Higher-order symmetries and creation operators for linear equations via Maxima and SymPy
Exercises in solving overdetermined systems of differential equations

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Introduction
Symmetries - general description
The physical model
Symmetries and general differential creation and annihilation operators
Lie symmetries of Bose-Hubbard model
Conditional symmetries

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Motto:

Mathematical Sciences form the crown and ultimate goal of all human activity.

Therefore, do not ask what mathematics and mathematical physics can do for society. That question is meaningless.

A meaningful question - which you should ask - is what your state and society can do for the development of Mathematics.

(Notengolmo, *Opera omnia* Vol. 1, p. (i))
Computation of symmetries of systems of partial differential equations is one of the oldest applications of computer algebra in the field of differential equations and mathematical physics. Already in the late eighties and early nineties several packages to compute symmetries have been developed in Macsyma, Reduce, Mathematica and Maple[1, 2]. Today, it is actually difficult to imagine not to use computer algebra when one faces analysis of complex differential (or difference) system. Skillful application of existent packages leads to efficient analysis of even very complicated systems like those encountered in theory of elasticity, see, e.g., [3].
General first-order symmetries

\[ U = 0, \quad (1) \]

and let \( X \) denotes the so-called infinitesimal generator of symmetries which is a first-order linear partial differential operator. Then there exists the following infinitesimal criterion of symmetry (please see, e.g., [4]):

\[ X^{(pr)} U|_{U=0} = 0, \quad (2) \]

where \( X^{(pr)} \) is the prolongation of the operator \( X \). The above formula has a simple geometric meaning: the symmetry of \( U \) is such a transformation (in the space of independent variables, dependent variables and their derivatives) which leaves the hypersurface of solutions invariant.
From the above condition a system of linear partial differential equations can be obtained to compute $X$. They are called *determining equations*. Even writing down all the determining equations is a very tedious procedure, ideally suited for computers. In the case of linear equations calculations of symmetries quite radically simplify as specified below. Nonetheless, computer algebra is still needed!
Symmetries in Maxima

- The package MACSYMA (of which Maxima is a descendant) was one of the first, if not *the* first, for which a program calculating determining equations and finding symmetries has been written. It is the famous `cartan` package by Estabrook and Wahlquist.

- In our applications, `cartan` and other packages known to us are, on one hand, too general, comprising analysis of non-linear systems, and, on the other hand, not general enough, since it does not allow for symmetry operators of the order higher than one.
Bargmann-Segal representation

Definition

The Bargmann-Segal representation consists in writing creation and annihilation operators as differential operators which act in the Hilbert space of analytic functions. Thus, wave functions are analytic functions of many complex variables, \( \Psi(z_1, z_2, ..., z_n) \) with the scalar product:

\[
\frac{1}{\pi^n} \int \Psi^*(z_1, z_2, ..., z_n) \Psi(z_1, z_2, ..., z_n) \exp(-\sum_k |z_k|^2) \tag{3}
\]

Creation operators \( a_k^\dagger \), \( k = 1, 2, ..., n \) are represented as multiplications by \( z_k \), and annihilation operators \( a_k \) as differential operators \( \partial/\partial z_k \). E.g. \( a_k^\dagger a_l \Psi = z_k (\partial \Psi / \partial z_l) \).
Basic Hamiltonian

Definition

The extended Bose-Hubbard model is one of the most important models describing system of particles evolving on a lattice. It is defined by the Hamiltonian:

\[ H = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{V}{2} \sum_i a_i^\dagger a_i^2 + W \sum_{\langle i,j \rangle} a_i^\dagger a_i a_i^\dagger a_j, \]  

(4)

where \( \langle i,j \rangle \) denotes that only nearest neighbours contribute to summation.

It is the term containing \( W \) which is responsible for the adjective “extended”.

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Higher-order symmetries and creation operators for linear equations via Maxima and SymPy
Definition

By (possibly time-dependent) constant of motion we understand an operator $C$ which commutes with the Hamiltonian:

$$[C, H] = 0$$
 Constants of motion and first-order symmetry operators

**Definition**

By (possibly time-dependent) constant of motion we understand an operator $C$ which commutes with the Hamiltonian:

$$[C, H] = 0$$

**Definition**

Let $Q$ be a linear partial differential operator. By first-order symmetry operator we understand a linear partial differential operator $L$ of the first order such that:

$$[L, Q] = RQ,$$

where $R$ is a function of independent variables.
Remark

*The above operator equation has to be satisfied identically for all admissible functions.*
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Remark
The above operator equation has to be satisfied identically for all admissible functions.

Remark
First-order symmetry operators form a Lie algebra!
Higher-order symmetries and creation operators

Definition

By $n$th-order symmetry operator we understand a linear partial differential operator $L^{(n)}$ of the order $n$ such that:

$$[L^{(n)}, Q] = S^{(n-1)} Q,$$

where $S$ is a differential operator of the order $n - 1$. 

Remark

Higher-order symmetry operators usually do not form a Lie algebra.
Definition

By \( n \)th-order symmetry operator we understand a linear partial differential operator \( L^{(n)} \) of the order \( n \) such that:

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[L^{(n)}, Q] = S^{(n-1)} Q,
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Definition

By $n$th-order symmetry operator we understand a linear partial differential operator $L^{(n)}$ of the order $n$ such that:

$$[L^{(n)}, Q] = S^{(n-1)} Q,$$  \hspace{1cm} (6)

where $S$ is a differential operator of the order $n - 1$.

Remark

Higher-order symmetry operators usually do not form a Lie algebra.
Definition

We call an operator $A^\dagger$ a creation operator if there exists a real positive constant $k$ such that $[H, A^\dagger] = kA^\dagger$. 
Fact

The only non-trivial symmetry of the Bose-Hubbard model for $W = 0$ is, unfortunately, that generated by the excitation-number operator:

$$\hat{N} = \sum_i z_i \frac{\partial}{\partial z_i} = \sum_i a_i^\dagger a_i.$$ 

with $R = 0$. 
What are symmetries of partial differential equations good for?

- There is a connection with conservations laws.
- New (non-trivial) solutions can be generated from known (possibly trivial) ones upon using a Lie theorem.
- Special solutions of partial differential equations can be obtained on using differential invariants.
- Separation of variables can (sometimes) be achieved.
Separation of variables in BHM

Example

Let $W = 0, M = 2$. Let us solve the eigenvalue problem for $\hat{N}$:

$$z_1 \frac{\partial \chi}{\partial z_1} + z_2 \frac{\partial \chi}{\partial z_2} = \lambda \chi,$$

and find an invariant, $\hat{N} \phi = 0$. We have, e.g.,

$$\phi = \phi(z_1/z_2) = z_1/z_2 = w, \quad \chi = (z_1 z_2)^{\lambda/2}.$$ We can attempt the following simple separation of variables in the time-independent Schrödinger equation $H \psi = E \psi$:

$$\psi(z_1, z_2) = (z_1 z_2)^{\lambda/2} u(w).$$
Example

Then $u(w)$ satisfies an ordinary differential equation:

$$w^2 u''(w) + (w + (w^2 - 1)(J/V))u'(w) +
(\lambda^2 - \lambda - (J/V)\lambda(w + 1/w))u(w) = \frac{E}{V}u(w).$$

For instance, for $\lambda = 1$ we obtain the solution $u = w^{1/2} - w^{-1/2}$, $\psi = z_1 - z_2$, $E = J$. 
Generation of new solutions by solving Lie equations

Example

The Bose-Hubbard model admits the following symmetry generator for $M = 2, V = 2W$:

$$X = z_1 \frac{\partial}{\partial z_2} + z_2 \frac{\partial}{\partial z_1}$$

It generates finite symmetry transformation which can be obtained from the solution to the Lie equations:

$$\frac{d\tilde{z}_1}{d\epsilon} = \tilde{z}_2, \quad \frac{d\tilde{z}_2}{d\epsilon} = \tilde{z}_1,$$

with the initial conditions $\tilde{z}_1(0) = z_1, \tilde{z}_2(0) = z_2$. 
If $\Psi(t, z_1, z_2)$ satisfies the Schrödinger equation, so does $\Psi(t, z_1 \cosh(\epsilon) + z_2 \sinh(\epsilon), z_1 \sinh(\epsilon) + z_2 \cosh(\epsilon))$. 
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Reduction of the number of variables and special solutions

Example

Let $M = 3$, $W = 0$, we use the symmetry generator

$$\hat{N} = \sum_{i=1}^{M} z_i \frac{\partial}{\partial z_i}.$$ 

Solving $\hat{N} \chi = 0$ we obtain invariants, e.g., $w_1 = z_1/z_2$, $w_2 = z_3/z_2$. We can then look for the solution to the Schrödinger equation in terms of $\Psi = \exp(-iEt/\hbar)\phi(w_1, w_2)$ to obtain $(\phi_{20} = \partial^2 \phi/(\partial w_1^2)$, etc.):
Reduction of the number of variables and special solutions

Example

\[-(E/V)\phi_{00} + w_1^2 \phi_{20} + w_1 w_2 \phi_{11} + w_2^2 \phi_{02} +
\]
\[ ((J/V)(w_1^2 - 1) + w_1 + (J/V)w_1 w_2)\phi_{10} +
\]
\[ ((J/V)(w_2^2 - 1) + w_2 + (J/V)w_1 w_2)\phi_{01} = 0. \]
Conditional symmetries of linear equations

Definition

An operator $X$ is a generator of a first-order conditional symmetry of a linear partial differential equation if there exists a function $R$ of independent variables and a first-order linear partial differential operator $S$ such that:

$$[Q, X] = RQ + SX$$
Proposition (J. Kaleta, A. Zembrzuski)

The most general symmetry in the above class for BHM with \( W = 0 \) is that generated by:

\[
X = A(t, \{z_i\}) \left( \tau \frac{\partial}{\partial t} + \sum_i \xi_i \frac{\partial}{\partial z_i} + \phi \right),
\]

where \( A(t, \{z_i\}) = \exp(\sum_i c_i(t)z_i) \), \( \tau = \tau_0 \), \( \xi_i = c_0 z_i \), \( \phi = \phi_0 \).
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References


Miller W., *Symmetry and separation of variables*, Addison-Wesley, Reading (1977)
Thank you for your attention