mahavidyalaya Shirur Anantpal 413544

Abstract:-

The Main aim of this paper is to study properties of second order differential operators on directed graphs Different types of functions spaces are defined on the graphs. Wedefine, in terms of both differential systems and known function spaces, boundary value problems on graphs. "It is shown that original boundary value problem on graph is equivalent to the system of boundary value problems with differential equation and boundary conditions". A counter example is given to explain the fact that, for Sturm-Liouville Differential operators on graphs, self-adjointness does always imply regularity. A differential operator on directed graph with weighted edges is specified by a system of ordinary differential operators. A class of local operators is introduced to clarify which operators should be considered as defined on graphs. When the lower bound of edge length is positive then all local Self -adjoint extensions of minimal symmetric operator can distinguished by boundary conditions at vertices.

Keyword :- Differential Equation, Sturm-Liouville, self-adjointness, boundary conditions.

Introduction:-

Let G be a graph with finitely many edges, say K, each of finite length. Denote the edges by $e_i, i = 1, \dots, K$, and the corresponding lengths of the edges by $l_i, i= 1, \dots, K$.

We consider the formal second order differential operator.

$$ly: = -\frac{d^2y}{dx^2} + q(x)y = \lambda y \quad \dots\dots\dots(I)$$

on G where, throughout this paper q is a real valued function on G. Restrictions are imposed on q as additional structure is needed it is assumed that q is essentially bounded.

At the vertices or nodes of G we impose boundary conditions with respect to which l_i is formally self-adjoint (see [15] for the definition in the case of systems and [2] for graphs). Such boundary conditions will be called formally self-adjoint boundary conditions.

In particular by equation (I) we mean the system of equations

$$-\frac{d^2y_i}{dx^2} + q_i(x)y_i = \lambda y_i, x \in (0, l_i), \quad i = 1, \dots, K$$

where q_i and y_i denote q and y restricted to e_i and e_i is identified with $(0, l_i)$. We consider boundary conditions of the form

$$\sum_{j=1}^k [\alpha_{ij}y_j + \beta_{ij}y'_j](0) + \sum_{j=1}^k [\gamma_{ij}y_j + \delta_{ij}y'_j](l_j) = 0, \quad i = 1, \dots, 2K,$$

where the number of linearly independent boundary conditions is 2K. This number of linearly independent boundary conditions is necessary (but not sufficient) for the self-adjointness of the boundary value problem on G. Self-adjoint boundary conditions for the Sturm-Liouville operator on a graph have been characterized by Harmer, Kostrykin and Schrader, and Kuchment in [06, 07, 12]. Carlson, in [2], gives a description of adjoints and domains of essential self-adjointness for a class of differential operators on a weighted graphs. Although our researches show that historically the first graph model was used in chemistry, see [04, 05, 16, 17], the development

of the theory of differential operators on graphs is recent with most of the research in this area having been conducted in the last couple of decades. It should however be noted that both multipoint boundary value problems (less general than boundary value problems on graphs) and differential systems (more general than boundary value problems on graphs) were studied far earlier than this. Differential operators on graphs arise naturally in chemistry, physics and engineering (nanotechnology), and are mathematically interesting. Amongst these applications of differential operators on graphs are the free-electron theory of conjugated molecules in chemistry, see [04, 05, 17], quantum wires and quantum chaos, see [07, 08, 09, 10], and scattering theory and photonic crystals, see [03, 11, 13].

1.1 Boundary Value Problems on Graphs

The differential equation (I) on the graph G can now be considered as the system of equations

$$-\frac{d^2 y_i}{dx^2} + q_i(x)y_i = \lambda y_i, \quad x \in (0, l_i), \quad i = 1, \dots, K \quad \dots\text{(II)}$$

Where q_i and y_i denote $q|_{e_i}$ and $y|_{e_i}$.

The boundary conditions at the node v are specified in terms of the values of y and y' at v on each of the incident edges. In particular if the edges which start at v are $e_i, i \in \Lambda_s(v)$ and the edges which end at v are $e_i, i \in \Lambda_e(v)$ then the boundary conditions at v can be expressed as

$$\sum_{j \in \Lambda_s(v)} \alpha_{ij} y_j + \beta_{ij} y'_j(0) + \sum_{j \in \Lambda_e(v)} \gamma_{ij} y_j + \delta_{ij} y'_j(l_j) = 0 \quad \dots\text{(III)}$$

for $i = 1, \dots, N(v)$, where $N(v)$ is the number of linearly independent boundary conditions at node v . Let $\alpha_{ij} = 0 = \beta_{ij}$ for $i = 1, \dots, N(v)$ and $j \notin \Lambda_s(v)$ and similarly let $\gamma_{ij} = 0 = \delta_{ij}$ for $i = 1, \dots, N(v)$ and $j \notin \Lambda_e(v)$. The boundary conditions (III) considered over all nodes v , after possible relabeling, may thus be written as

$$\sum_{j=1}^K [\alpha_{ij} y_j + \beta_{ij} y'_j](0) + \sum_{j=1}^K [\gamma_{ij} y_j + \delta_{ij} y'_j](l_j) = 0, \quad i = 1, \dots, 2K \quad \dots\text{(IV)}$$

where $2K$ is the total number of linearly independent boundary conditions. It should be noted that the complete geometry of the graph G (other than the number of and length of the edges) is encapsulated in the boundary conditions.

To ensure formal self-adjointness we require the Lagrange form, $(lf, g) - (f, lg)$, to vanish for all $f, g \in C^2(G)$ obeying (III). For formally self-adjoint boundary conditions $N(v) = \square(\Lambda_s(v)) + \square(\Lambda_e(v))$ and $\sum_v N(v) = 2k$. The formulation of self-adjoint boundary value problems on graphs was studied in detail in [2], and the class of self-adjoint boundary conditions was characterized in [06] and [07]. The boundary value problem (II)-(III) on G can be formulated as an operator eigenvalue problem in $\mathcal{L}^2(G)$, [1, 2, 18], for the closed densely defined operator

$$Lf = -f'' + qf \quad \dots\text{(V)}$$

With domain

$$D(L) = \{f \mid f, f' \in AC, Lf \in \mathcal{L}^2(G), f \text{ obeying (III)}\}, \quad \dots\text{(VI)}$$

or equivalently

$$D(L) = \{f \mid f \in \mathcal{H}^2(G), f \text{ obeying (III)}\},$$

since \mathcal{H}^m spaces can be defined in terms of absolutely continuous functions, see [14].

The formal self-adjointness of (II)-(III) ensures that L is a closed densely defined self-adjoint

Corollary:- If L_0 is a closed symmetric operator, with finite defect indices, bounded from below on a complex Hilbert space and L is a self-adjoint extension of L_0 then L is lower semibounded.

Theorem:- The operator L is lower semibounded

Proof: From the above corollary as L is self adjoint, we need only show that L is lower semibounded on $C_0^\infty(G)$. If $f \in C_0^\infty(G)$. Then

$$(Lf, f) = \int_G (-f'' - f + q|f|^2) dx = \int_G (|f'|^2 + q|f|^2) dx \geq -\|f\|^2 \text{ess sup } |q|.$$

1.2 System Formulation

We now show that the boundary value problem on a graph can be reformulated as a boundary value problem for a system on the interval $(0, 1)$.

Consider the edge e_i of length l_i , we then have

$$-y_i''(x) + q_i(x)y_i(x) = \lambda y_i(x) \text{ on } (0, l_i)$$

Let $t = \frac{x}{l_i}$ and $\tilde{y}_i(t) = y_i(l_i t)$. Then

$$-\frac{d^2}{dt^2} [\tilde{y}_i(t)] = -l_i^2 y_i''(l_i t) = l_i^2 (\lambda y_i(l_i t) - q_i(l_i t) y_i(l_i t)) = l_i^2 (\lambda - Q_i(t)) \tilde{y}_i(t),$$

Where

$$Q_i(t) = q_i(l_i t)$$

Thus for each $i=1, \dots, K$ our transformed equation is

$$-(\tilde{y}_i'') + l_i^2 (Q_i - \lambda) \tilde{y}_i = 0 \text{ on } (0,1)$$

giving the system

$$\tilde{L}\tilde{Y} := -W\tilde{Y}'' + Q\tilde{Y} = \lambda\tilde{Y}. \quad \dots(\text{VII})$$

where $W = \text{diag} \left[\frac{1}{l_1^2}, \dots, \frac{1}{l_k^2} \right]$, $\tilde{Y} = \begin{bmatrix} \tilde{Y}_1 \\ \vdots \\ \tilde{Y}_K \end{bmatrix}$ and $Q = \text{diag} [Q_1, \dots, Q_K]$.

We now consider the boundary conditions. After performing the above transformation on each edge we have that all our edges are now of length 1 and thus we only have the endpoints at 0 and 1. Hence the boundary conditions may be written in matrix form as

$$\tilde{Y}(0) + \tilde{B}\tilde{Y}'(0) + \tilde{C}\tilde{Y}(1) + \tilde{D}\tilde{Y}'(1) = 0 \quad \dots(\text{VIII})$$

Where $\tilde{A} = [\alpha_{ij}]$, $\tilde{B} = \begin{bmatrix} \beta_{ij} \\ l_j \end{bmatrix}$, $\tilde{C} = [\gamma_{ij}]$ and $\tilde{D} = \begin{bmatrix} \delta_{ij} \\ l_j \end{bmatrix}$.

Thus our original boundary value problem on the graph G is equivalent to the system boundary value problem with differential equation (VII) and boundary conditions (VIII).

Let \mathcal{L}_K^2 denote the weighted vector space \mathcal{L}^2

$$\mathcal{L}_K^2 = \{F: (0,1) \rightarrow \mathbb{C}^k \mid F_i \in \mathcal{L}^2(0,1), i = 1, \dots, K\}$$

with inner product

$$\langle F, G \rangle_w = \sum_{i=1}^k l_i \int_0^1 F_i \bar{G}_i dt = \int_0^1 F^T W^{-\frac{1}{2}} \bar{G} dt. \quad (\text{IX})$$

It should be noted that \mathcal{L}_k^2 is isometrically isomorphic to $\mathcal{L}^2 G$ under the identification $\mathcal{L}^2 G \rightarrow \mathcal{L}_k^2$ defined by

$$f(x) \mapsto \begin{bmatrix} f|_{e_1}(l_1 t) \\ \vdots \\ f|_{e_k}(l_k t) \end{bmatrix}$$

where $x \in G$ and $t \in (0, 1)$.

The boundary value problem (VII) and (VIII) can be reformulated as an operator eigenvalue problem, [19], by setting

$$\bar{L}F = -WF'' + QF$$

with domain

$$D(\bar{L}) = \{F | F, F' \in AC, \bar{L}F \in \mathcal{L}^2(G), F \text{ Obeying (VIII)}\}$$

Theorem:- The system (VII) and (VIII) is formally self-adjoint in \mathcal{L}_k^2 if and only if the boundary value problem (II) and (III) in $\mathcal{L}^2(G)$ is formally self-adjoint.

Proof:

Let $F, G : (0, 1) \rightarrow C^k$ be C^2 and denote by f and g the functions on G defined by $f|_{e_i}(l_i t) = F_i(t)$ and $g|_{e_i}(l_i t) = G_i(t)$ for $i = 1, \dots, K$ and $t \in (0, 1)$, then under this identification

$$\begin{aligned} \langle \bar{L}F, G \rangle_w - \langle F, \bar{L}G \rangle_w &= - \sum_{i=1}^k l_i^{-1} \int_0^1 [F_i'' \bar{G}_i - F_i \bar{G}_i''] dt \\ &= - \sum_{i=1}^k l_i^{-1} \int_0^1 [F_i' \bar{G}_i - F_i \bar{G}_i']_0^1 \end{aligned}$$

$$= \sum_{i=1}^k [(f' \bar{g} - f \bar{g}')|_{e_i}]_0^{l_i}$$

$$= (LF, g) - (f, Lg)$$

and (III) holds if and only if (VIII).

In this setting the formal self-adjointness of (VII) and (VIII) ensures that the operator \bar{L} on \mathcal{L}_k^2 is a closed densely defined self-adjoint operator and thus the formal self-adjointness of (II) and (III) ensures that \bar{L} is a closed densely defined self-adjoint operator in \mathcal{L}_k^2 , see [20].

1.3 Irregularity

In this section we show that self-adjointness does not necessarily imply regularity, in fact in most cases it does not.

Without loss of generality we may assume that our boundary conditions are normalised, i.e. of the form

$$U_1(Y) = U_{10}(Y) - U_{11}(Y) = 0$$

$$U_2(Y) = U_{20}(Y) - U_{21}(Y) = 0$$

Where

$$U_{10}(Y) = A_1 Y'(0) + A_{10} Y(0)$$

$$U_{20}(Y) = A_2 Y'(0) + A_{20} Y(0)$$

$$U_{11}(Y) = B_1 Y'(1) + B_{10} Y(1)$$

$$U_{21}(Y) = B_2 Y'(1) + B_{20} Y(1)$$

where for each $i = 1, 2$, at least one of the matrices A_i, B_i is different from zero. If $A_i = 0$ then by the normalisation process given in [15] we will obtain that A_{i0} will then become A_i and similarly for $B_i = 0$.

Following [15] we define regularity of boundary conditions as follows.

Definition :- The normalised boundary conditions, above, are said to be regular if both the numbers χ^- and χ^+ defined by

$$\chi^- = i^{2n} \det \begin{bmatrix} W^{-\frac{1}{2}}B_1 & -A_1 \\ W^{-\frac{1}{2}}B_2 & -A_2 \end{bmatrix}, \chi^+ = i^{2n} \det \begin{bmatrix} A_1 & -W^{-\frac{1}{2}}B_1 \\ A_2 & -W^{-\frac{1}{2}}B_2 \end{bmatrix}$$

do not vanish. Where W is the constant, positive, diagonal weight matrix of (VII).

We make use of a counter example to show that even a simple self-adjoint boundary value problem on a graph need not be regular.

Consider the graph

with one node, v , and the second order operator

$$\frac{-d^2y}{dx^2} + qy = \lambda y,$$

with boundary conditions of the form

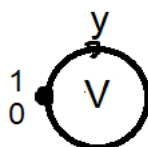
$$y(0) = y(1),$$

$$y'(0) = y'(1),$$

at v .

We then have that

$$\chi^+ = -\det \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} = 0$$



i.e. we don't have regularity.

Most self-adjoint problems on graphs are not regular, as is evident from the above example.

Conclusion:-

In this paper we have proved that a self-adjoint boundary value problem on a graph can be considered as a self adjoint system. This system was then shown to be equivalent to a system of twice the dimension but with separated boundary conditions. Abstract Prufer angle methods were then used to find eigenvalue asymptotic. We then returned to original graph structure, where using techniques from partial differential equations. We set up a variational formulation for boundary value problems on graphs. From this we were able to give a type of Dirichlet – Neumann bracketing for boundary problems on graphs. Consequently, eigenvalue and eigenfunction asymptotic approximations were obtained.

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