

Lie point symmetries: An alternative approach to wave-functions

K Andriopoulos and PGL Leach

Abstract

We apply Lie's theory of symmetries of differential equations to construct solutions of the time-dependent Schrödinger equation. We compare this approach with the traditional method based on separation of variables and Sturm-Liouville theory and also the operator method developed by Dirac.

Keywords: Lie Symmetries, Time-dependent Schrödinger equation

1. Introduction

We discuss different methods for the derivation of solutions for some problems occurring in Quantum Mechanics. We use as a vehicle for the demonstration of this derivation the Schrödinger equation for the simple harmonic oscillator [10]. Up to now two approaches were generally known. The first approach used the rather *ad hoc* method of separation of variables and the second used the operator method developed by Dirac. Unfortunately the former can be employed but in a few problems occurring in Quantum Mechanics, and Physics generally, since, as it is well-known, the technique of separation of variables only works if the variables are separable.

The time-dependent Schrödinger equation with the potential of a simple harmonic oscillator in suitably rescaled variables is

$$2i \frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} - x^2 u = 0, \quad u(\pm\infty) = 0. \quad (1)$$

For the method of separation of variables one seeks nontrivial solutions of (1) of the form

$$u(x, t) = G(t)F(x) \exp \left[-\frac{1}{2}x^2 \right], \quad (2)$$

in which one has included a term which satisfies the conditions at $\pm\infty$, *ie* an asymptotic solution.

The form of solutions, (2), when substituted in (1) yields the two equations

$$F''(x) - 2xF'(x) + (2\lambda - 1)F(x) = 0 \quad (3)$$

$$\dot{G}(t) + i\lambda G(t) = 0, \quad (4)$$

where λ is the constant of separation.

For a polynomial solution of (3) and hence a bounded solution of (1) it is necessary for λ to take the values $n + \frac{1}{2}$, $n = 0, 1, 2, \dots$, where n is the degree of the polynomial.

Thus we obtain

$$u_n(x, t) = H_n(x) \exp \left[-\frac{1}{2} (x^2 + it) - int \right], \quad (5)$$

where $H_n(x)$ are the Hermite Polynomials [3][p 1033].

An alternative, operator, approach was introduced by Dirac [2] who recognised the connection between the canonical formalism of Hamiltonian Mechanics and Quantum Mechanics and expressed the time-dependent Schrödinger equation as

$$\hat{H}u = i \frac{\partial u}{\partial t},$$

where \hat{H} is the classical Hamiltonian with the canonical variables, p and q , replaced by the operators, \hat{p} and \hat{q} , with commutator $[\hat{q}, \hat{p}] = i$. In the case of the simple harmonic oscillator

$$\hat{H} = \frac{1}{2} (\hat{p}^2 + \hat{q}^2)$$

one introduces two operators

$$\hat{a} = \hat{q} + i\hat{p} \quad \text{and} \quad \hat{a}^\dagger = \hat{q} - i\hat{p}, \quad [\hat{a}, \hat{a}^\dagger] = 2,$$

which act as annihilation and creation operators for the eigenfunctions of

$$\hat{H}\psi = E\psi.$$

The ground state is found from

$$\hat{a}\psi_0 = 0 \quad \Rightarrow \quad \left(x + \frac{d}{dx} \right) \psi_0 = 0 \quad \Rightarrow \quad \psi_0 = \exp \left[-\frac{1}{2} x^2 \right]$$

in the position representation (up to a normalisation constant). Higher states, ψ_n , are obtained using \hat{a}^\dagger , ie

$$\psi_n = (\hat{a}^\dagger)^n \psi_0.$$

Naturally these are the same as obtained by the method of separation of variables. The requirement that E be nonnegative leads to

$$E_n = n + \frac{1}{2}.$$

In this paper we apply Lie's theory of symmetries of differential equations, to construct solutions of the time-dependent Schrödinger equation. We show how the construction of these solutions comes naturally by using Lie's techniques, that is, the symmetries that the differential equation possesses. The only restriction to the application of Lie's method is that equations for such problems should possess a

sufficient number of Lie point symmetries. Then it is possible to construct a basic solution using one of the symmetries and, by operating another symmetry on the solution surface produced by the former, to generate an infinite number of linearly independent solutions, which provide a basis for the general solution of the problem being solved.

The existence of Lie symmetries is extrinsic to our ability to solve a differential equation by means of analytical methods. Without the existence of some sort of suitable symmetry the differential equation, in this instance the time-dependent Schrödinger equation of Quantum Mechanics, simply does not admit the possibility of a solution in closed form.

The outline of this paper is as follows. In the following section we introduce and develop the derivation of the general solution of a class of problems, using as a vehicle the quantal simple harmonic oscillator, making use of the symmetries the equation possesses. In §3 we make some observations.

2. Lie point symmetries

The concept of symmetry is well established in Physics and is naturally associated with the existence of conservation laws. Hamiltonian systems can possess a variety of conservation laws.

For example, if

$$\frac{\partial H}{\partial t} = 0 \quad \Leftrightarrow \quad H = H(q, p), \quad (6)$$

the energy ($= H$) is conserved. The first half of (6), $\partial H/\partial t = 0$ means that H is invariant under time translation, *ie* it possesses the symmetry ∂_t ($:= \partial/\partial t$). Conservation of energy is invariably associated with the presence of this symmetry.

In three dimensions, if the Hamiltonian possesses spherical symmetry, *ie*

$$H = H(r, \mathbf{p}), \quad \Leftrightarrow \quad \frac{\partial H}{\partial \theta} = 0, \quad \frac{\partial H}{\partial \phi} = 0,$$

the angular momentum, $\mathbf{L} := \dot{\mathbf{r}} \times \mathbf{r}$, is conserved. The Hamiltonian is invariant under the transformations associated with the rotation group $SO(3)$.

The algebraic representation of the group in terms of the components of the angular momentum is given by

$$[L_i, L_j]_{PB} = \epsilon_{ijk} L_k.$$

There is an equivalent representation in terms of differential operators given by

$$\begin{aligned} \Gamma_1 &= \partial_\phi \\ \Gamma_{2\pm} &= e^{\pm i\phi} (\partial_\theta \pm i \cot \theta \partial_\phi). \end{aligned}$$

The algebraic properties are represented by the Lie Brackets

$$[\Gamma_1, \Gamma_{2\pm}]_{LB} = \pm i\Gamma_{2\pm} \quad \text{and} \quad [\Gamma_{2+}, \Gamma_{2-}]_{LB} = 2i\Gamma_1.$$

This is just another representation of the algebra $so(3)$.

The application of Group Theory to Physics has been one of the success stories of modern science. To a large extent the initiation of the application is due to Herman Weyl who extracted the physical essence from the Theory of Continuous Groups developed by Sophus Lie.

The analysis of differential equations in terms of invariance under infinitesimal transformation was initiated by Lie in the 1870s and extended by him in succeeding decades with a series of lengthy publications [7, 8, 9]. Lie commenced with the study of continuous groups and their realisations in terms of infinitesimal transformations and was concerned with the properties of invariance under these transformations. The infinitesimal transformation, say in two variables (the generalisation to more variables is not one of conceptual complexity), is

$$\begin{aligned} \bar{t} &= t + \epsilon\tau & \Leftrightarrow & \quad \bar{t} = (1 + \epsilon\Gamma)t \\ \bar{x} &= x + \epsilon\eta & & \quad \bar{x} = (1 + \epsilon\Gamma)x, \end{aligned} \quad (7)$$

where the infinitesimal transformation is generated by the differential operator

$$\Gamma = \tau\partial_t + \eta\partial_x. \quad (8)$$

In particular

$$\Gamma t = \tau \quad \text{and} \quad \Gamma x = \eta.$$

When Γ is associated with an invariant such as in the case of time translation and the consequent conservation of energy, it is called a symmetry.

The infinitesimal transformations (7) generated by the differential operator (8) cause infinitesimal transformations in derivatives. For example, if the x in (7) is the dependent variable and t is the independent variable, the corresponding infinitesimal transformation in the first derivative is computed as follows.

$$\begin{aligned} \frac{d\bar{x}}{d\bar{t}} &= \frac{d(x + \epsilon\eta)}{d(t + \epsilon\tau)} = \frac{dx + \epsilon d\eta}{dt + \epsilon d\tau} \\ &= \left(\frac{dx}{dt} + \epsilon \frac{d\eta}{dt} \right) \left(1 + \epsilon \frac{d\tau}{dt} \right)^{-1} \\ &= \frac{dx}{dt} + \epsilon \left(\frac{d\eta}{dt} - \frac{dx}{dt} \frac{d\tau}{dt} \right) + O(\epsilon^2), \end{aligned}$$

where in the last step we have used Newton's binomial expansion and $O(\epsilon^2)$ stands for the sum of all terms of second order or greater. The differential operator which generates this infinitesimal transformation is $(\dot{\eta} - \dot{x}\dot{\tau})\partial_{\dot{x}}$ and can be appended to the original Γ to give

$$\Gamma^{[1]} = \tau\partial_t + \eta\partial_x + (\dot{\eta} - \dot{x}\dot{\tau})\partial_{\dot{x}}$$

which is known as the first extension of Γ . The process of extension may be continued indefinitely. A similar process may be applied in the case of functions of many variables.

A differential equation

$$E(x, u, u^{(1)}, \dots, u^{(n)}) = 0,$$

be it ordinary or partial (in which case x is a multivariable and $u^{(j)}$ represents all possible derivatives of the j th order), possesses a Lie symmetry, Γ , if

$$\Gamma^{[n]}E|_{E=0} = 0, \quad (9)$$

where $\Gamma^{[n]}$ is the n th extension of Γ required to deal with the n th derivatives in E . The subscript $E = 0$ means that the constraint of the differential equation is taken into account.

The solution of (9) is a nontrivial task for all but the simplest equations and is best performed using one of the symbolic manipulation codes designed for the purpose. For a review of the packages available see Hereman [5, 6]. A standard text such as that of Bluman and Kumei [1] can be consulted for the more technical aspects of the theory.

The time-dependent Schrödinger equation, (1), has the $5 + 1 + \infty$ Lie point symmetries¹

$$\begin{aligned} \Gamma_1 &= i\partial_t & \Gamma_5 &= e^{-it}(\partial_x + ux\partial_u) \\ \Gamma_2 &= e^{2it}[\partial_t + ix\partial_x - iu(\frac{1}{2} + x^2)\partial_u] & \Gamma_6 &= u\partial_u \\ \Gamma_3 &= e^{-2it}[\partial_t - ix\partial_x + iu(\frac{1}{2} - x^2)\partial_u] & \Gamma_f &= f(x, t)\partial_u \\ \Gamma_4 &= e^{it}(\partial_x - ux\partial_u), \end{aligned} \quad (10)$$

where ∂_t , ∂_x and ∂_u represent $\partial/\partial t$, $\partial/\partial x$ and $\partial/\partial u$, respectively.

One observes that the symmetries Γ_1, Γ_2 and Γ_3 constitute the subalgebra $sl(2, R)$, Γ_4 and Γ_5 are known as the solution symmetries, Γ_6 is the homogeneity symmetry and Γ_f produces the infinite number of Lie point symmetries, where $f(x, t)$ is any solution of (1). One notes that the five symmetries $\Gamma_1 - \Gamma_5$ correspond to the Noether symmetries of the Lagrangian $L = \frac{1}{2}(\dot{x}^2 - x^2)$ of the classical simple harmonic oscillator. Γ_4 and Γ_5 are called the solution symmetries since they correspond to the two Noether symmetries, $\exp[\pm it]\partial_x$, of L and $\exp[\pm it]$ are two linearly independent solutions of the Euler-Lagrange equation of L . The homogeneity symmetry Γ_6 is a consequence of the linearity of (1). Note that there is a slight difference between the Noether symmetries of the classical Lagrangian for the oscillator and the Lie symmetries of the Schrödinger equation. For the former Γ_4 and Γ_5 constitute an abelian subgroup – a feature common to solution symmetries – and in the case of the latter Γ_6 is needed to produce closure of the algebra which is, appropriately enough, the Weyl algebra. Lie symmetries have two attractive features relevant to our discussion. They enable

¹We used Program LIE [4, 11].

one to construct solutions of differential equations and the action of a symmetry on a solution produces a solution. To produce a new solution one introduces the concept of a solution surface. If a solution is

$$u = f(t, x),$$

then the corresponding solution surface is

$$\Sigma = u^{-1}f(t, x)$$

in (t, x, u) space. The action of a symmetry on Σ is to map the surface to a new surface

$$\bar{\Sigma} = u^{-1}\bar{f}(t, x)$$

so that the new solution is

$$u = \bar{f}(t, x).$$

Some symmetries are more effective than others and we skip the less useful and start with the reasonable candidate, Γ_4 , the associated Lagrange's system of which is

$$\frac{dt}{0} = \frac{dx}{1} = \frac{du}{-ux},$$

with characteristics (which can be used as similarity variables)

$$v = t \quad \text{and} \quad w = u \exp\left[\frac{x^2}{2}\right] \quad \text{so that} \quad u = f(t) \exp\left[-\frac{x^2}{2}\right]. \quad (11)$$

When (11) is substituted into (1) to compute $f(t)$, we obtain

$$f(t) = \exp\left[-\frac{1}{2}it\right].$$

Thus

$$u_0 = \exp\left[-\frac{1}{2}(it + x^2)\right]$$

which is the basic similarity solution. This similarity solution, u_0 , has no finite zeros, represents the ground-state solution of (1) and defines a surface in (t, x, u) space through

$$\Sigma_0 = u^{-1} \exp\left[-\frac{1}{2}(it + x^2)\right].$$

We can now generate further solutions by using the other symmetries. The repeated action of Γ_5 on the solution surface computed in each step provides a whole class of solutions, *ie*

$$\begin{aligned} u_1 &= -2x \exp\left[-\frac{1}{2}(3it + x^2)\right] \\ u_2 &= (4x^2 - 2) \exp\left[-\frac{1}{2}(5it + x^2)\right] \\ u_3 &= (12x - 8x^3) \exp\left[-\frac{1}{2}(7it + x^2)\right] \\ &\vdots \end{aligned}$$

with the general formula of their production being of the form

$$u_{2n} = \left(\sum_{j=0}^n a_j x^{2j} \right) \exp \left[-\frac{1}{2} ((4n+1)it + x^2) \right] \quad (12)$$

$$u_{2n+1} = \left(\sum_{j=0}^n b_j x^{2j+1} \right) \exp \left[-\frac{1}{2} ((4n+3)it + x^2) \right]. \quad (13)$$

To determine the $a_j, j = 0, n$, we substitute (12) in (1) to obtain

$$\begin{aligned} & (4n+1) \sum_{j=0}^n a_j x^{2j} + \sum_{j=0}^n 2j(2j-1)a_j x^{2j-2} - 4 \sum_{j=0}^n j a_j x^{2j} - \sum_{j=0}^n a_j x^{2j} = 0 \\ \Leftrightarrow & \sum_{j=0}^n 4(j-n)a_j x^{2j} = \sum_{j=0}^n 2j(2j-1)a_j x^{2j-2} \\ \Leftrightarrow & \sum_{j=0}^{n-1} 4(j-n)a_j x^{2j} = \sum_{j=1}^n 2j(2j-1)a_j x^{2j-2} \\ \Leftrightarrow & \sum_{j=0}^{n-1} 4(j-n)a_j x^{2j} = \sum_{j=0}^{n-1} 2(j+1)(2j+1)a_{j+1} x^{2j} \\ \Leftrightarrow & a_{j+1} = \frac{2(j-n)}{(j+1)(2j+1)} a_j \quad \Leftrightarrow \quad a_j = \frac{(-1)^j 2^{2j} n!}{(2j)!(n-j)!} a_0. \end{aligned}$$

Similarly the $b_j, j = 0, n$, are found, when (13) is substituted in (1), to be

$$b_{j+1} = \frac{2(j-n)}{(j+1)(2j+3)} b_j \quad \Leftrightarrow \quad b_j = \frac{(-1)^j 2^{2j} n!}{(2j+1)!(n-j)!} b_0.$$

Thus, if we set $a_0 = b_0 = 1$, we obtain the solutions

$$u_{2n}(t, x) = \left(\sum_{j=0}^n \frac{(-1)^j 2^{2j} n!}{(2j)!(n-j)!} x^{2j} \right) \exp \left[-\frac{1}{2} ((4n+1)it + x^2) \right] \quad (14)$$

$$u_{2n+1}(t, x) = \left(\sum_{j=0}^n \frac{(-1)^j 2^{2j} n!}{(2j+1)!(n-j)!} x^{2j+1} \right) \exp \left[-\frac{1}{2} ((4n+3)it + x^2) \right]. \quad (15)$$

We note that the polynomials in (14) and (15) coincide with those obtained by the method of separation of variables and are identified with the well-known Hermite polynomials of §1.

3. Observations

We have treated the solution of the quantal simple harmonic oscillator in three different ways, two in outline and one in detail. The first method, the more traditional of three, is that of separation of variables. The second is based upon the elegant operator approach to Quantum Mechanics developed by Dirac. The third made use of the intrinsic symmetry properties of the Schrödinger wave-equation.

In the method of separation of variables one has to make use of the necessity for the wave-function to tend towards zero as the spatial variable tends towards infinity at two levels. The first is in the use of the asymptotic behaviour of the solution of the time-independent Schrödinger equation and the second in the demand that the series solution attached to the acceptable asymptotic behaviour terminates, *ie* is a polynomial, to avoid divergence of the solution at infinity. The second demand produces the eigenvalue of the Hamiltonian, *ie* the energy.

The properties of the two operators, \hat{a}^\dagger and \hat{a} , as creation and annihilation operators, coupled with the positive semidefiniteness of the norm of the wave-function, again lead to the specific value for the energy and the ground-state solution. The creation operator attends to the construction of the solutions for higher levels of energy.

The Lie point symmetries of the time-dependent Schrödinger equation provided a natural way to approach the solution of the equation by using the fundamental connection between the symmetries of differential equation and solutions. After one has found a solution which is invariant under the action of a particular symmetry, the other symmetries may be used to construct new solutions. These solutions naturally arose as polynomials times the basis solution. The solutions obtained are automatically solutions of the time-dependent equation. In our demonstration of the method to construct the solutions we simply used only the second ‘solution’ symmetry. However, one could equally use Γ_3 to construct additional solutions. The only difference is that the creation is by an even number of steps so that one either creates the even series of wave-functions or the odd series. When one is at a higher state, the symmetries Γ_2 and Γ_4 can both be used as annihilation operators with the former annihilating in steps of two. The energy eigenvalue comes from the single remaining nontrivial symmetry, *videlicet* Γ_1 .

The various methods for the solution of differential equations are based on symmetry. One of the great values of the work of Lie was to provide a unified approach to the solution of differential equations, be they partial or ordinary, in place of the plethora of specific methods developed over the roughly two centuries before his seminal work. In this respect we must recognise the closeness of the operator method to the use of Lie symmetries. In fact, when one writes the creation and annihilation operators, \hat{a}^\dagger and \hat{a} , as differential operators in the position representation, one realises that they are simply Γ_4 and Γ_5 stripped of their time-dependent part. Consequently it is fair to claim that the very existence of the operator approach of Dirac is based upon

the existence of the Lie symmetries Γ_1 , Γ_4 and Γ_5 . In Γ_4 and Γ_5 we have Dirac's operators coupled with a time-dependent multiplier and the existence of Γ_1 enables one to separate time and space.

In this note we have used a simple carrier problem, that of the harmonic oscillator, in an attempt to make obvious the essential features of the different methods we have discussed. We emphasise the centrality of the Lie symmetries of the Schrödinger equation to the possibility of its solution in closed form. Without the symmetries any other method, apart from numerical, cannot be possible.

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◇ K Andriopoulos
Department of Mathematics and
Center for Research and
Applications in Nonlinear Systems
University of Patras
Patras, 26500, Greece
kand@aegean.gr

◇ PGL Leach
School of Mathematical Sciences
University of KwaZulu-Natal
Durban 4041
Republic of South Africa
leachp@ukzn.ac.za and
leach@math.aegean.gr