Lie symmetries of semi-linear Schrödinger equations and applications

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Abstract. Conditional Lie symmetries of semi-linear 1D Schrödinger and diffusion equations are studied in case the mass (or the diffusion constant) is considered as an additional variable and/or where the couplings of the non-linear part have a non-vanishing scaling dimension. In this way, dynamical symmetries of semi-linear Schrödinger equations become related to certain subalgebras of a three-dimensional conformal Lie algebra (conf\textsubscript{3}). The representations of these subalgebras are classified and the complete list of conditionally invariant semi-linear Schrödinger equations is obtained. Applications to the phase-ordering kinetics of simple magnets and to simple particle-reaction models are briefly discussed.

1. Introduction
The understanding of the long-time kinetics of non-equilibrium continues to pose challenging problems. Here we are interested in the long-standing problem of phase-ordering kinetics of simple magnets which arises when, say, a ferromagnet is rapidly quenched from a disordered initial state to below its critical temperature $T < T_c$. We restrict attention here to the case with a non-conserved order-parameter, when a common description [1] is given in terms of a Langevin equation for the coarse-grained order-parameter $\Phi$ (referred to as ‘model A’)

$$\frac{\partial \Phi}{\partial t} = \Gamma \nabla^2 \Phi - \frac{dV(\Phi)}{d\Phi} + \eta$$

(1.1)

where $V$ describes the self-interaction of $\Phi$, $\eta$ is a gaussian delta-correlated thermal noise of variance $T$ and white-noise initial conditions (which come from the disordered initial state) are assumed. The task is to obtain the long-time behaviour of solutions of equation (1.1); in particular one would like to be able to understand the origin of the dynamical scaling which has been observed in numerous exactly solvable systems, in many numerical simulations and in several experiments, see [1–4] and references therein. These results are conveniently formulated in terms of the two-time autocorrelation and the (linear) autoresponse functions defined as

$$C(t, s) := \langle \Phi(t)\Phi(s) \rangle = s^{-b}f_C(t/s)$$

$$R(t, s) := \frac{\delta \langle \Phi(t) \rangle}{\delta h(s)} \bigg|_{h=0} = s^{-1-a}f_R(t/s)$$

(1.2)

where $h(s)$ is time-dependent magnetic field conjugate to the non-conserved order-parameter $\Phi$. We have also included here the conventionally admitted scaling forms, which are valid in the
double scaling limit \( t, s \gg t_{\text{micro}} \) and \( t - s \gg t_{\text{micro}} \) where \( t_{\text{micro}} \) is some ‘microscopic’ reference time. The *ageing behaviour* of the system is expressed through the breaking of time-translation invariance, that is \( C(t, s) \) or \( R(t, s) \) depend on both \( t \) and \( s \) and *not* merely on the difference \( t - s \). Physically, ageing comes from the existence of at least two stable, equivalent and competing stationary states of the system, such that although locally a stationary state is rapidly reached, globally the system never manages to decide to which of the possible stationary states it should relax [1–4].

In view of the complexity of the problem, an approach based on the dynamical symmetries of the ageing phenomenon would be helpful. Such an approach is possible since the behaviour of solutions of (1.1) actually only depends on the deterministic part of that equation, provided that this deterministic part is Galilei-invariant.

**Theorem.** [5] Consider the deterministic part of eq. (1.1), which is obtained by setting \( \eta = 0 \). If that deterministic part is Galilei-invariant, then all \( n \)-point correlation and response functions of the full stochastic theory can be exactly expressed in terms of \((n+1)\)- or \((n+2)\)-functions determined from the deterministic part alone.

In particular, the two-time response function \( R(t, s) \) can in this way be shown to be independent of the noises in eq. (1.1). The requirement of Galilei-invariance in phase-ordering kinetics is a natural one, because the dynamical exponent \( z = 2 \) in this case [1]. Furthermore, the form of \( R(t, s) \) and also of \( C(t, s) \) can be predicted and is found in very good agreement with simulational data [6–8]. Therefore, the time-dependent properties of the system follow from quantities calculable from the deterministic part alone. In turn, the dynamical symmetries of that deterministic part (following from eq. (1.1)) will be enough for a characterization of phase-ordering kinetics. Here, we take up the question of how to establish non-trivial dynamical symmetries of such deterministic partial differential equations.

2. **Dynamical symmetries with fixed masses**

As a first example of our procedure, we consider the case when the ‘mass’ \( \mathcal{M} \) is a fixed constant. The non-linear Schrödinger equation reads (for simplicity in \( d = 1 \) space dimension)

\[
2\mathcal{M}\partial_t \Phi - \partial_r^2 \Phi = gF(t, r, \Phi, \Phi^*)
\]

(2.1)

where \( F \) is referred to as a potential, \( g \) is a coupling constant and the ‘mass’ \( \mathcal{M} \) is inversely proportional to the kinetic coefficient \( \Gamma \) in (1.1). If \( F = 0 \), the equation becomes linear and its well-known dynamical symmetry is given by the Schrödinger algebra \( \mathfrak{sch}_1 \) [9], spanned by the generators (\( x \) is the scaling dimension of the field \( \Phi \))

\[
\begin{align*}
X_{-1} &= -\partial_t, \quad Y_{-\frac{1}{2}} = -\partial_r, \quad M_0 = -\mathcal{M} \\
Y_{\frac{1}{2}} &= -t\partial_r - \mathcal{M}r, \quad X_0 = -t\partial_t - \frac{1}{2}r\partial_r - \frac{x}{2} \\
X_1 &= -t^2\partial_t - tr\partial_r - \frac{\mathcal{M}}{2}r^2 - xt
\end{align*}
\]

(2.2)

It is also well-known that, for a dimensionless \( g \), the non-linear equation is only Schrödinger-invariant for the special choice of the potential \( F = (\Phi\Phi^*)^2 \Phi \) [10].

However, the equation (2.1) has in general complex solutions while for an application to the kinetic equation (1.1) one needs real-valued solutions. Furthermore, the available empirical evidence in favour of Schrödinger-invariance in the kinetic Ising model in \( d = 1, 2 \) and 3 [5, 6] goes against the mathematical result cited above. In order to overcome these difficulties, we
recognize that \( g \) is in general a dimensionful quantity and hence we shall look for the dynamical symmetries algebra of (2.1) taking this into account [11, 12].

If the dimensionful coupling constant enters into theory, the generators (2.2) are in general modified by additional \( g \)-dependent terms. We take the generator of scale-transformation in the form [11]

\[
X_0 = -t \partial_t - \frac{1}{2} r \partial_r - y g \partial_y - \frac{x}{2},
\]

where the dimensionful coupling \( g \) enters together with its scaling dimension \( y \), and other generators are calculated such that the commutators of \( \text{sch}_1 \) are kept and the free Schrödinger operator \( S = 2M_0 X_{-1} - Y_{-1/2}^2 \) remains unchanged in this new representation. We find that only the generator of special transformations is modified with respect to (2.2) and reads

\[
X_1 = -t^2 \partial_t - tr \partial_r - 2ytg \partial_y - \frac{M_0^2}{2} - xt.
\]

Furthermore if the time-translation invariance is broken, merely invariance under the ageing algebra \( \text{agc}_1 := \langle X_{0,1}, Y_{-1/2}, M_0 \rangle \) should hold. In this case we obtain a more general form of special transformations

\[
X_1 = -t^2 \partial_t - tr \partial_r - 2ytg \partial_y - m_0 g^{1+1/y} \partial_y - \frac{M_0^2}{2} - xt,
\]

where \( m_0 \) is a constant which characterizes the representations of \( \text{agc}_1 \) (for \( \text{sch}_1, m_0 = 0 \)).

Now standard methods [16] lead to the following form of non-linear part in equation (2.1) [11]

\[
F = \Phi (\Phi \Phi^*)^{1/y} f \left( (\Phi \Phi^*)^y \left[ g^{-1/y} \left( \frac{m_0}{y} \right)^{-xy} \right] \right).
\]

Consequently, in the long-time limit the equations invariant under \( \text{sch}_1 \) \((m_0 = 0)\) and \( \text{agc}_1 \) \((m_0 \neq 0)\) become indistinguishable. It is a property of theories with fixed masses that the potential still depends on both \( \Phi \) and its ‘complex conjugate’ \( \Phi^* \). In applications to non-equilibrium dynamics, the latter can be identified with the response field \( \Phi \) associated to the order-parameter field. We have shown recently that the exact results obtained for the bosonic variants of the contact-process and the pair-contact process for \( C(t,s) \) and \( R(t,s) \) [13, 14] can be completely explained in terms of local scale-invariance, where the action of the effective field-theory is split into a Schrödinger-invariant term leading to an equation of motion with a non-linearity of the form (2.5) and a pure noise term [11, 14].

3. Dynamic symmetries with variable masses

We now extend the scope of our investigation and also consider the ‘mass’ \( M \) as a new coordinate in the problem. Then the Schrödinger algebra \( \text{sch}_d \) in \( d \) spatial dimensions can be embedded into the complexified conformal algebra \( \text{conf}_{d+2} \) in \( d + 2 \) dimensions. One may see this in a simple way by writing \( M = im \) and then performing a Fourier transformation which defines a new wave function [15]

\[
\Phi = \Phi_m(t, r) = \frac{1}{\sqrt{2\pi}} \int_R d\zeta \ e^{-im\zeta} \Psi(\zeta, t, r)
\]

The one-dimensional free Schrödinger equation then becomes \((2\partial_\zeta \partial_{\zeta} - \partial_\zeta^2) \Psi = 0\) which can be rewritten through a further change of variables as a massless Klein-Gordon/Laplace equation in three dimensions,\(^1\) which has the simple Lie algebra \( \text{conf}_3 \) as a dynamical symmetry. The root diagram of the latter is shown in part (a) of figure 1, from which the correspondence between the roots and the generators of \( \text{sch}_1 \) can be read off. Four additional generators \( N, V, W, V^+ \) should be added in order to get the full conformal algebra \( \text{conf}_3 \).\(^2\)

\(^1\) We point out that the ‘mass’ \( M \) is a non-relativistic mass, which plays a completely different rôle than the masses of relativistic theories.

\(^2\)
In what follows, the so-called 'parabolic subalgebras' of $\text{conf}_3$ are of interest. Up to isomorphisms, these are [15]

- $\tilde{\text{sch}}_1 := \langle X_{-1,0,1}, Y_{-\frac{1}{2},\frac{1}{2}}, M_0, N \rangle$, see black dots in part (b) of the figure.
- $\tilde{\text{age}}_1 := \langle X_{0,1}, Y_{-\frac{1}{2},\frac{1}{2}}, M_0, N \rangle$, see black dots in part (c) of the figure.
- $\tilde{\text{alt}}_1 := \langle D, X_1, Y_{-\frac{1}{2},\frac{1}{2}}, M_0, N, V_+ \rangle$, see part (d) of the figure.

Here the generator $D = 2X_0 - N$ of the full dilatations is used. The corresponding "almost-parabolic subalgebras" [12] are the same as above but without the generator $N$.

For notational simplicity we shall work in one space dimension and look for a semi-linear extension of the linear "Schrödinger equation" of the form [12]

$$\hat{S} \Psi := \left(2\partial_\zeta \partial_t - \partial_t^2 \right) \Psi = F(g, \zeta, t, r, \Psi, \Psi^*)$$

which is invariant under one of the parabolic subalgebras of $(\text{conf}_3)_C$. We first construct new differential-operator representations of the algebras defined above which contain also a dimensionful coupling $g$. Then we explicitly give the admissible forms of $F$ in (2.1).

### 3.1. Invariant linear equations

The new representations with dimensionful coupling constants of (almost) parabolic subalgebras of $(\text{conf}_3)_C$ are constructed as follows. As before, we take for the dilatation generators

$$X_0 = -t \partial_t - \frac{1}{2} r \partial_r - yg \partial_g - \frac{x}{2}, \quad D = -t \partial_t - r \partial_r - \zeta \partial_\zeta - sg \partial_g - x.$$  (3.3)

The exponents $y$ and $s$ describe the scaling behaviour of the coupling $g$. Space- and time-translations $Y_{-\frac{1}{2}} = -\partial_r, X_{-1} = -\partial_t$ are also fixed, while the remaining generators read

$$
\begin{align*}
M_0 &= -\partial_\zeta - L(t, r, \zeta, g) \partial_g, & Y_{1/2} &= -t \partial_t - r \partial_r - Q(t, r, \zeta, g) \partial_g \\
X_1 &= -t^2 \partial_t - tr \partial_r - \frac{1}{2} r^2 \partial_\zeta - P(t, r, \zeta, g) \partial_g - xt \\
N &= -t \partial_\zeta + \zeta \partial_\zeta - K(t, r, \zeta, g) \partial_g \\
V_+ &= -2tr \partial_t - 2\zeta r \partial_\zeta - (r^2 + 2\zeta t) \partial_r - F(t, r, \zeta, g) \partial_g - 2xr. & \quad (3.4)
\end{align*}
$$
The unknown functions $L, Q, P, K, F$ are found from the commutation relations and the requirement that the linear equation $\hat{S}\Psi = 0$ is left invariant under above transformations. Our results are presented in the following table.

| case | subalgebra | representation | $x$ | $S$ |
|------|------------|----------------|-----|-----|
| 1    | $\mathfrak{age}_1$ | NMG | $L = 0, Q = 0$, $P = p_{01}tg$ | $= 1/2$ | $2\partial_t \partial_t - \partial_r^2$ |
|      | $\mathfrak{age}_1$ | $K = k_0g$ | $\neq 1/2$ | $2\partial_t \partial_t - \partial_r^2$ |
| 2    | $\mathfrak{age}_1$ | MMG | $L = -2y g/\zeta$, $Q = -2y g r/\zeta$, $P = -y g r^2/\zeta$ | $= 1/2$ | $2\partial_t \partial_t - 4yg\zeta^{-1}\partial_r\partial_t - \partial_r^2$ |
|      | $\mathfrak{age}_1$ | $K = k_0g$ | $\neq 1/2$ | $(2\partial_t \partial_t - \partial_r^2)\Psi = 0$ |
| 3    | $\mathfrak{alt}_1$ | $L = sg/\zeta$, $Q = srg/\zeta$, $P = sr^2 g/2\zeta$, $F = 2srg$ | $= 1/2$ | $2\partial_t \partial_t + 2sg\zeta^{-1}\partial_r\partial_t - \partial_r^2$ |
| 4    | $\mathfrak{alt}_1$ | $K = k_0g$ | $\neq 1/2$ | $\partial_\zeta \partial_t$ |
| 5    | $\mathfrak{sch}_1$ | $L = Q = P = 0$, $L = Q = 0$, $P = 2yg$ | $= 1/2$ | $2\partial_t \partial_t - \partial_r^2$ |
|      | $\mathfrak{sch}_1$ | $K = k_0g$ | $\neq 1/2$ | $2\partial_t \partial_t - \partial_r^2$ |

We obtain two distinct representations (see [12] for details):
1. representations with $L = 0$ for $\mathfrak{age}_1$, $\mathfrak{sch}_1$ which we call ‘non-modified’ (NMG).
2. representations with $L \neq 0$ for $\mathfrak{age}_1$, $\mathfrak{alt}_1$ which we call ‘modified’ (MMG).
We see that for $x \neq 1/2$ auxiliary condition(s) lead to modified forms of $\hat{S}$ [12].

### 3.2. Invariant non-linear equations

From these representations, standard methods [10,16] allow to calculate the potential $F$ in the invariant equation $\hat{S}\Psi = F$. Our results [12] are listed in the following table where we give

(i) Generic solutions for the potential $F$.
(ii) Non-generic solutions with certain conditions on parameters of the algebras and where $f$ stands for an arbitrary function.

| case | subalgebra | potential $F$ | condition |
|------|------------|---------------|------------|
| 1    | $\mathfrak{age}_1$ | $a^{x+2} f(a^x \Psi, \Psi/\Psi^*)$ | $p_{01} \neq 2y - k_0$ |
| 2    | $\mathfrak{age}_1$ | $a^{x+2} f(a^x \Psi, \Psi/\Psi^*)$ | $p_{01} = 2y - k_0$ |
| 3    | $\mathfrak{age}_1$ | $b^{x+2} f(b^x \Psi, \Psi/\Psi^*)$ | $k_0 \neq 4y$ |
| 4    | $\mathfrak{age}_1$ | $b^{x+2} f(b^x \Psi, \Psi/\Psi^*)$ | $k_0 = 4y$ |
| 5    | $\mathfrak{alt}_1$ | $c^{-x^2} f(c^x g, c^x \Psi, \Psi/\Psi^*)$ | $k_0 \neq 0$ |
| 6    | $\mathfrak{alt}_1$ | $c^{-x^2} f(c^x g, c^x \Psi, \Psi/\Psi^*)$ | $k_0 = 0$ |
| 7    | $\mathfrak{sch}_1$ | $g^{-x+2}/2y f(g^{x+2} \Psi, \Psi/\Psi^*)$ | $k_0 \neq 0$ |
| 8    | $\mathfrak{sch}_1$ | $g^{-x+2}/2y f(g^{x+2} \Psi, \Psi/\Psi^*)$ | $k_0 = 0$ |
4. An application to phase-ordering

Consider the equations invariant under \( \mathfrak{gc}_1 \) or \( \mathfrak{sch}_1 \) with a corresponding auxiliary condition for the wave function. If the potential does not depend on the second variable \( \Psi / \Psi^* \) (a ‘phase’) we obtain the following invariant semi-linear equation [12]

\[
(2 \partial_t + \partial_x^2) \psi = \psi^5 \bar{f} (g \psi^{4y})
\]  

(4.1)

where \( \bar{f} \) is an arbitrary function (see cases 2, 8). This kind of invariant equations with a real potential looks quite similar to the Langevin equation (1.1) at zero temperature \( T = 0 \) as it is studied in phase-ordering kinetics, see [1–3]. However, we stress that in order to obtain an invariant equation, we need to take the non-vanishing scaling dimension of the coupling \( g \) into account and/or must consider the ‘mass’ as a further variable. Our invariant equation (4.1) is not fully identical with (1.1) and might be called model A’.

Remarkably, the representation of the invariance algebra is independent of the choice of the function \( \bar{f} \) which characterizes the potential. This is in keeping with the folklore knowledge on universality in phase-ordering, namely that the details in the form of the potential should not affect the long-time behaviour. Indeed, universality of phase-ordering can be precisely formulated through the Allen-Cahn equation which follows from (1.1) and states that the velocity of the domain walls between the ordered domains (of time-dependent size \( L(t) \sim t^{1/2} \) with \( z = 2 \)) only depends on the curvature of these walls and is independent on more detailed system properties such as the surface tension [1]. For an experimental check on the Allen-Cahn relation in the ordering kinetics of the alloy \( \text{Cu}_{0.79}\text{Pd}_{0.21} \) see [17].

Summarizing, realizing that the couplings in semi-linear equations are in general dimensionful has allowed us to extend previous results on the existence of non-trivial dynamical symmetries. This also brings the mathematical theory into much closer contact with simulational results. Furthermore, going over to variable masses appears to bring the possibility of actually proving dynamical scaling and also further non-anticipated symmetries within reach. We hope to return to this in the future.

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