LA-13978
Approved for public release;
distribution is unlimited.

Applications of Lie Groups and Gauge Functions to the Construction of Exact Difference Equations for Initial and Two-Point Boundary Value Problems

Los Alamos
NATIONAL LABORATORY

Edited by Patricia W. Mendius, Group IM-1
Prepared by Wendy Burditt, Group IM-1

LA-13978
Issued: August 2002

Applications of Lie Groups and Gauge Functions to the Construction of Exact Difference Equations for Initial and Two-Point Boundary Value Problems

Roy Axford*

*Consultant at Los Alamos. Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, 103 S. Goodwin, Urbana, IL 61801

Los Alamos
NATIONAL LABORATORY

CONTENTS

Applications of Lie Groups and Gauge Functions to the Construction of Exact Difference Equations for Initial and Two-Point Boundary Value Problems

by

Roy A. Axford*

ABSTRACT

New methods are developed to construct exact difference equations from which numerical solutions of both initial value problems and two-point boundary value problems involving first and second order ordinary differential equations can be computed. These methods are based upon the transformation theory of differential equations and require the identification of symmetry properties of the differential equations. The concept of the divergence-invariance of a variational principle is also applied to the construction of difference equations. It is shown how first and second order ordinary differential equations that admit groups of point transformations can be integrated numerically by constructing any number of exact difference equations.

1.0. Introduction

The general objective of this study is to develop methods that are capable of producing exact difference equations which can provide precise numerical solutions of initial value problems involving first and second order ordinary differential equations and two-point boundary value problems involving Sturm-Liouville second order differential operators. The methods developed herein are based upon the transformation group theory of both differential equations and variational principles. A given initial value or two-point boundary value problem is transformed into canonical variables in terms of which an exact difference equation can be more directly constructed. The canonical variables are found with the generators of groups of point transformation that are admitted by first and second order differential equations that appear in initial value and two-point boundary value problems. New variables in terms of which an exact difference equation can be constructed are not unique. In principle, an infinite number of new sets of dependent and independent variables can be determined from the symmetries of first and second order ordinary differential equations. It is shown that this fact permits the introduction of new variables in such a way as to simplify the explicit construction of exact difference equations.

When a linear second order ordinary differential equation is written in its self-adjoint form, it can be thought of as the Euler-Lagrange equation of a variational

* Consultant at Los Alamos: Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, 103 S. Goodwin, Urbana, Illinois 61801.

principle. A variational principle can be a divergence-invariant of a subgroup of point transformations of a higher dimensional group admitted by the corresponding Euler-Lagrange equation. The divergence-invariance property of a variational principle leads to the construction of a gauge function in terms of which Noether's theorem yields a conservation law. Conservation laws can be worked out for each group of point transformations for which the variational principle is a divergence-invariant and then used to construct exact two-term recurrence relations that yield exact numerical results for the solutions of two-point boundary value problems. Exact two-term recurrence relations that come out of divergence-invariance symmetries can also be used to construct exact second order difference equations to solve numerically second order ordinary differential equations. Numerical algorithms that can be developed on the basis of the concepts discussed above are illustrated by the construction of numerical Green's functions for the Sturm-Liouville second order differential operator that appears in two-point boundary value problems and by the construction of numerical solutions of the neutron diffusion equation. It is shown that two-term recurrence relations provide more effective numerical algorithms than second order difference equations for the construction of numerical solutions of two-point boundary value problems that involve second order ordinary differential equations.

2.0. Exact Difference Equations for Initial Value Problems

Suppose that a first order ordinary differential equation, namely,

$$y^1(x) = f(x,y) \quad , \tag{1}$$

is given and that a numerical solution is sought subject to the initial condition at $x = x_0$,

$$y(x_0) = y_0 \quad . \tag{2}$$

Many numerical techniques have appeared in the past to provide approximate solutions to this initial value problem with finite difference simulations. Although approximate results with acceptable accuracy can be obtained, how is it possible to construct an **exact** difference equation simulation, rather than an approximate, in a systemic way to provide an exact numerical solution to the above initial value problem? An exact difference equation simulation is defined by the properties that follow: (1) it produces numerically the exact solution to the differential equation, (2) the solution $y(x+h)$ at $x+h$ can be computed from the solution $y(x)$ at x for an increment h in the independent variable with arbitrary value, that is, the difference equation is valid for any size increment in the independent variable, and (3) the difference equation and the differential equation it simulates are both invariant under the same group of point transformations.

2.1. First Method for Constructing Exact Difference Equations

Assume that the ordinary differential equation $y^1 = f(x,y)$ admits a one-parameter group of point transformations whose infinitesimal transformation is represented by the group generator,

$$\hat{U} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} \quad , \tag{3}$$

in which $\xi(x,y)$ is the Lie derivative of the independent variable x and $\eta(x,y)$ is the Lie derivative of the dependent variable $y(x)$. Let $X(x,y)$ and $Y(x,y)$ be a new set of variables in terms of which the group generator becomes

$$\hat{\hat{U}} = \hat{U}X \frac{\partial}{\partial X} + \hat{U}Y \frac{\partial}{\partial Y} \quad . \tag{4}$$

If these new variables are determined as solutions of the linear first order partial differential equations,

$$\hat{U}X = \xi(x,y)\frac{\partial X}{\partial x} + \eta(x,y)\frac{\partial X}{\partial y} = 0 \quad , \tag{5}$$

and

$$\hat{U}Y = \xi(x,y)\frac{\partial Y}{\partial x} + \eta(x,y)\frac{\partial Y}{\partial y} = 1 \quad , \tag{6}$$

then the transformed group generator becomes

$$\hat{\hat{U}} = \frac{\partial}{\partial Y} \quad . \tag{7}$$

The general form of a first order ordinary differential equation that admits the group of point transformations with this generator is

$$\frac{dY}{dX} = H(X) \quad , \tag{8}$$

in which the function $H(X)$ depends only on the new independent variable X. By introducing the new variables $X(x,y)$ and $Y(x,y)$ the differential equation $y^1 = f(x,y)$ can be transformed to the alternative form given in Eq. (8) in which the variables are separated.

Integration of Eq. (8) produces the following difference equation:

$$Y\big(x+h, y(x+h)\big) = Y\big(x, y(x)\big) + \int_{X(x,y(x))}^{X(x+h,y(x+h))} dX \;\; H(X) \quad . \tag{9}$$

In general, this is a transcendental equation for $y(x+h)$, but it is an **exact** difference equation that is valid for any increment h in the independent variable. An alternative integration of Eq. (8) yields

$$Y\big(x, y(x)\big) = Y\big(x_0, y(x_0)\big) + \int_{X(x_0,y(x_0))}^{X(x,y(x))} dX \;\; H(X) \quad , \tag{10}$$

which contains the initial condition $y(x_0) = y_0$ at $x = x_0$ explicitly. By comparing the results obtained in Eqs. (9) and (10) it is seen that the difference equation given by Eq. (9) can be obtained from Eq. (10) by making the following replacements. In Eq. (10) replace x_0 with x, $y(x_0)$ with $y(x)$, x with $x+h$, and $y(x)$ with $y(x+h)$ for any arbitrary value h.

An exact difference equation to integrate the linear first order ordinary differential equation,

$$y^1(x) + P(x)y(x) = Q(x) \quad , \tag{11}$$

can be constructed as follows. This equation admits the group of point transformations generated by

$$\hat{U} = \eta(x)\frac{\partial}{\partial y} \quad , \tag{12}$$

where the coordinate function is a solution of

$$\eta^1(x) + P(x)\eta(x) = 0 \quad , \tag{13}$$

that is,

$$\eta(x) = \exp\left(-\int P(x)dx\right) \quad . \tag{14}$$

The canonical variables of this group are given by

$$X(x,y) = x \quad , \tag{15}$$

and

$$Y(x,y) = \frac{y}{\eta(x)} \quad . \tag{16}$$

Since $dX = dx$, and

$$dY = \frac{-y\eta^1(x)dx}{\eta^2(x)} + \frac{dy}{\eta(x)} \quad , \tag{17}$$

transforming Eq. (11) to canonical variables yields

$$\frac{dY}{dX} = \frac{Q(X)}{\eta(X)} \quad . \tag{18}$$

Integrating between the *nth* and *(n + 1)st* arbitrarily located grid points produces the exact difference equation,

$$y(x_{n+1}) = \frac{\eta(x_{n+1})}{\eta(x_n)}y(x_n) + \eta(x_{n+1})\int_{x_n}^{x_{n+1}} dx\frac{Q(x)}{\eta(x)} \tag{19}$$

The preceeding analysis shows that many exact difference equations can be constructed to obtain numerical solutions of first order ordinary differential equations. To illustrate the method developed above for a nonlinear first order differential equation, consider the one-parameter group that is generated by

$$\hat{U} = \phi(x)y^v\frac{\partial}{\partial y} \quad , \tag{20}$$

where $\phi(x)$ is an arbitrary function and v is a constant. We first derive the general form of a first order ordinary differential equation that admits this group and then show how to construct an exact difference equation to obtain its solution numerically.

The first prolongation of the group generator given in Eq. (20) is

$$\hat{U}^{(1)} = \phi(x)y^{v}\frac{\partial}{\partial y} + \left[\phi^{1}(x)y^{v} + v\phi(x)y^{v-1}y^{1}\right]\frac{\partial}{\partial y^{1}} \quad . \tag{21}$$

An invariant function and first differential invariant are found for this group by solving the characteristic equations of the first order partial differential equation, $\hat{U}^{(1)}f = 0$. These are

$$\frac{dx}{0} = \frac{dy}{\phi(x)y^{v}} = \frac{dy^{1}}{\phi^{1}(x)y^{v} + v\phi(x)y^{v-1}y^{1}} \quad . \tag{22}$$

The first and the second members show that

$$u(x,y) = x \tag{23}$$

is an invariant function, while a first differential invariant is obtained by integrating the differential equation obtained from the second and the third members, namely,

$$\frac{dy^{1}}{dy} = \frac{\phi^{1}(x)y^{v} + v\phi(x)y^{v-1}y^{1}}{\phi(x)y^{v}} = \frac{\phi^{1}(x)}{\phi(x)} + \frac{vy^{1}}{y} \quad . \tag{24}$$

A first differential invariant is found to be

$$v\left(x,y,y^{1}\right) = y^{-v}y^{1} + \frac{\phi^{1}(x)}{\phi(x)}\frac{y^{1-v}}{(v-1)} \quad . \tag{25}$$

Since the general solution of a linear first order partial differential equation is an arbitrary function of solutions of its characteristic equations, we find that

$$y^{1} + \frac{\phi^{1}(x)}{\phi(x)}\frac{y}{(v-1)} = y^{v}F(x) \quad , \tag{26}$$

in which *F(x)* is an arbitrary function, is the general form of a first order ordinary differential equation that admits the group with the generator give in Eq. (20).

To obtain an exact difference equation to obtain numerical solutions of this Bernoulli equation we first transform it to new variables computed with Eqs. (5) and (6), which for this case become

$$\phi(x)y^{v}\frac{\partial X}{\partial y} = 0 \quad , \tag{27}$$

and

$$\phi(x)y^{v}\frac{\partial Y}{\partial y} = 1 \quad . \tag{28}$$

Accordingly, the new variables are

$$X(x,y) = x \quad , \tag{29}$$

and

$$Y(x,y)=\frac{1}{\phi(x)}\left(\frac{y^{1-v}}{1-v}\right) \quad . \tag{30}$$

Since

$$dX = dx \quad , \tag{31}$$

and

$$dY = -\frac{\phi^1(x)}{\phi^2(x)}\frac{y^{1-v}}{(1-v)}dx+\frac{y^{-v}}{\phi(x)}y^1 \quad , \tag{32}$$

it follows that

$$\frac{dY}{dX}=-\frac{\phi^1(x)}{\phi^2(x)}\frac{y^{1-v}}{(1-v)}+\frac{y^{-v}}{\phi(x)}y^1 \quad . \tag{33}$$

Accordingly, the Bernoulli equation (26) transforms to

$$\frac{dY}{dX}=\frac{F(X)}{\phi(X)} \quad . \tag{34}$$

From the exact difference equation found in Eq. (9) specialized for this case, it is seen that the Bernoulli equation,

$$y^1+\frac{\phi^1(x)}{(v-1)\phi(x)}y=y^vF(x) \quad , \tag{35}$$

can be integrated numerically with the exact difference equation,

$$y^{1-v}(x+h)=\frac{\phi(x+h)}{\phi(x)}y^{1-v}(x)+(1-v)\phi(x+h)\int_x^{x+h}dX\frac{F(X)}{\phi(X)} \quad , \tag{36}$$

which is valid for an arbitrary increment h in the independent variable. The indicated quadrature can be done once the two arbitrary functions $F(x)$ and $\phi(x)$ have been specified.

In the limit as the mesh size h goes to zero, the exact difference equation (36) should reduce to the Bernoulli equation (26). That this does, in fact, occur can be demonstrated as follows. By putting the approximations,

$$\phi(x+h)=\phi(x)+h\phi^1(x)+\ldots \quad , \tag{37}$$

$$y^{1-v}(x+h)=y^{1-v}(x)+(1-v)hy^{-v}(x)y^1(x)+\ldots \quad , \tag{38}$$

and

$$\int_x^{x+h}dX\frac{F(X)}{H(X)}=\frac{F(x)}{H(x)}h+\ldots \quad , \tag{39}$$

into Eq. (36) and taking the limit as the mesh spacing goes to zero, the Bernoulli equation (26) is recovered.

2.2. Second Method for Constructing Exact Difference Equations

The new variables *X(x,y)* and *Y(x,y)* that are obtained by solving the two first order linear partial differential equations (5) and (6) are sometimes called Lie's canonical variables. The method for constructing exact difference equations for obtaining numerical solutions of first order ordinary differential equations that was developed in the previous section follows from the introduction of Lie's canonical variables, which put the differential equation into a form that is invariant under translations along the *Y*-axis and directly integrable. Variables other than Lie's canonical variables may also be introduced to construct exact difference equations.

Suppose that new variables *X(x,y)* and *Y(x,y)* are introduced as solutions of the two linear first order partial differential equations,

$$\hat{U}X = \xi(x,y)\frac{\partial X}{\partial x} + \eta(x,y)\frac{\partial X}{\partial y} = 0 \quad , \tag{40}$$

and

$$\hat{U}Y = \xi(x,y)\frac{\partial Y}{\partial x} + \eta(x,y)\frac{\partial Y}{\partial y} = Y \quad . \tag{41}$$

Then the transformed group generator is

$$\hat{\bar{U}} = Y\frac{\partial}{\partial Y} \quad , \tag{42}$$

and the general form of a first order differential equation that admits the group generated by Eq. (42)

$$\frac{dY}{dX} = G(X)Y \quad , \tag{43}$$

where *G(X)* is an arbitrary function of the new independent variable. Integration of Eq. (43) produces an exact difference equation, namely,

$$Y\big(x+h, y(x+h)\big) = Y\big(x, y(x)\big)\exp\int_{X(x,y(x))}^{X(x+h,y(x+h))} dX \;\; G(X) \quad . \tag{44}$$

This is, in general, a transcendental equation to compute $y(x + h)$ from $y(x)$ for an arbitrary increment in the independent variable equal to h.

Accordingly, we have the following result. If the differential equation,

$$y^1 = f(x,y) \quad , \tag{45}$$

admits a one-parameter group of point transformation whose infinitesimal transformation is represented by the group generator,

$$\hat{U} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} \quad , \tag{46}$$

and if new variables *X(x,y)* and *Y(x,y)* are introduced as solutions of the two first order partial differential equations (40) and (41), then the result given in Eq. (44) is an exact difference equation from which exact numerical solutions of Eq. (45) can be computed for any grid size *h*.

To illustrate this theorem, a second exact difference equation to integrate numerically the Bernoulli equation,

$$y^1 + \frac{\phi^1(x)}{\phi(x)}\frac{y}{v-1} = y^v F(x) \quad , \tag{47}$$

will be constructed by applying Eq. (44). Since equation (47) admits the group of point transformations generated by

$$\hat{U} = \phi(x) y^v \frac{\partial}{\partial y} \quad , \tag{48}$$

the new variables are solutions of

$$0\frac{\partial X}{\partial x} + \phi(x) y^v \frac{\partial X}{\partial y} = 0 \quad , \tag{49}$$

and

$$0\frac{\partial Y}{\partial x} + \phi(x) y^v \frac{\partial Y}{\partial y} = Y \quad . \tag{50}$$

Hence, we have

$$X(x,y) = x \quad , \tag{51}$$

and

$$Y(x,y) = \exp\left[\frac{1}{(1-v)\phi(x)} y^{1-v}(x)\right] \quad , \tag{52}$$

so that Eq.(47) transforms to

$$\frac{dY}{dX} = Y\frac{F(X)}{\phi(X)} \quad . \tag{53}$$

Hence, the exact difference equation (44) reduces to

$$Y\big(x+h, y(x+h)\big) = Y\big(x, y(x)\big)\exp\int_x^{x+h} dX \frac{F(X)}{\phi(X)} \quad , \tag{54}$$

from which numerical solutions of (47) can be computed.

2.3. Proof that Invariant Difference Equations are Exact

Any number of exact difference equations can be constructed to obtain numerical solutions of first order nonlinear differential equations provided that a symmetry property of the differential equation is known. The methods developed above follow directly by introducing new variables computed with the group generator of a transformation group admitted by the differential equation.

The fact that the difference equations constructed by the above methods are exact can be demonstrated by the following argument. Consider the difference equation (36) found for the Bernoulli equation (35), which can be rewritten in the form,

$$\begin{aligned}\Phi\big(x, x+h, y(x), y(x+h)\big) = y^{1-\nu}(x+h) - \frac{\phi(x+h)}{\phi(x)}\, y^{1-\nu}(x) \\ -(1-\nu)\phi(x+h)\int_x^{x+h} dX\, \frac{F(X)}{\phi(X)} = 0 \quad .\end{aligned} \tag{55}$$

For equation (55) to be an exact difference equation, it must admit the same group as the Bernoulli equation itself. This group has the generator given in Eq. (20). Let $\hat{U}^{(G)}$ denote the prolongation of this generator to the grid point values of the dependent variable. This prolongation is given by

$$\hat{U}^{(G)} = \phi(x)y^{\nu}(x)\frac{\partial}{\partial y(x)} + \phi(x+h)y^{\nu}(x+h)\frac{\partial}{\partial y(x+h)} \quad . \tag{56}$$

The necessary and sufficient condition that the difference equation (55) admits the same group as the Bernoulli equation it simulates is that

$$\hat{U}^{(G)}\Big[\Phi\big(x, x+h, y(x), y(x+h)\big)\Big] = 0 \quad , \quad \mathrm{mod}(\Phi = 0) \tag{57}$$

That this condition is, in fact, satisfied can be verified by the evaluation of the left hand side of Eq. (57). Accordingly, the difference equation is exact because it and the Bernoulli equation (35) it simulates do admit the same group of point transformations.

3.0. Exact Difference Equations for Two-Point Boundary Value Problems

Methods for obtaining numerical solutions of two-point boundary value problems that involve second order ordinary differential equations include (1) the shooting method, which inherits all the stability issues that arise in the numerical solution of initial value problems, and (2) reduction to systems of algebraic equations by finite differences, finite elements, and finite volumes. In this section a new method for solving two-point boundary value problems numerically is developed. It will be shown how the symmetries of second order ordinary differential equations and relevant variational principles can be used to derive two-point recurrence relations with which numerical results for two-point boundary value problems can be computed. These two-term recurrence relations can also be used to construct exact second order difference equations that simulate second order ordinary differential equations.

3.1. Gauge Functions and Invariant Variational Principles

The self-adjoint form of a second order ordinary differential equation, namely,

$$\frac{d}{dx}\left[p(x)y^1(x)\right]-q(x)y(x)+s(x)=0 \quad , \tag{58}$$

for $x_1 \le x \le x_2$, can be regarded as the Euler-Lagrange equation of the variational principle functional,

$$J=\int_{x_1}^{x_2} dx\left[p(x)\left(y^1\right)^2+q(x)y^2-2ys(x)\right] \quad , \tag{59}$$

when homogeneous Dirichlet, Neumann or Robin boundary conditions are specified at the end points of the interval, $x_1 \le x \le x_2$. The Euler-Lagrange equation is

$$\frac{\partial F}{\partial y}-D_x\left(\frac{\partial F}{\partial y^1}\right)=0 \quad , \tag{60}$$

where

$$F\left(x,y,y^1\right)=p(x)\left(y^1\right)^2+q(x)y^2-2ys(x) \quad , \tag{61}$$

and D_x is the total derivative operator, namely

$$D_x=\frac{\partial}{\partial x}+y^1\frac{\partial}{\partial y}+y^{11}\frac{\partial}{\partial y^1}+\ldots \quad . \tag{62}$$

The variational principle functional (59) can be an integral invariant of a group of point transformations. Let the once-extended group have the infinitesimal transformation,

$$\bar{x}=x+\xi(x,y)\delta a \quad , \tag{63}$$

$$\bar{y}=y+\eta(x,y)\delta a \quad , \tag{64}$$

and

$$\bar{y}^1=y^1+\eta^{(1)}\left(x,y,y^1\right)\delta a \quad , \tag{65}$$

where δa is a small change in the group parameter away from the identity value. The functional (59) is said to be divergence-invariant under the group of point transformations with the once-extended infinitesimal transformations given by Eqs. (63)–(65) with

$$\eta^{(1)}\left(x,y,y^1\right)=D_x\eta(x,y)-y^1D_x\xi(x,y) \tag{66}$$

provided that the following condition is satisfied:

$$\int_{\bar{x}_1}^{\bar{x}_2} d\bar{x}\;\; F\left(\bar{x},\bar{y},\bar{y}^1\right)-\int_{x_1}^{x_2} dx\;\; F\left(x,y,y^1\right)=\delta a\int_{x_1}^{x_2} dx\;\; D_x\phi(x,y) \quad , \tag{67}$$

in which the function $\phi(x,y)$ is called the gauge function. If $\phi(x,y)=0$, the functional (59) is said to be absolutely invariant under the group. By introducing the Jacobian of the infinitesimal transformation, namely,

$$\frac{d\bar{x}}{dx} = 1 + D_x \xi(x,y)\delta a \quad , \tag{68}$$

the first integral in Eq. (67) becomes

$$\int_{\bar{x}_1}^{\bar{x}_2} d\bar{x} F\left(\bar{x}, \bar{y}, \bar{y}^1\right) = \int_{x_1}^{x_2} dx \frac{d\bar{x}}{dx} F\left(\bar{x}, \bar{y}, \bar{y}^1\right) \quad . \tag{69}$$

With a multidimensional Taylor series to terms of order δa, we have

$$F\left(\bar{x}, \bar{y}, \bar{y}^1\right) = F\left(x, y, y^1\right) + \hat{U}^{(1)} F\left(x, y, y^1\right)\delta a + \ldots \quad , \tag{70}$$

where the symbol $\hat{U}^{(1)}$ of the once-extended infinitesimal transformation is given by

$$\hat{U}^{(1)} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} + \eta^{(1)}\left(x,y,y^1\right)\frac{\partial}{\partial y^1} \quad . \tag{71}$$

Substituting Eqs. (68) and (70) into Eq. (69) yields

$$\begin{aligned} \int_{\bar{x}_1}^{\bar{x}_2} d\bar{x} F\left(\bar{x}, \bar{y}, \bar{y}^1\right) &= \int_{x_1}^{x_2} dx\left[1 + D_x \xi(x,y)\delta a\right]\left[F\left(x,y,y^1\right) + \hat{U}^{(1)} F\left(x,y,y^1\right)\delta a\right] \ , \\ &= \int_{x_1}^{x_2} dx F\left(x,y,y^1\right) + \delta a \int_{x_1}^{x_2} dx\left[F\left(x,y,y^1\right) D_x \xi(x,y) + \hat{U}^{(1)} F\left(x,y,y^1\right)\right] \ , \end{aligned} \tag{72}$$

to first order terms in δa. With Eq. (72) the divergence-invariance condition given in Eq. (67) reduces to

$$\hat{U}^{(1)} F\left(x,y,y^1\right) + F\left(x,y,y^1\right) D_x \xi = D_x \phi(x,y) \ , \tag{73}$$

which becomes, when written out in full,

$$\xi(x,y)\frac{\partial F}{\partial x} + \eta(x,y)\frac{\partial F}{\partial y} + \left[D_x \eta(x,y) - y^1 D_x \xi(x,y)\right]\frac{\partial F}{\partial y^1} + F\, D_x \xi(x,y) = D_x \phi(x,y) \quad . \tag{74}$$

This equation can be used to determine groups of point transformations admitted by the functional (59) when the Lagrangian $F(x,y,y^1)$ is given.

With the Lagrangian,

$$F\left(x,y,y^1\right) = p(x)\left(y^1\right)^2 + q(x)y^2 - 2ys(x) \quad , \tag{75}$$

in the variational principle (59) for which the differential equation (58) is the Euler-Lagrange equation, the divergence-invariance condition (74) reduces to

$$\begin{aligned}&\xi\left[p^1\left(y^1\right)^2+q^1y^2-2ys^1\right]+2(qy-s)\eta\\&+2py^1\left[\frac{\partial\eta}{\partial x}+y^1\left(\frac{\partial\eta}{\partial y}-\frac{\partial\xi}{\partial x}\right)-\left(y^1\right)^2\frac{\partial\xi}{\partial y}\right]\\&+\left[p\left(y^1\right)^2+qy^2-2ys\right]\left(\frac{\partial\xi}{\partial x}+y^1\frac{\partial\xi}{\partial y}\right)=\frac{\partial\phi}{\partial x}+\frac{\partial\phi}{\partial y}y^1\quad.\end{aligned}\tag{76}$$

This equation must be an identity in the derivative y^1, so equating coefficients of like powers of y^1 on both sides produces the following four relations:

$$p(x)\frac{\partial\xi}{\partial y}(x,y)=0\quad,\tag{77}$$

$$\xi(x,y)p^1(x)+2p(x)\left[\frac{\partial\eta}{\partial y}(x,y)-\frac{\partial\xi}{\partial x}(x,y)\right]+p(x)\frac{\partial\xi}{\partial x}(x,y)=0\quad,\tag{78}$$

$$2p(x)\frac{\partial\eta}{\partial x}(x,y)+q(x)y^2\frac{\partial\xi}{\partial y}(x,y)-2ys(x)\frac{\partial\xi}{\partial y}(x,y)=\frac{\partial\phi}{\partial y}(x,y)\quad,\tag{79}$$

and

$$\begin{aligned}&\xi(x,y)q^1(x)y^2-2y\xi(x,y)s^1(x)+2\left[q(x)y-s(x)\right]\eta(x,y)\\&+q(x)y^2\frac{\partial\xi}{\partial x}(x,y)-2ys(x)\frac{\partial\xi}{\partial x}(x,y)=\frac{\partial\phi}{\partial x}(x,y)\quad.\end{aligned}\tag{80}$$

These last four equations are the determining equations for the coordinate functions $\xi(x.y)$ and $\eta(x,y)$ in the group generator,

$$\hat{U}=\xi(x,y)\frac{\partial}{\partial x}+\eta(x,y)\frac{\partial}{\partial y}\quad,\tag{81}$$

and the gauge function $\phi(x,y)$ such that the functional (59) is divergence-invariant under the group of point transformations with this generator. From Eq. (77) it follows that

$$\xi(x,y)=\xi(x)\quad,\tag{82}$$

a function of only the independent variable x. This means that the symmetry transformations generated by (81) are fiber preserving. In view of Eq. (82) the three remaining determining equations (78) to (80) simplify to

$$\xi(x)p^1(x)+2p(x)\left[\frac{\partial\eta}{\partial y}(x,y)-\xi^1(x)\right]+p(x)\xi^1(x)=0\quad,\tag{83}$$

$$2p(x)\frac{\partial\eta}{\partial x}(x,y)=\frac{\partial\phi}{\partial y}(x,y)\quad,\tag{84}$$

and

$$\xi(x)q^1(x)y^2 - 2y\xi(x)s^1(x) + 2\big[q(x)y - s(x)\big]\eta(x,y)$$
$$+q(x)y^2 s^1(x) - 2ys(x)\xi^1(x) = \frac{\partial\phi}{\partial x}(x,y) \quad . \tag{85}$$

A special case of the determining equations (83) to (85) that is useful in working out numerical solutions of the two-point boundary value problem based on the inhomogeneous second order differential equation (58) is found by setting $\xi(x) = 0$. Then from Eq. (83) we have

$$\frac{\partial\eta}{\partial y}(x,y) = 0 \quad , \tag{86}$$

so that

$$\eta(x,y) = \eta(x) \quad , \tag{87}$$

a function of the independent variable x only when $\xi(x) = 0$. In this case we have from Eqs. (84) and (85)

$$\frac{\partial\phi}{\partial y}(x,y) = 2p(x)\eta^1(x) \quad , \tag{88}$$

and

$$\frac{\partial\phi}{\partial y}(x,y) = 2\big[q(x)y - s(x)\big]\;\eta(x) \quad . \tag{89}$$

Integrating Eq. (88) gives

$$\phi(x,y) = 2p(x)\eta^1(x)y + A(x) \quad . \tag{90}$$

The function $A(x)$ is to be determined from

$$\frac{\partial\phi}{\partial x}(x,y) = 2\frac{d}{dx}\Big[p(x)\eta^1(x)\Big]y + A^1(x) \tag{91}$$

and Eq. (89). Comparing Eqs. (89) and (91) shows that

$$\frac{d}{dx}\Big[p(x)\eta^1(x)\Big] = q(x)\eta(x) \quad , \tag{92}$$

and

$$A^1(x) = -2s(x)\eta(x) \quad , \tag{93}$$

so that

$$A(x) = -2\int dx \;\; s(x)\eta(x) \quad , \tag{94}$$

and the gauge function is given by

$$\phi(x,y) = 2p(x)\eta^1(x)y - 2\int dx \;\; s(x)\eta(x) \quad . \tag{95}$$

The above calculations may be summarized by the following theorem. The variational principle functional,

$$J = \int_{x_1}^{x_2} dx \left[p(x)\left(y^1\right)^2 + q(x)y^2 - 2ys(x) \right] \quad , \tag{96}$$

for which the Euler-Lagrange satisfying homogeneous Dirichlet, Neumann, or Robin boundary conditions is the second order ordinary differential equation,

$$\frac{d}{dx}\left[p(x)y^1 \right] - q(x)y + s(x) = 0 \quad , \tag{97}$$

is divergence-invariant under the group of point transformations generated by

$$\hat{U} = \eta(x)\frac{\partial}{\partial y} \quad , \tag{98}$$

where the coordinate function $\eta(x)$ is a solution of the homogenous counterpart of Eq. (97), namely,

$$\frac{d}{dx}\left[p(x)\eta^1(x) \right] - q(x)\eta(x) = 0 \quad , \tag{99}$$

and the gauge function is given by

$$\phi(x,y) = 2p(x)\eta^1(x)y - 2\int dx \;\; s(x)\eta(x) \quad . \tag{100}$$

This theorem leads to a conservation law which is a form of Noether's theorem with a gauge function.

To derive this conservation law we start from

$$\int_{x_1}^{x_2} dx \left[F D_x \xi + \hat{U}^{(1)} F - D_x \phi \right] = 0 \quad , \tag{101}$$

the divergence-invariance condition, which in expanded form is given by

$$\int_{x_1}^{x_2} dx \left[F D_x \xi + \xi \frac{\partial F}{\partial x} + \eta \frac{\partial F}{\partial y} + \left(D_x \eta - y^1 D_x \xi \right) \frac{\partial F}{\partial y^1} - D_x \phi(x,y) \right] = 0 \quad . \tag{102}$$

With the identities,

$$F D_x \xi = D_x(\xi F) - \xi D_x F \quad , \tag{103}$$

$$D_x \eta \frac{\partial F}{\partial y^1} = D_x\left(\eta \frac{\partial F}{\partial y^1} \right) - \eta D_x \left(\frac{\partial F}{\partial y^1} \right) \quad , \tag{104}$$

$$y^1 D_x \xi \frac{\partial F}{\partial y^1} = D_x\left(y^1 \frac{\partial F}{\partial y^1} \xi \right) - \xi y^1 D_x \left(\frac{\partial F}{\partial y^1} \right) - \xi y^{11} \frac{\partial F}{\partial y^1} \quad , \tag{105}$$

and

$$D_x F = \frac{\partial F}{\partial x} + y^1 \frac{\partial F}{\partial y} + y^{11} \frac{\partial F}{\partial y^1} \quad , \tag{106}$$

the divergence-invariance condition of Eq. (102) takes the alternative form,

$$\int_{x_1}^{x_2} dx \left\{ D_x\left[\xi F - \xi y^1 \frac{\partial F}{\partial y} + \eta \frac{\partial F}{\partial y^1} - \phi(x,y)\right] + \left(\eta - \xi y^1\right)\left[\frac{\partial F}{\partial y} - D_x\left(\frac{\partial F}{\partial y^1}\right)\right]\right\} = 0 \quad . \tag{107}$$

This equation can be interpreted as follows. On solutions of the Euler-Lagrange equation,

$$\frac{\partial F}{\partial y} - D_x\left(\frac{\partial F}{\partial y'}\right) = 0 \quad , \tag{108}$$

the conservation law,

$$\xi\left[F - y^1 \frac{\partial F}{\partial y^1}\right] + \eta \frac{\partial F}{\partial y^1} - \phi(x,y) = \text{constant} \quad , \tag{109}$$

holds and is, in fact, a first integral of (97). Accordingly, it follows that, when the coordinate functions of the group generator,

$$\hat{U} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} \quad , \tag{110}$$

are $\xi(x,y)=0$ and $\eta(x,y)=\eta(x)$, a solution of the homogeneous equation,

$$\frac{d}{dx}\left[p(x)\eta^1\right] - q(x)\eta(x) = 0 \quad , \tag{111}$$

a first integral obtained from Eqs. (100) and (108) for the second order differential equation,

$$\frac{d}{dx}\left[p(x)y^1\right] - q(x)y + s(x) = 0 \quad , \tag{112}$$

is given by

$$p(x)\eta(x)y^1 - p(x)\eta^1(x)y + \int dx\eta(x)s(x) = \text{constant} \quad . \tag{113}$$

This is a first order ordinary differential equation that admits the group generated by

$$\hat{U} = \eta(x)\frac{\partial}{\partial y} \quad , \tag{114}$$

with first extension,

$$\hat{U}^{(1)} = \eta(x)\frac{\partial}{\partial y} + \eta^1(x)\frac{\partial}{\partial y^1} \quad , \tag{115}$$

the same group admitted by both the second order differential equation (112) and variational principle functional (59). The canonical variables $X(x,y)$ and $Y(x,y)$ of this group are solutions of the first order partial differential equations,

$$0\frac{\partial X}{\partial x} + \eta(x)\frac{\partial X}{\partial y} = 0 \quad , \tag{116}$$

and

$$0\frac{\partial Y}{\partial x}+\eta(x)\frac{\partial Y}{\partial y}=1 \quad . \tag{117}$$

These solutions are

$$Y(x,y)=\frac{y}{\eta(x)} \quad , \tag{118}$$

and

$$X(x,y)=x \quad . \tag{119}$$

Since

$$dY=-\frac{\eta^1(x)}{\eta^2(x)}ydx+\frac{dy}{\eta(x)} \quad , \tag{120}$$

and

$$dX=dx \quad , \tag{121}$$

we have

$$\frac{dY}{dX}=\frac{1}{\eta^2(x)}\left[\eta(x)y^1-\eta^1(x)y\right] \quad . \tag{122}$$

Hence, in terms of the canonical variables the first integral in Eq. (113) of Eq. (112) is given by

$$\frac{dY}{dX}=\frac{(-1)}{p(X)\eta^2(X)}\int dX\eta(X)s(X)+\frac{\text{constant}}{\mathrm{p}(X)\eta^2(X)} \quad . \tag{123}$$

This relation can be applied in the following way to construct two-term recurrence relations with which numerical solutions of the two-point boundary value problem based on the second order differential equation (112) with homogeneous boundary conditions can be constructed. Let

$$H(X)=\frac{(-1)}{p(X)\eta^2(X)}\int dX\eta(X)s(X)+\frac{\text{constant}}{\mathrm{p}(X)\eta^2(X)} \quad , \tag{124}$$

so that Eq. (124) becomes

$$\frac{dY}{dX}=H(x) \quad . \tag{125}$$

Then integrating this equation yields the two difference equations that follow:

$$Y\big(x+h,y(x+h)\big)=Y\big(x,y(x)\big)+\int_{X(x,y(x))}^{X(x+h,y(x+h))}dX\,H(X) \quad , \tag{126}$$

and

$$Y\big(x,y(x)\big)=Y\big(x-h,y(x-h)\big)+\int_{X(x-h,y(x-h))}^{X(x,y(x))} dX\, H(X) \quad . \tag{127}$$

These difference equations are exact because the simultaneous symmetry properties of the second order ordinary differential equation (112) and its corresponding variational principle functional (59) are not lost in the discretisation process, which is, accordingly, symmetry preserving. Also, by subtracting Eq. (127) from Eq. (126) a second order difference equation that is exact is obtained.

3.2. Exact Difference Equations for Computing Green's Functions

Green's functions for the self-adjoint differential operator in Eq. (58) satisfy the differential equation,

$$\frac{d}{dx}\left[p(x)\frac{d}{dx}K\big(x|\xi\big)\right]-q(x)K\big(x|\xi\big)+\delta\big(x-\xi\big)=0 \quad , \tag{128}$$

on a domain $x_1 \le x \le x_2$ such that $x_1 \le \xi \le x_2$ with two-point homogeneous Dirichlet, Neumann or Robin boundary conditions specified at $x=x_1$ and $x=x_2$. At $x=\xi$ the Green's function is continuous, and its derivative is discontinuous with the discontinuity,

$$\lim_{\varepsilon \to 0}\left[\frac{d}{dx}K\big(\xi+\varepsilon|\xi\big)-\frac{d}{dx}K\big(\xi-\varepsilon|\xi\big)\right]=\frac{(-1)}{p(\xi)} \quad . \tag{129}$$

In this section two-term recurrence relations, which are exact difference equations, are obtained for computing numerical solutions of Eq. (128) for three cases. These are for (1) a single region domain in slab geometry, (2) a single region domain in spherical symmetry, and (3) a two region composite domain in slab geometry.

3.2.1. Numerical Green's Function for a Single Region Domain in Slab Geometry

In this case we want a numerical solution of the differential equation,

$$D\frac{d^2}{dx^2}K\big(x|\xi\big)-\Sigma_a K\big(x|\xi\big)+\delta\big(x-\xi\big)=0 \quad , \tag{130}$$

that satisfies the two-point boundary conditions,

$$\frac{dK}{dx}\big(0|\xi\big)=0 \quad , \tag{131}$$

and

$$K\big(a|\xi\big)=0 \quad , \tag{132}$$

on the domain $0 \le x \le a$. Within the context of the neutron diffusion equation, the notation in Eq. (130) is that Σ_a is the absorption cross section, and D is the diffusion coefficient. We can interpret Eq. (130) as the Euler-Lagrange equation of the variational principle,

$$J = \int_0^a dx \left\{ D\left[\frac{d}{dx}K\left(x|\xi\right)\right]^2 + \sum_a \left[K\left(x|\xi\right)\right]^2 - 2K\left(x|\xi\right)\delta\left(x-\xi\right) \right\} \quad . \tag{133}$$

Both the Green's function differential equation (130) and its corresponding functional admit the group of point transformations generated by

$$\hat{U} = \eta(x)\frac{\partial}{\partial K} \quad , \tag{134}$$

where the coordinate function η(x) is a solution of

$$\eta^{11}(x) - \alpha^2\eta(x) = 0 \quad . \tag{135}$$

Here α is the inverse diffusion length given by

$$\alpha^2 = \frac{\sum_a}{D} \quad . \tag{136}$$

The functional (133) is divergence-invariant under this group with the gauge function,

$$\phi\left(x,K\right) = 2D\eta^1(x)K\left(x|\xi\right) - 2\int dx\eta(x)\delta\left(x-\xi\right) \quad . \tag{137}$$

which takes one of two forms depending upon whether or not $x<\xi$ or $x>\xi$. For the interval $0\leq x\leq\xi$, the gauge function is

$$\phi\left(x,K\right) = 2D\eta^1(x)K\left(\mathrm{x}|\xi\right) \quad . \tag{138}$$

For the interval $\xi\leq x\leq a$, the gauge function is given by

$$\phi\left(x,K\right) = 2D\eta^1(x)K\left(x|\xi\right) - 2\eta\left(\xi\right) \quad . \tag{139}$$

The conservation law,

$$D\eta(x)\frac{d}{dx}K\left(x|\xi\right) - D\eta^1(x)K\left(x|\xi\right) + \int dx\,\eta(x)\delta\left(x-\xi\right) = \text{constant} \quad , \tag{140}$$

can be simplified by using the boundary condition at $x=0$ on the derivative of the Green's function and taking the solution of Eq. (135) for the coordinate function $\eta(x)$ that satisfies the boundary condition,

$$\eta^1(0) = 0 \quad . \tag{141}$$

That is, for these boundary conditions, we have

$$\eta(x) = \cosh\left(\alpha x\right) \quad . \tag{142}$$

Hence, the constant in the conservation law given by Eq. (140) can be taken to be zero, so it now takes two forms. These are

$$\eta(x)\frac{d}{dx}K\left(x|\varsigma\right) - \eta^1(x)K\left(x|\xi\right) = 0 \quad , \tag{143}$$

for the interval $0\leq x\leq\xi$, and

$$D\eta(x)\frac{d}{dx}K\left(x|\xi\right)-D\eta^{1}(x)K\left(x|\xi\right)+\eta\left(\xi\right)=0 \quad , \tag{144}$$

for the interval $\xi\le x\le a$. These last two equations can be written in the alternative forms,

$$\frac{d}{dx}\left[\frac{K\left(x|\xi\right)}{\eta(x)}\right]=0 \quad , \tag{145}$$

for $0\le x\le\xi$, and

$$\frac{d}{dx}\left[\frac{K\left(x|\xi\right)}{\eta(x)}\right]=\frac{(-1)\eta\left(\xi\right)}{D\eta^{2}(x)} \quad , \tag{146}$$

for $\xi\le x\le a$.

We now introduce grid points x_i for $1\le i\le N_1$ for $0\le x_i\le\xi$ and grid points x_j for $1\le j\le N_2$ for $\xi\le x_j\le a$. The grid points need not be uniformly spaced but can be arbitrarily selected. Integrating Eq. (146) between two grid points x_j and x_{j+1} in the interval $\xi\le x\le a$ produces

$$\frac{K\left(x_{j+1}|\xi\right)}{\cosh\left(\alpha x_{j+1}\right)}-\frac{K\left(x_{j}|\xi\right)}{\cosh\left(\alpha x_{j}\right)}=\frac{(-1)\cosh\left(\alpha\xi\right)}{D}\int_{x_j}^{x_{j+1}}\frac{dx}{\cosh^{2}\left(\alpha x\right)} \quad . \tag{147}$$

Since

$$\int\frac{dx}{\cosh^{2}\left(\alpha x\right)}=\frac{1}{\alpha}\left[\frac{\sinh\left(\alpha x\right)-\cosh\left(\alpha x\right)}{\cosh\left(\alpha x\right)}\right] \quad , \tag{148}$$

the two-term recurrence relation in Eq. (147) reduces to

$$K\left(x_{j}|\xi\right)=\frac{\cosh\left(\alpha x_{j}\right)}{\cosh\left(\alpha x_{j+1}\right)}K\left(x_{j+1}|\xi\right)+\frac{\cosh\left(\alpha\xi\right)\sinh\left[\alpha\left(x_{j+1}-x_{j}\right)\right]}{\alpha D\ \cosh\left(\alpha x_{j+1}\right)} \quad . \tag{149}$$

From the boundary condition on the Green's function at $x=a$, we have

$$K\left(x_{N_2}|\xi\right)=0 \quad , \tag{150}$$

so for $j=N_2-1$ we obtain from Eq. (149)

$$K\left(x_{N_2-1}|\xi\right)=\frac{\cosh\left(\alpha\xi\right)\sinh\left[x_{N_2}-x_{N_2-1}\right]}{\alpha D\ \cosh\left(\alpha x_{N_2}\right)} \quad . \tag{151}$$

Numerical values for the Green's function at all remaining grid points in the interval $\xi\le x\le a$ can be computed with the two-term recurrence relation of Eq. (149) by setting $j=N_2-2, N_2-3, N_2-4, \dots, 3, 2,$ 1 sequentially.

Integrating Eq. (145) between two grid points x_i and x_{i+1} that lie in the interval $0\le x\le\xi$ yields the two-term recurrence relation,

$$K\left(x_i|\xi\right) = \frac{\cosh\left(\alpha x_i\right)}{\cosh\left(\alpha x_{i+1}\right)} K\left(x_{i+1}|\xi\right) \quad , \tag{152}$$

which is evaluated sequentially for $i=N_1-1, N_1-2\ N_1-3, , 3, 2,$ 1 after using the fact that the Green's function is continuous at $x=\xi$, so that

$$K\left(x_{N_1}|\xi\right) = K\left(x_{j=1}|\varsigma\right) \quad . \tag{153}$$

The two-term recurrence relations found in Eqs. (149) and (152) produce exact values for the Green's function at arbitrarily located grid points in both the intervals $0 \le x \le \xi$ and $\xi \le x \le a$. The evaluations with these two recurrence relations proceed from right to left through the grid points because of the Dirichlet boundary condition imposed on the Green's function at the right boundary point, $x=a$.

3.2.2. Numerical Green's Function for a Single Region Domain in Spherical Geometry

The Green's function in this case satisfies the differential equation,

$$\frac{D}{r^2}\frac{d}{dr}\left[r^2 \frac{dK}{dr}\left(r|\xi\right)\right] - \Sigma_a K\left(r|\xi\right) + \frac{\delta\left(r-\xi\right)}{4\pi r^2} = 0 \quad , \tag{154}$$

together with the boundary conditions that $K\left(0|\xi\right)$ is finite and

$$K\left(a|\xi\right) = 0 \quad , \tag{155}$$

when the domain is defined by the inequality $0 \le r \le a$. This differential equation for the Green's function can be thought of as the Euler-Lagrange equation that corresponds to the variational principle functional,

$$J = \int_0^a dr \left\{ Dr^2 \left[\frac{d}{dr} K\left(r|\xi\right)\right]^2 + \Sigma_a \left[K\left(r|\xi\right)\right]^2 r^2 - \frac{K\left(r|\xi\right)\delta\left(r-\xi\right)}{2\pi} \right\} \quad . \tag{156}$$

The differential equation (154) defining the spherical geometry Green's function is a differential invariant of the group generated by

$$\hat{U} = \eta(r)\frac{\partial}{\partial K} \quad , \tag{157}$$

where the coordinate function $\eta(r)$ is a solution of

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 \frac{d\eta}{dr}(r)\right] - \alpha^2 \eta(r) = 0 \quad . \tag{158}$$

Since the Green's function is finite at $r=0$, we take this solution as

$$\eta(r) = \frac{\sinh(\alpha r)}{r} \quad . \tag{159}$$

The variational functional (156) is divergence-invariant under this same group with the gauge function,

$$\phi(r,K) = 2Dr^2\eta^1(r)K(r|\xi) - \frac{1}{2\pi}\int dr\eta(r)\delta(r-\xi) \quad . \tag{160}$$

The corresponding conservation law is given by

$$Dr^2\eta(r)\frac{d}{dr}K(r|\xi) - Dr^2\eta^1(r)K(r|\xi) = \frac{(-1)}{4\pi}\int dr\eta(r)\delta(r-\xi) \quad , \tag{161}$$

which takes one of two forms. These are

$$\frac{d}{dr}\left[\frac{K(r|\xi)}{\eta(r)}\right] = 0 \quad , \tag{162}$$

for the interval $0 \le r \le \xi$, and

$$\frac{d}{dr}\left[\frac{K(r|\xi)}{\eta(r)}\right] = \frac{(-1)\eta(\xi)}{4\pi Dr^2\eta^2(r)} \quad , \tag{163}$$

for the interval $\xi \le r \le a$. To derive a two-term recurrence relation for the interval $\xi \le r \le a$ from Eq. (163), we can use the fact that

$$\int \frac{dr}{r^2\eta^2(r)} = \int \frac{dr}{\sinh^2(\alpha r)} = \frac{1}{\alpha}\left[\frac{\sinh(\alpha r) - \cosh(\alpha r)}{\sinh(\alpha r)}\right] \quad . \tag{164}$$

Let r_j be the *jth* grid point in the interval $\xi \le r \le a$ for $1 \le j \le N_2$. Then integration of Eq. (63) produces

$$\frac{K(r_j|\xi)}{\eta(r_j)} = \frac{K(r_{j+1}|\xi)}{\eta(r_{j+1})} + \frac{\eta(\xi)}{4\pi\alpha D}\int_{\alpha r_j}^{\alpha r_{j+1}} \frac{dX}{\sinh^2(X)} \quad . \tag{165}$$

This reduces to the two-term recurrence relation,

$$K(r_j|\xi) = \frac{\sinh(\alpha r_j)}{\sinh(\alpha r_{j+1})}\frac{(r_{j+1})}{(r_j)}K(r_{j+1}|\xi) + \frac{\sinh(\alpha\xi)\sinh\left[\alpha(r_{j+1} - r_j)\right]}{4\pi\alpha D\xi r_j \sinh(\alpha r_{j+1})} \quad , \tag{166}$$

for $j=N_2-2, N_2-3, N_2-4, \ldots, 3, 2,$ 1. From the Dirichlet boundary condition at $r=a$, we have

$$K(r_{N_2}|\xi) = 0 \quad . \tag{167}$$

Hence, evaluating Eq. (166) at r_{N_2-1} yields

$$K(r_{N_2-1}|\xi) = \frac{\sinh(\alpha\xi)\sinh\left[\alpha(r_{N_2} - r_{N_2-1})\right]}{4\pi\alpha D r_{N_2-1}\sinh(\alpha r_{N_2})} \tag{168}$$

to start the grid point evaluations of the Green's function with Eq. (166) in the interval $\xi \le r \le a$. Let r_i be the *ith* grid point in the interval $0 \le r \le \xi$ for $1 \le i \le N_1$ with $r_1=0$. Integration of Eq. (162) produces

$$K\left(r_i\middle|\xi\right)=\frac{\sinh(\alpha r_i)K\left(r_{i+1}\middle|\xi\right)}{\sinh(\alpha r_{i+1})}\left(\frac{r_{i+1}}{r_i}\right) \tag{169}$$

as the two-term recurrence relation to obtain numerical values of the Green's function in the interval $0 \le r \le \xi$ for $i=N_1-1, N_1-2, N_1-3, \ldots, 3, 2, 1$. It may be noted that $K\left(r_{N_1}\middle|\xi\right)$ is known from the computations in the interval $\xi \le r \le a$, so computations for the interval $0 \le r \le \xi$ can be started by using the continuity of the Green's function at $r=\xi$. Also, since

$$\lim_{r\to 0}\left[\frac{\sinh(\alpha r)}{r}\right]=\alpha \quad , \tag{170}$$

the recurrence relation (169) yields a finite value for the Green's function at $r_1=0$ which is

$$K\left(r_1\middle|\xi\right)=\frac{\alpha r_2 K\left(r_2\middle|\xi\right)}{\sinh(\alpha r_2)} \quad . \tag{171}$$

The locations of the grid points in the two regions can be selected arbitrarily. The two recurrence relations (166) and (169) produce exact numerical values for the Green's function in the two intervals $0 \le r \le \xi$ and $\xi \le r \le a$, irrespective of the locations of the grid points because they are exact difference equations that preserve symmetry properties of the Green's function differential equation (154) and the corresponding variational principle given in Eq. (156).

3.2.3. Numerical Green's Function for a Two-Region Composite Domain in Slab Geometry

When the material properties are spatially dependent, the Green's function for the neutron diffusion operator satisfies the differential equation,

$$\frac{d}{dx}\left[D(x)\frac{d}{dx}K\left(x\middle|\xi\right)\right]-\Sigma_a(x)K\left(x\middle|\xi\right)+\delta\left(x-\xi\right)=0 \quad , \tag{172}$$

on a specified domain in slab geometry together with homogeneous two-point boundary conditions. This differential equation can be regarded as the Euler-Lagrange equation of the variational principle,

$$J=\int_{x_1}^{x_2} dx\left\{D\left(x\right)\left[\frac{d}{dx}K\left(x\middle|\xi\right)\right]^2+\Sigma_a(x)\left[K\left(x\middle|\xi\right)\right]^2-2\delta\left(x-\xi\right)K\left(x\middle|\xi\right)\right\} \quad . \tag{173}$$

Numerical solutions of Eq. (172) are found below for the case of a two-region composite domain in which the material properties are assumed to be piecewise constant. That is, it is assumed that

$$D(x)=\begin{cases} D_1 & \text{for } \ 0 \le x \le a \ , \\ D_2 & \text{for } \ a \le x \le a+T \ , \end{cases} \tag{174}$$

and

$$\sum_a = \begin{cases} \sum_{a_1} & \text{for } 0 \le x \le a \ , \\ \sum_{a_2} & \text{for } a \le x \le a+T \ . \end{cases} \tag{175}$$

It will also be assumed that $0 \le \xi \le a$ and that the Green's function satisfies the two end point boundary conditions,

$$\frac{d}{dx} K(0|\xi) = 0 \quad , \tag{176}$$

and

$$K(a+T|\xi) = 0 \quad . \tag{177}$$

The Green's function is continuous at $x=\xi$, and its first derivative is discontinuous at $x=\xi$ with the discontinuity,

$$\lim_{\varepsilon \to 0} \left[\frac{d}{dx} K(\xi+\varepsilon|\xi) - \frac{d}{dx} K(\xi-\varepsilon|\xi) \right] = \frac{(-1)}{D_1} \quad . \tag{178}$$

The interface between the two regions is at $x=a$, and at this interface the Green's function and its corresponding net currents are continuous, that is,

$$\lim_{\varepsilon \to 0} \left[K(a+\varepsilon|\xi) - K(a-\varepsilon|\xi) \right] = 0 \quad , \tag{179}$$

and

$$\lim_{\varepsilon \to 0} \left[D_1 \frac{d}{dx} K(a+\varepsilon|\xi) - D_1 \frac{d}{dx} K(a-\varepsilon|\xi) \right] = 0 \quad . \tag{180}$$

The Green's function differential equation (172) and the variational principle (173) both admit the group of point transformations that is generated by

$$\hat{U} = \eta(x) \frac{\partial}{\partial K} \quad , \tag{181}$$

where the coordinate function $\eta(x)$ is given by

$$\eta(x) = \begin{cases} \eta_1(x) & \text{for } 0 \le x \le a \ , \\ \eta_2(x) & \text{for } a \le x \le a+T \ , \end{cases} \tag{182}$$

with solutions of

$$\eta_1^{11}(x) - \alpha_1^2 \eta_1(x) = 0 \quad , \tag{183}$$

$$\eta_2^{11}(x) - \alpha_2^2 \eta_2(x) = 0 \quad , \tag{184}$$

where the following inverse diffusion lengths are defined by

$$\alpha_1^2 = \frac{\sum_{a1}}{D_1} \quad , \tag{185}$$

and

$$\alpha_2^2 = \frac{\Sigma_{a2}}{D_2} \quad . \tag{186}$$

Since the Green's function satisfies a homogeneous Neumann boundary condition at $x=0$, the solution of (183) used is

$$\eta_1(x) = \cosh(\alpha_1 x) \ , \ (0 \le x \le a) \quad . \tag{187}$$

Also, the solution of (184) is given by

$$\eta_2(x) = A_1 \cosh(\alpha_2 x) + A_2 \sinh(\alpha_2 x) \ , \ (0 \le x \le a+T) \quad . \tag{188}$$

The coordinate function must satisfy the boundary conditions,

$$\eta_1(a) = \eta_2(a) \quad , \tag{189}$$

and

$$D_1 \eta_1'(a) = D_2 \eta_2'(a) \quad , \tag{190}$$

at the interface between the two regions. These two boundary conditions become

$$\cosh(\alpha_2 a) A_1 + \sinh(\alpha_2 a) A_2 = \cosh(\alpha_1 a) \quad , \tag{191}$$

and

$$\sinh(\alpha_2 a) A_1 + \cosh(\alpha_2 a) A_2 = \frac{D_1 \alpha_1}{D_2 \alpha_2} \sinh(\alpha_1 a) \quad . \tag{192}$$

Solving these last two equations yields

$$A_1 = \cosh(\alpha_2 a)\cosh(\alpha_1 a) - \frac{D_1 \alpha_1}{D_2 \alpha_2} \sinh(\alpha_2 a)\sinh(\alpha_1 a) \quad . \tag{193}$$

and

$$A_2 = -\sinh(\alpha_2 a)\cosh(\alpha_1 a) + \frac{D_1 \alpha_1}{D_2 \alpha_2} \cosh(\alpha_2 a)\sinh(\alpha_1 a) \quad , \tag{194}$$

and combining Eqs. (193) and (194) with Eq. (188) produces

$$\eta_2(x) = \cosh(\alpha_1 a)\cosh[\alpha_2(x-a)] + \frac{D_1 \alpha_1}{D_2 \alpha_2} \sinh(\alpha_1 a)\sinh[\alpha_2(x-a)] \quad . \tag{195}$$

Evaluating this expression gives at $x=a+T$

$$\eta_2(a+T) = \cosh(\alpha_1 a)\cosh(\alpha_2 T) + \frac{D_1 \alpha_1}{D_2 \alpha_2} \sinh(\alpha_1 a)\sinh(\alpha_2 T) \quad , \tag{196}$$

which will be used to simplify the notations for further results.

Let the Green's function for the two regions be denoted by

$$K(x|\xi) = \begin{cases} y_1(x) & \text{for } 0 \le x \le a \ , \\ y_2(x) & \text{for } a \le x \le a+T \quad . \end{cases} \tag{197}$$

Then the conservation law in the first region defined by $0 \le x \le a$ is given by

$$D_1\eta_1(x)y_1^1(x) - D_1\eta_1^1(x)y_1(x) + \int dx\eta_1(x)\delta(x-\xi) = E_1 \quad , \tag{198}$$

and the conservation law in the second region, $a \le x \le a+T$ is given by

$$D_2\eta_2(x)y_2^1(x) - D_x\eta_2^1(x)y_2(x) = E_2 \quad , \tag{199}$$

since $0 \le \xi \le a$. Here E_1 and E_2 are constants. For a homogeneous Neumann boundary condition at $x=0$, we have

$$E_1 = 0 \quad , \tag{200}$$

but $E_2 \neq 0$ as shown below.

Assume that $0 \le x \le \xi$. Then the conservation law (198) becomes

$$\frac{d}{dx}\left[\frac{y_1(x)}{\eta_1(x)}\right] = 0 \ , \ \left(0 \le x \le \xi\right) \quad . \tag{201}$$

With the assumption that $\xi \le x \le a$, the conservation law reduces to

$$\frac{d}{dx}\left[\frac{y_1(x)}{\eta_1(x)}\right] = \frac{(-1)\eta_1(\xi)}{D_1\eta_1^2(x)} \quad , \quad \left(\xi \le x \le a\right) \quad . \tag{202}$$

To apply the conservation law (199) for the second region $a \le x \le a+T$, it is necessary to evaluate the constant, E_2, which can be done as follows: From the conservation law (198) evaluated at $x=a$, we have

$$D_1\eta_1(a)y_1^1(a) - D_1\eta_1^1(a)y_1(a) = -\eta_1(\xi) \quad , \tag{203}$$

and from (199) evaluated at $x=a$,

$$D_2\eta_2(a)y_2^1(a) - D_2\eta_2^1(a)y_2(a) = E_2 \quad . \tag{204}$$

By subtracting Eq. (203) from Eq. (204) and noting the continuity of net currents at $x=a$ it is found that

$$E_2 = -\eta_1(\xi) \quad . \tag{205}$$

With this result the conservation law (199) for the region a $a \le x \le a+T$ can be written in the form,

$$\frac{d}{dx}\left[\frac{y_2(x)}{\eta_2(x)}\right] = \frac{(-1)\eta_1(\xi)}{D_2\eta_2^2(x)} \quad . \tag{206}$$

Numerical algorithms in the form of two-point recurrence relations to compute the composite domain Green's function can be found with the forms of the conservation theorems given in Eqs. (201), (202), and (206).

Grid points are required in three intervals as defined by

$$a \le x_k \le a+T \ , \ \text{for} \ 1 \le k \le N_3 \ ,$$
$$\xi \le x_j \le a \ , \ \text{for} \ 1 \le j \le N_2 \ ,$$

and

$$0 \le x_i \le \xi \ , \ \text{for } 1 \le i \le N_1 \ .$$

These grid points can be located at arbitrary positions. Since the Green's function satisfies a homogeneous Dirichlet boundary condition at $x=a+T$, the numerical evaluations are done by moving through the grid points from right to left. To start with the conservation law (206) in the region $a \le x \le a+T$, we need the intigral,

$$\int \frac{dx}{\eta_2^2(x)} = \frac{\sinh(\alpha_2 x) - \cosh(\alpha_2 x)}{\alpha_2 (A_1 + A_2) \eta_2(x)} \quad , \tag{207}$$

where $\eta_2(x)$ is as given in Eq. (188). Then it is found that, from the conservation law (206), the integral between adjacent grid points,

$$\int_{x_k}^{x_{k+1}} dx \ \frac{d}{dx}\left[\frac{y_2(x)}{\eta_2(x)}\right] = \frac{(-1)\eta_1(\xi)}{D_2} \int_{x_k}^{x_{k+1}} \frac{dx}{\eta_2^2(x)} \quad , \tag{208}$$

simplifies to the following two-term recurrence relation:

$$y_2(x_k) = \frac{\eta_2(x_k)}{\eta_2(x_{k+1})} y_2(x_{k+1}) + \frac{\eta_1(\xi)\sinh\left[\alpha_2(x_{k+1} - x_k)\right]}{\alpha_2 D_2 \eta_2(x_{k+1})} \quad . \tag{209}$$

In this expression $\eta_2(x_k)$ and $\eta_2(x_{k+1})$ are evaluated with

$$\eta_2(x_2) = \cosh(\alpha_1 a)\cosh\left[\alpha_2(x_2 - a)\right] + \frac{D_1 \alpha_1}{D_2 \alpha_2}\sinh(\alpha_1 a)\sinh\left[\alpha_2(x_k - a)\right] \quad , \tag{210}$$

and so forth. Since

$$y_2\left(x_{N_3}\right) = 0 \quad , \tag{211}$$

the calculation is started with

$$y_2\left(x_{N_3-1}\right) = \frac{\eta_1(\xi)\sinh\left[\alpha_2\left(a + T - x_{N_3-1}\right)\right]}{\alpha_1 D_2 \eta_2(a+T)} = K\left(x_{N_3-1} \middle| \xi\right) \quad . \tag{212}$$

Then the Green's function at grid points such that $a \le x_h \le a+T$ is found numerically with the two-term recurrence relation,

$$K\left(x_k \middle| \xi\right) = \frac{\eta_2(\eta_k)}{\eta_2(\eta_{k+1})} K\left(x_{k+1} \middle| \xi\right) + \left(\frac{\eta_1(\xi)\sinh\left[\alpha_2(x_{k+1} - x_k)\right]}{\alpha_2 D_2 \eta_2(x_{k+1})}\right) \quad , \tag{213}$$

for $k=N_3-2, N_3-3, \ldots, 3, 2,$ 1.

For grid points in the first region such that $\xi \le x_j \le a$, the conservation law (202) integrated between two adjacent grid points becomes

$$\int_{x_j}^{x_{j+1}} dx \ \frac{d}{dx}\left[\frac{y_1(x)}{\eta_1(x}\right] = \frac{(-1)\eta_1(\xi)}{D_1} \int_{x_j}^{x_{j+1}} \frac{dx}{\eta_1^2(x)} \quad , \tag{214}$$

which, in view of the integral given in Eq. (148) reduces to the two-term recurrence relation,

$$K\left(x_j|\xi\right)=\frac{\cosh\left(\alpha_1 x_j\right)K\left(x_{j+1}|\xi\right)}{\cosh\left(\alpha_1 x_{j+1}\right)}+\frac{\cosh(\alpha_1\xi)\sinh\left[a_1\left(x_{j+1}-x_j\right)\right]}{\alpha_1 D_1\cosh\left(\alpha_1 x_{j+1}\right)} \quad . \tag{215}$$

The computation runs through the sequence $j=N_2-1, N_2-2, N_2-3, \ldots, 3, 2, 1$ because $K\left(x_{N_2}|\xi\right)$ is known from the continuity of the Green's function at the interface $x=a$ between the two regions. For grid points in the first region such that $0\leq x_i\leq\xi$, the conservation law (201) gives

$$y_1\left(x_i\right)=\frac{\eta_1\left(x_i\right)}{\eta_1\left(x_{i+1}\right)}y\left(x_{i+1}\right) \quad , \tag{216}$$

which is the same as

$$K\left(x_i|\xi\right)=\frac{\cosh\left(\alpha_1 x_i\right)}{\cosh\left(\alpha_1 x_{i+1}\right)}K\left(x_{i+1}|\xi\right) \quad , \tag{217}$$

where $i=N_1-1, N_1-2, N_1-3, \ldots, 3, 2, 1$. The Green's functions in this equation at $i=N_1$, namely is known from continuity at $x=\xi$, that is,

$$\lim_{\varepsilon\to 0}\left[K\left(x_{N_1}-\varepsilon|\xi\right)-K\left(x_{j-1}+\varepsilon|\xi\right)\right]=0 \quad , \tag{218}$$

and

$$\cosh\left(\alpha_1 x_{N_1}\right)=\cosh\left(\alpha_1|\xi\right) \quad . \tag{219}$$

The three two-term recurrence relations, (213), (215), and (217), are exact difference equations that yield exact numerical results for the composite domain Green's function for arbitrary locations of the grid points in each of the three intervals.

3.3. Exact Difference Equations for the Neutron Diffusion Equation

The self-adjoint form of the neutron diffusion equation is given by

$$\frac{1}{x^N}\frac{d}{dx}\left[D(x)x^N y^1\right]-\sum_a(x)y+Q(x)=0 \quad , \tag{220}$$

where $N=0$ for slab geometry, $N=1$ for cylindrical geometry and $N=2$ for spherical geometry. This equation can be regarded as the Euler-Lagrange equation of the variational principle,

$$J=\int_{x_1}^{x_2}dx\left[D(x)x^N\left(y^1\right)^2+x^N\sum_a(x)y^2-2x^N yQ(x)\right] \quad . \tag{221}$$

For a region with spatially uniform properties these last two equations can be written in the simpler forms,

$$\frac{1}{x^N}\frac{d}{dx}\left[x^N y^1\right] - y + S(x) = 0 \quad , \tag{222}$$

and

$$J = \int_{x_1}^{x_2} dx \left[x^N \left(y^1\right)^2 + x^N y^2 - 2yx^N S(x)\right] \quad , \tag{223}$$

when distance is measured in units of the diffusion length L given by

$$L = \left(D / \Sigma_a\right)^{1/2}, \tag{224}$$

and the volumetric source term is replaced with

$$S(x) = \frac{Q(x)}{\Sigma_a} \quad . \tag{225}$$

Symmetry properties of homogeneous and inhomogeneous second order ordinary differential equations and their corresponding variational principles can be used to construct exact difference equations. The homogeneous second order differential equation,

$$a(x)y^{11} + b(x)y^1 + c(x)y = 0 \quad , \tag{226}$$

or its corresponding self-adjoint form

$$\frac{d}{dx}\left[p(x)y^1\right] - q(x)y = 0 \quad , \tag{227}$$

where

$$p(x) = \exp\int dx \frac{b(x)}{a(x)} \quad , \tag{228}$$

and

$$q(x) = (-1)p(x)\frac{c(x)}{a(x)} \quad , \tag{229}$$

both admit an eight-parameter group of point transformations. Let $u_2(x)$ and $u_1(x)$ be two linearly independent solutions of the self-adjoint form given in Eq. (227) with the Wronskian $W(x)$ which satisfies

$$\frac{dW(x)}{dx} = (-1)\frac{W(x)}{p(x)}\frac{d}{dx}p(x) \quad . \tag{230}$$

Then the Lie algebra of the generators of the eight-parameter group that is admitted by the self-adjoint form (227), or by the nonself-adjoint form (226), can be written with the following basis:

$$\hat{U}_1 = y\frac{\partial}{\partial y} \quad , \tag{231}$$

$$\hat{U}_2 = \mu_1(x)\frac{\partial}{\partial y} \quad , \tag{232}$$

$$\hat{U}_3 = \mu_2(x)\frac{\partial}{\partial y} \quad , \tag{233}$$

$$\hat{U}_4 = \frac{y}{W(x)}\left[\mu_1(x)\frac{\partial}{\partial x} + y\mu_1^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{234}$$

$$\hat{U}_5 = \frac{y}{W(x)}\left[\mu_2(x)\frac{\partial}{\partial x} + y\mu_2^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{235}$$

$$\hat{U}_6 = \frac{\mu_1(x)}{W(x)}\left[\mu_1(x)\frac{\partial}{\partial x} + y\mu_1^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{236}$$

$$\hat{U}_7 = \frac{\mu_2(x)}{W(x)}\left[\mu_2(x)\frac{\partial}{\partial x} + y\mu_2^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{237}$$

and

$$\hat{U}_8 = \frac{1}{W(x)}\left[2\mu_1(x)\mu_2(x)\frac{\partial}{\partial x} + y\frac{d}{dx}\big(\mu_1(x)\mu_2(x)\big)\frac{\partial}{\partial y}\right] \quad . \tag{238}$$

The variational principle for which the self-adjoint form (227) is the Euler-Lagrange equation is given by

$$J = \int_{x_1}^{x_2} dx\left[p(x)\left(y^1\right)^2 + q(x)y^2\right] \quad . \tag{239}$$

This functional is a divergence-invariant of a five-parameter subgroup of the eight-parameter group admitted by the corresponding Euler-Lagrange equation (227). The Lie algebra of the five-parameter subgroup admitted by the functional is given by the five generators, $\hat{U}_2$, $\hat{U}_3$, $\hat{U}_6$, $\hat{U}_7$, and $\hat{U}_8$, in Eqs. (231)–(238). This fact leads to five conservation laws from each of which difference equations can be constructed by the methods of Section 2 to compute numerical solutions of two-point boundary value problems based upon the self-adjoint form (227) of a homogeneous second order ordinary differential equation.

The inhomogeneous case is exemplified by the neutron diffusion equation (220) and its variational principle (221). If the volumetric neutron source term *S(x)* in the diffusion equation is an arbitrary function of position, then the diffusion equation and its variational principle will both admit the two-parameter group with the Lie algebra basis given by

$$\hat{U}_1 = \mu_1(x)\frac{\partial}{\partial y} \quad , \tag{240}$$

and

$$\hat{U}_2 = \mu_2(x)\frac{\partial}{\partial y} \quad , \tag{241}$$

where the coordinate functions $\mu_1(x)$ and $\mu_2(x)$ are solutions of the homogeneous diffusion equation,

$$\frac{d}{dx}\left[x^N \frac{d\mu}{dx}(x)\right] - x^N \mu(x) = 0 \quad . \tag{242}$$

On the other hand, if the volumetric source term in the diffusion equation is spatially uniform, that is, if

$$s(x) = s = \text{constant} \quad , \tag{243}$$

then the neutron diffusion equation is invariant under an eight-parameter group with the Lie algebra of generators that follows:

$$\hat{U}_1 = y\frac{\partial}{\partial y} \quad , \tag{244}$$

$$\hat{U}_2 = \mu_1(x)\frac{\partial}{\partial y} \quad , \tag{245}$$

$$\hat{U}_3 = \mu_2(x)\frac{\partial}{\partial y} \quad , \tag{246}$$

$$\hat{U}_4 = \frac{(y-s)}{W(x)}\left[\mu_1(x)\frac{\partial}{\partial x} + (y-s)\mu_1^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{247}$$

$$\hat{U}_5 = \frac{(y-s)}{W(x)}\left[\mu_2(x)\frac{\partial}{\partial x} + (y-s)\mu_2^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{248}$$

$$\hat{U}_6 = \frac{\mu_1(x)}{W(x)}\left[\mu_1(x)\frac{\partial}{\partial x} + (y-s)\mu_1^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{249}$$

$$\hat{U}_7 = \frac{\mu_2(x)}{W(x)}\left[\mu_2(x)\frac{\partial}{\partial x} + (y-s)\mu_2^1(x)\frac{\partial}{\partial y}\right] \quad , \tag{250}$$

and

$$\hat{U}_8 = \frac{1}{W(x)}\left[2\mu_1(x)\mu_2(x)\frac{\partial}{\partial x} + (y-s)\frac{d}{dx}\big(\mu_1(x)\mu_2(x)\big)\frac{d}{dy}\right] \quad , \tag{251}$$

where $\mu_1(x)$ and $\mu_2(x)$ are linearly independent solutions of Eq. (242), and $W(x)$ is their Wronskian. The associated variational principle, namely,

$$J = \int_{x_1}^{x_2} dx\left[x^N\left(y^1\right)^2 + x^N y^2 - 2yx^N s\right] \quad , \tag{252}$$

for the case of a spatially uniform source is a divergence-invariant of the five-parameter subgroup with Lie algebra basis given by $\hat{U}_2$, $\hat{U}_3$, $\hat{U}_6$, $\hat{U}_7$, and $\hat{U}_8$ in Eqs. (245), (246), (249), (250), and (251), respectively. In view of the symmetry properties found above, there are two conservations laws for the case of a spatially arbitrary source term and five conservation laws for the case of a spatially uniform volumetric source term from which exact difference equations to obtain numerical solutions of two-point boundary value problems involving the neutron diffusion equation can be constructed. Two examples of applying the above symmetries to determining gauge functions and exact difference equations are illustrated below.

In the first example we want to solve the diffusion equation with a spatially dependent source, namely,

$$y^{11} - y + s\left(1-\varepsilon x^2\right) = 0 \ , \quad \text{for} \quad 0 \le x \le a \ , \tag{253}$$

in slab geometry with a homogenous Neumann boundary condition,

$$y^1(0) = 0 \ , \tag{254}$$

at $x=0$, and a homogeneous Dirichlet boundary condition,

$$y(a) = 0 \ , \tag{255}$$

at $x=a$. The associated variational principle is given by

$$J = \int_0^a dx\left[\left(y^1\right)^2 + y^2 - 2ys\left(1-\varepsilon x^2\right)\right] \tag{256}$$

with the constant ε. Both the diffusion equation and the variational principle (256) admit the group of point transformations generated by

$$\hat{U} = \cosh(x)\frac{\partial}{\partial y} \ . \tag{257}$$

The condition that the functional in Eq. (256) be divergence-invariant under the group generated by (257), namely,

$$\xi\frac{\partial F}{\partial x} + \eta\frac{\partial F}{\partial y} + \eta^{(1)}\frac{\partial F}{\partial y^1} + FD_x\xi = D_x\phi \ , \tag{258}$$

from Eq. (73), reduces in this case to

$$2\cosh(x)\left[y - s\left(1-\varepsilon x^2\right)\right] + 2\sinh(x)y^1 = \frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y}y^1 \ . \tag{259}$$

Hence, we have

$$\frac{\partial\phi}{\partial y} = 2\sinh(x) \ , \tag{260}$$

and

$$\frac{\partial\phi}{\partial x} = 2\cosh(x)\left[y - s\left(1-\varepsilon x^2\right)\right] \ , \tag{261}$$

so that the gauge functions given by

$$\phi(x,y) = 2y \ \ \sinh(x) - 2\int dx \ \ \cosh(x) \ \ s\left(1-\varepsilon x^2\right) \quad . \tag{262}$$

The corresponding conservation law is

$$\cosh(x)y^1 - \sinh(x)y + \int dx \ \ \cosh(x) \ \ s\left(1-\varepsilon x^2\right) = \text{constant} \quad , \tag{263}$$

in which the constant can be taken as zero for the homogeneous Neumann boundary condition at $x=0$. The canonical variables of the group with the generator in Eq. (257) are

$$y(x,y) = \frac{y}{\cosh(x)} \quad , \tag{264}$$

and

$$X(x,y) = x \quad . \tag{265}$$

Since

$$\int dx \ \ \cosh(x) \ \ s\left(1-\varepsilon x^2\right) = s\left\{\sinh(x) - \varepsilon\left[x^2\sinh(x) - 2x\cosh(x) + 2\sinh(x)\right]\right\} \quad , \tag{266}$$

we obtain by writing the conservation law (263) in terms of canonical variables the result,

$$\frac{dY}{dx} = \frac{(-1)s}{\cosh^2(x)}\left\{\sinh(x) - \varepsilon\left[x^2\sinh(x) - 2x\cosh(x) + 2\sinh(x)\right]\right\} \quad . \tag{267}$$

By integrating this result from x to $x+h$ we obtain the exact difference equation,

$$\frac{y(x+h)}{\cosh(x+h)} = \frac{y(x)}{\cosh(x)} + s\left\{\frac{1}{\cosh(x+h)} - \frac{1}{\cosh(x)} - \varepsilon\left[\frac{(x+h)^2+2}{\cosh(x+h)} - \frac{x^2+2}{\cosh(x)}\right]\right\} \quad . \tag{268}$$

Also, integrating Eq. (267) from $x–h$ to x yields a second exact difference equation, namely,

$$\frac{y(x-h)}{\cosh(x-h)} = \frac{y(x)}{\cosh(x)} - s\left\{\frac{1}{\cosh(x)} - \frac{1}{\cosh(x-h)} - \varepsilon\left[\frac{x^2+2}{\cosh(x)} - \frac{(x+h)^2+2}{\cosh(x-h)}\right]\right\} \quad . \tag{269}$$

These two difference equations are exact, and can be used to show the limitations of a standard difference scheme to solve the diffusion equation (253). If the standard three-point difference formula is used to approximate the second order derivative in Eq. (253), the standard finite difference scheme for this equation is

$$\frac{y(x+h) + y(x-h) - 2y(x)}{h^2} - y(x) + s\left(1-\varepsilon x^2\right) = 0 \quad , \tag{270}$$

where h is a uniform grid spacing. By adding the two exact two-time recurrence relations found in Eqs. (268) and (269) we obtain the following exact second order difference equation:

$$y(x+h)+y(x-h)=\frac{\left[\cosh(x+h)+\cosh(x-h)\right]y(x)}{\cosh(x)}$$
$$+s\left\{1-\frac{\cosh(x+h)}{\cosh(x)}-\varepsilon\left[(x+h)^2+2-\frac{\left(x^2+2\right)\cosh(x+h)}{\cosh(x)}\right]\right\} \tag{271}$$
$$-s\left\{\frac{\cosh(x-h)}{\cosh(x)}-1-\varepsilon\left[\frac{\left(x^2+2\right)\cosh(x-h)}{\cosh(x)}-(x-h)^2-2\right]\right\} \ ,$$

or

$$y(x+h)+y(x-h)=2y(x)\cosh(h)$$
$$+s\left\{2-2\cosh(h)+\varepsilon\left[2\left(x^2+2\right)\cosh(h)-2x^2-2h^2-4\right]\right\} \ . \tag{272}$$

This exact second order difference equation that comes out of exact two-term recurrence relations simplifies to the form,

$$y(x+h)+y(x-h)=\left(2+h^2\right)y(x)+s\left(-h^2+h^2x^2\varepsilon\right) \ , \tag{273}$$

with the approximation that

$$\cosh(h)=1+\frac{h^2}{2}+\dots \ . \tag{274}$$

This result obtained by approximating exact two-term recurrence relations is the same as the standard second order difference equation written in Eq. (270) for the diffusion equation. This second order difference equation leads to a set of algebraic equations for approximate solutions of the diffusion equation at the grid points of a uniformly spaced grid. In contrast either of the two-term recurrence relations (268) and (269) will yield exact solutions of the diffusion equation at arbitrarily located grid points without solving a set of algebraic equations.

In the second example we want to develop exact difference equations to obtain numerical solutions of the neutron diffusion equation is spherical geometry with a spatially uniform source. The neutron balance in differential form is

$$\frac{d}{dx}\left(x^2y^1\right)-x^2y+x^2s=0 \ , \quad \text{for} \quad 0\le x\le a \ . \tag{275}$$

Let

$$w=xy \ , \tag{276}$$

so that

$$\frac{d^2w}{dx^2}-w+xs=0 \ , \tag{277}$$

with the associated variational principle,

$$J = \int_0^a dx \left[\left(w^1 \right)^2 + w^2 - 2xsw \right] \quad . \tag{278}$$

The boundary conditions are both homogeneous Dirichlet boundary conditions, that is,

$$w(0) = 0 \quad , \tag{279}$$

and

$$w(a) = 0 \quad . \tag{280}$$

Both the diffusion equation (277) and the variational principle admit the group of point transformations generated by

$$\hat{U} = \sinh(x) \frac{\partial}{\partial w} \quad . \tag{281}$$

The functional (278) is divergence-invariant under this group with the gauge function,

$$\phi(x,w) = 2w\cosh(x) - 2s\int dx\, x\sinh(x) \quad , \tag{282}$$

or

$$\phi(x,w) = 2w\cosh(x) - 2s[x\cosh - \sinh(x)] \quad . \tag{283}$$

The conservation law found with this gauge function is given by

$$\sinh(x)w^1 - \cosh(x)w + s[x\cosh(x) - \sinh(x)] = \text{constant} \quad . \tag{284}$$

The constant in this equation can be taken as zero because of the homogeneous Dirichlet boundary condition at *x=0*. The canonical variables of the group generated by (281) are

$$Y(x,w) = \frac{w}{\sinh(x)} \quad , \tag{285}$$

and

$$X = x \quad . \tag{286}$$

In terms of these canonical variables the conservation law (284) becomes

$$\frac{dY}{dx} = \frac{(-1)s}{\sinh^2(x)}[x\cosh(x) - \sinh(x)] \quad . \tag{287}$$

As

$$\int dx \frac{[x\cosh(x) - \sinh(x)]}{\sinh^2(x)} = \frac{x}{\sinh(x)} \quad , \tag{288}$$

we obtain from Eq. (287) the two two-term recurrence relations that follow:

$$\frac{w(x+h)}{\sinh(x+h)} = \frac{w(x)}{\sinh(x)} + s\left[\frac{x+h}{\sinh(x+h)} - \frac{x}{\sinh(x)}\right] \quad , \tag{289}$$

and

$$\frac{w(x-h)}{\sinh(x-h)} = \frac{w(x)}{\sinh(x)} - s\left[\frac{x}{\sinh(x)} - \frac{x-h}{\sinh(x-h)}\right] \quad . \tag{290}$$

These two results are exact, and can be added to produce an exact second order difference equation, namely,

$$\begin{aligned} w(x+h)+w(x-h) = {} & \frac{w(x)\left[\sinh(x+h)+\sinh(x-h)\right]}{\sinh(x)} \\ & +s\left\{2x - \frac{x\left[\sinh(x+h)+\sinh(x-h)\right]}{\sinh(x)}\right\} \end{aligned} \tag{291}$$

or

$$w(x+h)+w(x-h) = 2w(x)\cosh(h) + 2xs\left[1-\cosh(h)\right] \quad . \tag{292}$$

With the approximation,

$$\cosh(h) = 1 + \frac{h^2}{2} \quad , \tag{293}$$

this exact difference equation reduces to

$$w(x+h)+w(x-h)-2w(x)-h^2 w(x)+xsh^2 = 0 \quad , \tag{294}$$

which is a standard approximate second order difference equation for the diffusion equation (277) found with the standard three-point central difference formula for second order derivatives. Numerical solutions of the spherical geometry diffusion equation (276) can be computed with either of the exact two-term recurrence relations at grid points with arbitrary locations. These two-term recurrence relations produce exact numerical results without having to solve a system of algebraic equations as is required with the standard approximate second order difference equation (294).

This report has been reproduced directly from the best available copy. It is available electronically on the Web (http://www.doe.gov/bridge).

Copies are available for sale to U.S. Department of Energy employees and contractors from:
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831
(865) 576-8401

Copies are available for sale to the public from:
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22616
(800) 553-6847

Los Alamos
NATIONAL LABORATORY
Los Alamos NM 87545