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On the Diffusion in a Lattice Gas Model: Group-Theoretic Approach

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Motivated by some recent results concerning the model of a noninteracting one-dimensional lattice gas with an order preservation of particles where multiple occupancy of the sites is not excluded, we give new symmetries and new reductions of the corresponding continuum nonlinear partial differential equation. Closed-form analytic solutions are found.

KEY WORDS: Lattice gas models; diffusion processes; group analysis of differential equations.

1. INTRODUCTION

For situations in which a one-dimensional lattice gas with order preservation of particles where multiple occupancy of the sites is not excluded, the dynamics of this model was studied by Kutner *et al.*[1] and they developed the master equation which describes the dynamics of particle clusters. The corresponding continuum nonlinear diffusion equation is

$$C_t(x, t) = [D_0(1 + C)^{-2} C_x]_x - [V_0(1 + C)^{-1} C]_x \tag{1}$$

where $C(x, t)$ is the concentration of particles, D_0 and V_0 are lattice constants. In this model, the diffusion coefficient and the drift velocities become particle concentration dependent, in contrast to the standard model of independently diffusing particles. Equation (1) has the form of a continuity equation and the density current is the sum of a diffusive and a convective term

$$J(x, t) = -D_0(1 + C)^{-2} C_x + V_0(1 + C)^{-1} C \tag{2}$$

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It contains the coefficient of collective or chemical diffusion,

$$D(C) = D_0(1 + C)^{-2} \tag{3}$$

and the mean particle velocity

$$V(C) = V_0(1 + C)^{-1} \tag{4}$$

In the special case, where the transition rate of a particle in the direction of increasing the site number is equal to the transition rate when the site number is decreasing, one get $V_0 = 0$ and $D_0 = 1$, and Eq. (2) reads

$$J(x, t) = -C_x/(1 + C)^2 \tag{5}$$

and the diffusion processes without drift.[1]

The model of Kutner *et al.*,[11] in the general form, is mathematically equivalent to the partial differential equation (PDE)

$$D_0^{-1} u^3 u_t = u u_{xx} - 2u_x^2 - k u u_x \tag{6}$$

where

$$u(x, t) = C(x, t) + 1 \qquad \text{and} \qquad k = V_0/D_0$$

The importance of this system arises from the fact that it has a wide range of applications in physical and related sciences, e.g. in polymer diffusion,[2] transport of particles in disordered materials.[3] The nonlinear diffusion equations of the type studied here can be produced in a large variety, see e.g. the recent paper by Eyink *et al.*[4]

There is a continuing high level of interest in the construction of solutions to the generalized Burgers Eq. (1), see e.g. refs. 5–7. The majority of these authors consider problems such as existence of solutions, conditions for propagation speed, and asymptotic behavior near to equilibrium and stationary state, rather than exact solutions of (1). The similarity transformation method can help in finding exact solutions of Eq. (1).

The fundamental basis of the technique is that, when a nonlinear partial differential equation is invariant under a Lie group of transformations, a reduction transformation exists. With the help of these transformations the partial differential equation is reduced to ordinary differential equation (ODE) which may be solvable explicitly.[8–10] This similarity method has been applied to many physical problems.[11–16] A more comprehensive analysis for the class of inhomogeneous nonlinear diffusion-convection equations, with arbitrary coefficients, which possess symmetries and reductions will publish elsewhere. In this paper we shall apply the similarity method to Eq. (6). We shall study the invariance of (6) under continuous groups of transformations depending on one infinitesimal parameter (ε). The most extensive (ε) Lie-group of transformations, admitted by (6), will be shown to depend on four arbitrary group constants, and the general class of similarity solutions will be seen to separate into seven different subclasses according to the number of nonzero group constants. The reduction obtained from the optimal system of subalgebras is derived, and some new exact solutions can be obtained. In Section 2 we summarize the essentials of symmetry reduction of Eq. (6).

Section 3 contains the main ingredients and exact similarity solutions. Section 4 is devoted to conclusions and remarks.

2. SYMMETRY REDUCTION

First we sketch the derivation of the symmetry reductions of Eq. (6) using Lie group method.[8–10] Consider the one-parameter (ε) Lie group of infinitesimal transformations in x, t and u given by

$$\begin{aligned} \underline{x} &= x + \varepsilon X(x, t, u) + O(\varepsilon^2) \\ \underline{t} &= t + \varepsilon T(x, t, u) + O(\varepsilon^2) \\ \underline{u} &= u + \varepsilon U(x, t, u) + O(\varepsilon^2) \end{aligned} \tag{7}$$

Equation (7) is then extended to first and second order by the prolongation formulae, where, for example,

$$\partial \underline{u}/\partial \underline{x} = \underline{u}_{\underline{x}} = \partial u/\partial x + \varepsilon U^x + O(\varepsilon^2)$$

with

$$U^x = DU/Dx - (DX/Dx)\, u_x - (DT/Dx)\, u_t \tag{8}$$

and D/Dx is the total derivative operator with respect to x, that is,

$$\frac{D}{Dx} G(x, t, u) = \partial G/\partial x + u_x\, \partial G/\partial u$$

In a similar way, the infinitesimal transformations U^t, U^{xx} of the partial derivatives u_t and u_{xx} can be obtained from Eq. 7 (cf. ref. 8 Section 2) and we have

$$\underline{u}_t = u_t + \varepsilon U^t + O(\varepsilon^2)$$
$$\underline{u}_x = u_x + \varepsilon U^x + O(\varepsilon^2) \qquad (9)$$
$$\underline{u}_{xx} = u_{xx} + \varepsilon U^{xx} + O(\varepsilon^2)$$

We assume that the infinitesimal transformation (7) and (9) leave the governing Eq. (6) invariant, i.e., Eq. (6) holds when x and other variables are replaced by $\underline{x}$ and others.

By Eqs. (7) and(9), to first order in ε, Eq (6) becomes

$$-D_0^{-1} U^t + u^{-2} U^{xx} - 4u^{-3} u_x U^x - ku^{-2} U^x$$
$$+ 6u^{-4} u_x^2 U + 2ku^{-3} u_x U - 2u^{-3} u_{xx} U = 0 \qquad (10)$$

Conditions on the infinitesimals $X(x, t, u)$, $T(x, t, u)$ and $U(x, t, u)$ are determined by substituting Eq. 8 for U^x in Eq. 10, and so on for U^t and U^{xx} to get a polynomial in the variables $u_t, u_x, u_{xt}, \ldots$ which we regard as independent. Setting, successively, the coefficients of these variables, including powers and products between them, equal to zero we obtain a large number of partial differential equations in X, T and U which need to be satisfied. Therefore these equations enable us to derive the generators X, T, and U and consequently the desired Lie transformations. The resolution of this system gives

$$X = a_1 - a_2 e^{kx}/k$$
$$T = 2a_3 t + a_4 \qquad (11)$$
$$U = a_3 u + a_2 e^{kx} u$$

where a_i, $i = 1, 2, 3, 4$ are four arbitrary parameters. Equation (6) is hence invariant under the following infinitesimal generators:

$$A_1 = \partial_t$$
$$A_2 = \partial_x$$
$$A_3 = (-1/k)\, e^{kx}\, \partial_x + e^{kx} u\, \partial_u \qquad (12)$$
$$A_4 = 2t\, \partial_t + u\, \partial_u$$

A straightforward calculation gives the following commutating relations which define the infinitesimal Lie group:

$$[A_i, A_i] = [A_i, A_j] = 0, \qquad i, j = 1, 2, 3, 4$$

but

$$[A_2, A_3] = kA_3 \qquad \text{and} \qquad [A_1, A_4] = 2A_1 \tag{13}$$

The Lie algebras corresponding to the symmetry groups are characterized by the generators A_i, $i = 1, 2, 3, 4$. In general, the groups that leave (6) invariant depend on four parameters a_i, $i = 1, 2, 3, 4$. To each parameter there will correspond a family of group invariant solutions. We want to reduce the search for group invariant solutions to finding non-equivalent branches of solutions.

This leads to the concept of optimal system of group invariant solutions (see, e.g., ref. 9, Section 3.3 and Section 1.4), from which every other can be derived. Following Olver,[9] we are able to distinguish seven different types of solutions corresponding to the basic fields of an optimal system given by $A_1, A_3, A_4, A_1 + A_2, A_1 + A_3, A_2 + A_4$, and $A_3 + A_4$. The main use of these symmetries is to obtain a reduction of variables in Eq. (6), which can be obtained by solving the following characteristic equation [10; Section 28]:

$$\frac{dx}{X(x, t, u)} = \frac{dt}{T(x, t, u)} = \frac{du}{U(x, t, u)} \tag{14}$$

The general solution of these equations will involve two arbitrary constants one of which takes the role of similarity variable $s = s(x, t)$ and the other,

Table I. Similarity Variables and Similarity Forms for the Optimal System of Eq. (6) and the Reduced ODEs

	$s(x, t)$	$u(x, t)$	Reduced equations
A_1	x	$F(s)$	$F\,d^2F/ds^2 - 2(dF/ds)^2 - kF\,dF/ds = 0$
A_3	t	$e^{-kx}F$	$dF/ds = 0$
A_4	x	$t^{1/2}F$	$F\,d^2F/ds^2 - kF\,dF/ds - 2(dF/ds)^2 - F^4/2D_0 = 0$
$A_1 + A_2$	$(x - t)$	$F(s)$	$F\,d^2F/ds^2 - 2(dF/ds)^2 + \left(\frac{F^3}{D_0}\right) dF/ds - kF\,dF/ds = 0$
$A_1 + A_3$	$(e^{-kx} - t)$	$e^{kx}F$	$F\,d^2F/ds^2 - 2(dF/ds)^2 + (F^3/kV_0)\,dF/ds = 0$
$A_2 + A_4$	e^{2x}/t	$t^{1/2}F$	$4D_0s^2\,d^2F/ds^2 + (4D_0 - 2V_0)s\,dF/ds$ $- 8D_0s^2F^{-1}(dF/ds)^2 + sF^2\,dF/ds - F^3/2 = 0$
$A_3 + A_4$	$t^{-1/2}h(x)$	$e^{-kx}hF$	$s^2F\,d^2F/ds^2 - 2s^2(sF/ds)^2 - sF\,dF/ds - F^2$ $+ (D_0s^3F^3/2V_0^2)\,dF/ds = 0, \quad h(x) = \exp(e^{kx})$

say $F(s)$, plays the role of dependent variable, called the similarity function. By substituting the similarity forms in the partial differential Eq. (6), it will be reduced to an ordinary differential equation in $F(s)$. Solutions $F(s)$ lead by back substitution to the so-called similarity solutions $u(x, t)$ of Eq. 6. Table I shows the reduced ordinary differential equation and related symmetry invariants for each of the optimal systems, together with the corresponding similarity variables s and the similarity forms connecting $F(s)$ and $u(x, t)$. In the remaining part of the paper, these ordinary differential equations resulting from the reductions are investigated in detail to get similarity solutions.

3. EXPLICIT SIMILARITY SOLUTIONS OF EQ. 6

The resulting ordinary differential equations in Table I are of second order, except for the case where the symmetry A_3 with $s=t$ leads to a first order ODE, thus the explicit general solution is simple,

$$u(x) = 1 + C(x) = Ge^{-kx} \tag{15}$$

where G is arbitrary constant.

The ordinary differential equations of second order resulting from the reductions are nonlinear. All of them belong to the class of integrable and exactly solvable evolution equations, but the last one is not integrable and it may be solved by numerical methods. In the following we will focus our attention on the analytic solution of the integrable nonlinear ODEs listed in Table I.

Case 1. First integration of the first ODE in Table I is

$$\frac{dF}{ds} = C_1 F^2 - kF \tag{16}$$

and the second integration gives

$$F(x) = r(1 + \text{Coth}\, r(C_2 - C_1 s)), \qquad 0 > F > k/C_1 \tag{17}$$

where $r = k/2\ C_1$, C_1 and C_2 arbitrary constants.

Solution $F(s)$ lead by back substitution to so called similarity solution $u(x, t)$ of Eq. 6. In this case, Eq. 6 has the stationary solution

$$u(x, t) = r(1 + \text{Coth}\, r(C_2 - C_1 x)), \qquad 0 > u > k/C_1 \tag{18}$$

For the case, $r=1$, i.e., $C_1=k/2$, Eq. (1) has the solution

$$C(x,t)=u(x,t)-1=\mathrm{Coth}(C_2-kx/2), \qquad |C|>1 \tag{19}$$

Equation (16) has second integration, in another form

$$F(x)=r(1+\tanh r(C_2-C_1 s)), \qquad 0<F<k/C_1 \tag{20}$$

For the case, $r=1$ i.e. $k/C_1=2$ and $C_2=0$, Eq. (1) has solution

$$C(x,t)=u(x,t)-1=\tanh\left(\frac{-kx}{2}\right), \qquad |C|<1 \tag{21}$$

Case 2. For the third ODE in Table I, we write $dF/ds=1/P(F)$, then it reads

$$-dP/dF=2F^{-1}P+kP^2+F^3P^3/2D_0 \tag{22}$$

which is the Abel equation of first kind. Further simplification reduces (22) to a Bernoulli equation which, on substitution of $P(F)=1/Q(z)\,F^2$ and $z=k/F$, gives

$$-Q\,dQ/dz=Q+1/2\,D_0 z \tag{23}$$

For possible ways of finding a general solution of Eq. 23 consult [17, part II]. It is important to emphasize that the formal solution suggested here by using the similarity method $u=t^{1/2}F(x)$ agrees with the usual diffusive $t^{1/2}$-law.(18, 19)

Case 3. The fourth ODE in Table I has a travelling wave solution, where $s=(x-t)$ and $u=F(s)$. The first integration gives

$$dF/ds=C_1F^2-F^3/D_0-kF \tag{24}$$

where C_1 is an arbitrary constant. There are two cases:

(i) If $C_1=0$, Eq. 24 has solution

$$F(s)=V_0^{1/2}(C_2e^{2ks}-1)^{-1/2} \tag{25}$$

where C_2 is an arbitrary constant. Consequently, Eq. 1 has solution

$$C(x,t)=u(x,t)-1=V_0^{1/2}(C_2e^{2k(x-t)}-1)^{-1/2}-1 \tag{26}$$

(ii) If $C_1 \neq 0$, Eq. 24 has solution

$$F^p(F-y_1)^q(F-y_2)^r = C_2 e^s \tag{27}$$

where

$$\begin{aligned} p = 1/y_1 y_2, \quad q = 1/y_1(y_1 - y_2), \quad r = 1/y_2(y_2 - y_1) \\ y_{1,2} = C_1 D_0/2 \pm \tfrac{1}{2}(C_1^2 D_0^2 - 4k D_0)^{1/2} \end{aligned} \tag{28}$$

and C_2 is an arbitrary constant.

Case 4. For the fifth ODE in Table I, the ansatz connected with it is

$$s = (e^{-ks} - t) \qquad \text{and} \qquad u(x, t) = e^{-kx}F(x)$$

The ODE is integrated once to get

$$dF/ds = C_1 F^2 - F^3/kV_0 \tag{29}$$

where C_1 is an arbitrary constant.

Further integration of Eq. 29 gives

(i) For $C_1 = 0$,

$$F(s) = (C_2 + 2s/kV_0)^{-1/2} \tag{30}$$

where C_2 is an arbitrary constant. In this case Eq. 1 has solution

$$C(x, t) = u(x, t) - 1 = e^{-kx} \cdot \left(C_2 + \frac{2e^{-kx} - 2t}{kV_0}\right)^{-1/2} - 1 \tag{31}$$

(ii) For $C_1 \neq 0$,

$$F/(a - F) - e^{a/F} = \exp(a^2 \cdot (bs + C_2)) \tag{32}$$

where $b = kV_0$, $a = bC_1$ and C_2 is an arbitrary constant.

Case 5. For the sixth ODE in Table I, upon introducing the new variable $y = \ln s$, it becomes

$$d^2F/dy^2 + \frac{F^2}{4D_0} dF/dy - \frac{k}{2} dF/dy - \frac{2}{F}(dF/dy)^2 - F^3/8D_0 = 0 \tag{33}$$

On substitution of $p(F) = dF/dy$, Eq. 33 will be the Abel equation of second kind

$$p\,dp/dF = (k/2 - F^2/4D_0)\,p + 2p^2/F + p^3/8D_0 \tag{34}$$

which can be transformed into Abel equation of first kind

$$dR/dz = R^2 + G(z)\,R^3 \tag{35}$$

where

$$R(z) = F^2/p,\ G(z) = F/4V_0 - 2F^2 \quad \text{and} \quad z = F/4D_0 + k/2F$$

Further simplification arises on substitution of $R(z) = 1/H(z)$, which gives

$$-dH/dz = 1 + G(z)/H(z) \tag{36}$$

For details of the solution of Eqs. 36, 35, see [17, part I]

4. CONCLUSIONS

In this paper we have classified the Lie symmetries of the nonlinear diffusion equation with drift (1), which is the continuum form of the diffusion in one-dimensional lattice gas model with order preservation. We have found several new similarity reductions and explicit solutions of these reduced equations. With our calculations we have demonstrated that the Lie classical method can lead to an ansatz to separate independent variables. This method is very useful if we remember that there is more than one possibility for a separation. It should be mentioned that the model discussed here, for transport of particles in non-interacting lattice gas, represents not only the equilibrium or stationary state, but states that are far from equilibrium. The various functions of (t) that have been included in our results help provide a fundamental understanding of these complicated flows on a kinetic level.

It is worth noting that, in some circumstances, solutions of non-linear equations with appropriate boundary conditions converge to the similarity transformation forms as $t \to \infty$.[20, 21] So as a final comment, the similarity solutions have played an important role in mathematical analysis, particularly in nonlinear diffusion theory. This is not primarily because of their usefulness as global solutions but rather because of their crucial role in the asymptotic sense.

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