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Classical integrals as quantum mechanical differential operators: a comparison with the symmetries of the Schrödinger Equation

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Abstract. Superintegrable systems are characterised by the possession of many symmetries and integrals. We use the simple harmonic oscillator as an example and examine the relationship between the Noetherian integrals of a given Lagrangian as quantum operators and the Lie symmetries of the corresponding Schrödinger Equation.

1. Introduction

We use the simple harmonic oscillator as the vehicle for our discussion and demonstration. It has the standard Lagrangian[2]

$$\tfrac{1}{2}\left(\dot{x}^2 - x^2\right). \tag{1}$$

The Noether point symmetries and their associated integrals are calculated according to the formulae [2]

$$\begin{aligned} \dot{f}(t,\,x) = \tau(t,\,x)\frac{\partial L(t,\,x,\,\dot{x})}{\partial t} + \eta(t,\,x)\frac{\partial L(t,\,x,\,\dot{x})}{\partial x} \\ + \left(\dot{\eta} - \dot{x}\dot{\tau}\right)\frac{\partial L(t,\,x,\,\dot{x})}{\partial \dot{x}} + \dot{\tau}L(t,\,x,\,\dot{x}) \end{aligned} \tag{2}$$

and

$$\begin{aligned} I = f(t,\,x) - \big[\tau(t,\,x)L(t,\,x,\,\dot{x}) \\ + \left(\eta(t,\,x) - \dot{x}\tau(t,\,x)\right)\frac{\partial L(t,\,x,\,\dot{x})}{\partial \dot{x}}\bigg], \end{aligned} \tag{3}$$

where the point symmetry has the form $\Gamma = \tau(t,\,x)\partial_t + \eta(t,\,x)\partial_x$ and the function, $f(t,\,x)$, is the contribution consequent upon the possibility of a change in the endpoints when the variation of the Action Integral under the infinitesimal transformation generated by Γ is taken.

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[2] It is well known that there are many Lagrangians for the simple harmonic oscillator. For a sampling see [1]. The question to be addressed here is the relationship between the Noetherian integrals of a given Lagrangian as quantum operators and the corresponding Lie symmetries of the Schrödinger Equation.

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The Noether point symmetries and associated integrals for the Lagrangian (1) are

$$\begin{aligned}
\Gamma_1 &= \partial_t & I_1 &= \tfrac{1}{2}\left(\dot{x}^2 + x^2\right) \\
\Gamma_2 &= \mathrm{e}^{2it}\left(\partial_t + ix\partial_x\right) & I_2 &= \tfrac{1}{2}\,\mathrm{e}^{2it}\left(\dot{x}^2 - 2i\dot{x}x - x^2\right) \\
\Gamma_3 &= \mathrm{e}^{-2it}\left(\partial_t - ix\partial_x\right) & I_3 &= \tfrac{1}{2}\,\mathrm{e}^{-2it}\left(\dot{x}^2 + 2i\dot{x}x - x^2\right) \\
\Gamma_4 &= \mathrm{e}^{it}\partial_x & I_4 &= \mathrm{e}^{it}\left(ix - \dot{x}\right) \\
\Gamma_5 &= \mathrm{e}^{-it}\partial_x & I_5 &= -\mathrm{e}^{-it}\left(ix + \dot{x}\right) \\
\Gamma_6 &= 0 & I_6 &= 1.
\end{aligned}$$

The Hamiltonian corresponding to the Lagrangian (1) is

$$H = \tfrac{1}{2}\left(p^2 + x^2\right), \tag{4}$$

where the conjugate momentum is $p = \partial L/\partial\dot{x} = \dot{x}$. The Schrödinger Equation for (4) is

$$2i\frac{\partial u(t,\,x)}{\partial t} = -\frac{\partial^2 u(t,\,x)}{\partial x^2} + x^2 u(t,\,x) \tag{5}$$

and it has the Lie point symmetries

$$\begin{aligned}
\Sigma_1 &= \partial_t, \\
\Sigma_2 &= \mathrm{e}^{2it}\left[\partial_t + ix\partial_x - i\left(\tfrac{1}{2} + x^2\right)u\partial_u\right], \\
\Sigma_3 &= \mathrm{e}^{-2it}\left[\partial_t - ix\partial_x + i\left(\tfrac{1}{2} - x^2\right)u\partial_u\right], \\
\Sigma_4 &= \mathrm{e}^{it}\left(\partial_x - xu\partial_u\right), \\
\Sigma_5 &= \mathrm{e}^{-it}\left(\partial_x + xu\partial_u\right), \\
\Sigma_6 &= u\partial_u \quad \text{and} \\
\Sigma_\infty &= \phi(t,\,x)\partial_u,
\end{aligned}$$

where $\phi(t,\,x)$ is any solution of (5).

The Schrödinger Equation for the physical problem comes with the condition that $u(t,\,x)$ vanish at spatial infinity. There is no such condition on $\phi(t,\,x)$ unless the problem is stated with the boundary condition being part of the problem.

The Lie point symmetries, Σ_i, $i = 1,\,6$, are listed in parallel to the Noether point symmetries and integrals to make more readily a comparison of the properties reported below. In particular Σ_6 corresponds to the trivial integral I_6. We note that the coefficient functions for ∂_t and ∂_x are the same for the finite sets of symmetries.

The solution of the Schrödinger Equation is well known and is given by

$$u_n(t,\,x) = N_n \exp\left[-\left(n + \tfrac{1}{2}\right)it - \tfrac{1}{2}x^2\right]H_n(x), \tag{6}$$

where N_n is the normalisation constant for the nth-eigenstate and $H_n(x)$ is the nth Hermite polynomial which is the acceptable solution of the Hermite equation [3]

$$v''(x) - 2xv'(x) + 2nv(x) = 0. \tag{7}$$

2. Solution of the Schrödinger Equation using the Lie point symmetries of the equation

It is well known that the solution of (5) consistent with the boundary conditions can be obtained by means of separation of variables into time and space components and the use of the ladder operators introduced by Dirac [4], namely

$$a = D + x \quad \text{and} \quad a^\dagger = D - x, \tag{8}$$

where $a^\dagger$ is known as the creation operator and a is known as the annihilation operator since the former 'creates' states and the latter 'annihilates' states. What is obviously less well-known is that the Dirac operators are autonomous versions of two of the Lie point symmetries of (5) [5].

The Lie (point) symmetries of a differential equation constitute a Lie algebra under the operation of taking the Lie Bracket. In particular the Lie Brackets of the symmetries $\Sigma_i,\ i = 1, 6$ with Σ_∞ of the Schrödinger Equation, (5), produce another solution symmetry, *ie*,

$$[\Sigma_i,\, \Sigma_\infty]_{LB} = \tilde{\Sigma}_\infty, \tag{9}$$

where $\tilde{\Sigma}_\infty$ may be a constant multiple of Σ_∞ or a different solution symmetry[3]. Note that a solution symmetry (in this context) is a symmetry of the form $\phi(t,\, x)\partial_u$, where $\phi(t,\, x)$ is a solution of the Schrödinger Equation under consideration.

The Lie point symmetries of (5) all have the form

$$\Sigma = T(t)\partial_t + \Xi(t,x)\partial_x + \varepsilon(t,x)u\partial_u$$

apart from Σ_∞. The Lie Bracket of these two operators is [6]

$$[\Sigma,\, \Sigma_\infty]_{LB} = \left(T\phi_t + \Xi\phi_x - \varepsilon\phi\right)\partial_u. \tag{10}$$

The right side of (10) is a solution symmetry. One possibility is that it is trivial, *ie* zero. Then the expression on the right side of (10) is a linear first-order partial differential equation for $\phi(t,\, x)$. Consider Σ_5. The invariants of the first-order partial differential equation (10) can be calculated from the associated Lagrange's system,

$$\frac{\underset{\cdot}{\mathrm{t}}}{0} = \frac{\underset{\cdot}{\mathrm{x}}}{1} = \frac{\underset{\cdot}{\mathrm{u}}}{-xu},$$

from which the common exponential term has been cancelled. The invariants are t and $u \exp\left[\frac{1}{2}x^2\right]$.

We set

$$u(t,\, x) = \exp\left[-\tfrac{1}{2}x^2\right] f(t)$$

and substitute it into (5) to obtain the first-order equation

$$2i\dot{f}(t) - f(t) = 0$$

for $f(t)$ with solution

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

so that

$$u(t,\, x) = \exp\left[-\tfrac{1}{2}it - \tfrac{1}{2}x^2\right] \tag{11}$$

[3] A constant multiple, apart from zero, is of no consequence.

up to a constant of normalisation. The solution, (11), has no node and represents the groundstate solution. We denote it by u_0.

It is not necessary for the right side of (10) to be zero. Suppose it is some other solution, Φ. Then

$$T\phi_t + \Xi\phi_x - \varepsilon\phi = \Phi.$$

The action of Σ_5 on (11) is found by using the symmetry, Σ_∞, and the property that solutions are mapped into solutions. The Lie Bracket of the two symmetries, Σ_5 and Σ_∞, is

$$\left[\mathrm{e}^{-it}\left(\partial_x + xu\partial_u\right),\, \phi(t,\,x)\partial_u\right]_{LB} = \mathrm{e}^{-it}\left(\partial_x - x\right)\phi(t,\,x)\partial_u \tag{12}$$

so that, if we take the groundstate solution, u_0, in (11), the next eigenfunction is obtained from (12) when (11) is substituted, *ie*, the solution is mapped to the trivial solution. Consequently Σ_5 is the time-dependent creation operator and Σ_4 is the time-dependent annihilation operator. These Lie point symmetries of (5) are the origins of Dirac's famous operators.

Since the solution in (11) has no nodes and is annihilated by the action of Σ_4, it is the groundstate solution and we denote it by $u_0(t,\,x)$. Higher states may be obtained by the successive action of Σ_5. Thus

$$\begin{aligned}
u_1(t,\,x) &= \left[\Sigma_5,\, u_0(t,\,x)\partial_u\right]_{LB}\\
&= \left[\mathrm{e}^{-it}\left(\partial_x + xu\partial_u\right),\, \exp\left[-\tfrac{1}{2}it - \tfrac{1}{2}x^2\right]\partial_u\right]_{LB}\\
&= -2x\exp\left[-\tfrac{3}{2}it - \tfrac{1}{2}x^2\right]\partial_u,\\
u_2(t,\,x) &= \left[\Sigma_5,\, u_1(t,\,x)\partial_u\right]_{LB}\\
&= \left[\mathrm{e}^{-it}\left(\partial_x + xu\partial_u\right),\, \left(-2x\exp\left[-\tfrac{3}{2}it - \tfrac{1}{2}x^2\right]\right)\partial_u\right]_{LB}\\
&= \left(4x^2 - 2\right)\exp\left[-\tfrac{5}{2}it - \tfrac{1}{2}x^2\right]\partial_u
\end{aligned}$$

etc.

In a similar manner we find that Σ_1 is an eigenvalue operator and, if multiplied by i, is the energy operator; Σ_2 is a double annihilation operator and Σ_3 is a double creation operator.

3. Noetherian Integrals as differential operators

The Noetherian Integrals may be written as differential operators in the quantum scenario. They become

$$\begin{aligned}
I_1 &= \tfrac{1}{2}\left(-\partial_x^2 + x^2\right),\\
I_2 &= \tfrac{1}{2}\mathrm{e}^{2it}\left(-\partial_x^2 - (2x\partial_x + 1) - x^2\right),\\
I_3 &= \tfrac{1}{2}\mathrm{e}^{-2it}\left(-\partial_x^2 + (2x\partial_x + 1) - x^2\right)\\
I_4 &= i\mathrm{e}^{it}\left(x + \partial_x\right) \quad \text{and}\\
I_5 &= i\mathrm{e}^{-it}\left(-x + \partial_x\right).
\end{aligned}$$

(I_6 is an identity operator and we do not consider it further.)

The actions of each of these operators on the nth-eigenstate, given in (6), are given by

$$\begin{aligned}
I_1u_n(t,\,x) &= \left(n + \tfrac{1}{2}\right)N_n\exp\left[-i\left(n + \tfrac{1}{2}\right)t - \tfrac{1}{2}x^2\right]H_n(x),\\
I_2u_n(t,\,x) &= -2n(n-1)N_n\exp\left[-i\left(n - \tfrac{3}{2}\right)t - \tfrac{1}{2}x^2\right]H_{n-2}(x),\\
I_3u_n(t,\,x) &= -N_n\exp\left[-i\left(n + \tfrac{5}{2}\right)t - \tfrac{1}{2}x^2\right]H_{n+2}(x),\\
I_4u_n(t,\,x) &= 2inN_n\exp\left[-i\left(n - \tfrac{1}{2}\right)t - \tfrac{1}{2}x^2\right]H_{n-1}(x),\\
I_5u_n(t,\,x) &= -iN_n\exp\left[-i\left(n + \tfrac{3}{2}\right)t - \tfrac{1}{2}x^2\right]H_{n+1}(x).
\end{aligned}$$

In a less informative but conceptually clearer form these actions can be written as

$$\begin{aligned} I_1u_n(t,\,x) &= \left(n+\tfrac{1}{2}\right)u_n(t,\,x),\\ I_2u_n(t,\,x) &= -2n(n-1)N_nu_{n-2}(t,\,x),\\ I_3u_n(t,\,x) &= -\tfrac{1}{2}N_nu_{n+2}(t,\,x),\\ I_4u_n(t,\,x) &= 2inN_nu_{n-1}(t,\,x),\\ I_5u_n(t,\,x) &= -iN_nu_{n+1}(t,\,x). \end{aligned}$$

4. Variations on the Schrödinger Equation

We started from the standard Lagrangian, (1), and did all of the usual tricks to obtain the Schrödinger Equation, (5), its solutions and associated symmetries. We also have looked in the previous section at the action of the classical integrals when treated as operators on the solution. Now we examine what happens if we use these operators in a type of Schrödinger Equation. We should emphasise that one is looking at this from the point of view of symmetry and mathematics, not physics. Obviously there is no need to consider I_1 as that gives the standard quantal treatment.

The Schrödinger Equation corresponding to I_2 is

$$i\frac{\partial u}{\partial t} = \tfrac{1}{2}\mathrm{e}^{2it}\left(-\partial_x^2 - 2\left(x\partial_x+1\right) - x^2\right)u \tag{13}$$

which has the Lie point symmetries

$$\begin{aligned} \Gamma_1 &= \partial_t + ix\partial_x + \tfrac{1}{2}i\left(e^{2it}-2x^2\right)u\partial_u\\ \Gamma_2 &= e^{2it}\partial_t + 2ixe^{2it}\partial_x\\ &+i\left(-ie^{2it}+\tfrac{1}{2}e^{4it}-2x^2-2e^{2it}x^2\right)u\partial_u\\ \Gamma_3 &= e^{-2it}\partial_t\\ \Gamma_4 &= \partial_x - xu\partial_u\\ \Gamma_5 &= e^{2it}\partial_x - \left(2+e^{2it}\right)xu\partial_u \quad \text{and}\\ \Gamma_6 &= u\partial_u \end{aligned}$$

in addition to the usual infinite-dimensional abelian subalgebra of solution symmetries. The algebra of the finite subset is $sl(2,\,R)\oplus W_3$, *ie* the same algebra as in the case of the usual Schrödinger Equation, (5).

In the case of the Schrödinger Equation corresponding to I_3, namely

$$i\frac{\partial u}{\partial t} = \tfrac{1}{2}\mathrm{e}^{-2it}\left(-\partial_x^2 + 2\left(x\partial_x+1\right) - x^2\right)u, \tag{14}$$

a similar set of symmetries is obtained. Precisely the finite subalgebra comprises

$$\begin{aligned} \Delta_1 &= \partial_t - ix\partial_x - \tfrac{1}{2}i\left(2x^2-e^{-2it}x\right)u\partial_u\\ \Delta_2 &= e^{2it}\partial_t\\ \Delta_3 &= \partial_te^{-2it} - 2ie^{-2it}x\partial_x\\ &+i\left(e^{-2it}-\tfrac{1}{2}ie^{-4it}-2ix^2-2ie^{-2it}x^2\right)u\partial_u\\ \Delta_4 &= \partial_x + xu\partial_u\\ \Delta_5 &= e^{-2it}\partial_x + \left(2+e^{-2it}\right)xu\partial_u \quad \text{and}\\ \Delta_6 &= u\partial_u. \end{aligned}$$

There is not much point in discussing the equations corresponding to I_4 and I_5 as they are linear first-order partial differential equations and have an infinite number of symmetries. The equations can be solved by means of the method of characteristics and one obtains

$$u = \exp\left[\tfrac{1}{2}x^2\right] f(x - it) \quad \text{and}$$
$$u = \exp\left[2it + \tfrac{1}{2}x^2\right] g(\exp[2it] - 2x),$$

and

$$u = \exp\left[-\tfrac{1}{2}x^2\right] f(x - it) \quad \text{and}$$
$$u = \exp\left[-2it - x\right] g\left(2x + \exp[-2it]\right),$$

respectively, for the equations

$$i\tfrac{\partial u}{\partial t} = \tfrac{\partial u}{\partial x} - xu \quad \text{and}$$
$$i\tfrac{\partial u}{\partial t} = e^{2it}\tfrac{\partial u}{\partial x} - \left(2 + e^{2it}\right)xu,$$

and

$$i\tfrac{\partial u}{\partial t} = \tfrac{\partial u}{\partial x} + xu \quad \text{and}$$
$$i\tfrac{\partial u}{\partial t} = e^{-2it}\tfrac{\partial u}{\partial x} + \left(2 + e^{-2it}\right)xu,$$

which are the equations corresponding to I_4 and I_5.

It is not at all obvious how to interpret these solutions in terms of the desired behaviour of the solution, $u(t,\, x)$, at Infinity. Personally, even for the solutions which have a suitable exponential terms, we cannot see how one could possibly select a solution for the so far arbitrary functions which would give anything like proper behaviour.

5. Discussion

Conventional Quantum Mechanics uses (5) derived from the Lagrangian, (1), via the quantisation of the corresponding Hamiltonian. Behind all of this there is a considerable body of theory applying to Classical Mechanics. On one hand, a matter not treated here, the Lagrangian is far from unique. All one needs to do is to glance at [1] to find a modest sampling. The critical point is that from the Lagrangian, whatever it is, one must be able to obtain the Newtonian Equation of Motion. The Theories of Lagrange and Hamilton are really mathematical constructs whereas the Equation of Newton is based upon a Law of Physics. Consequently one must be cautious in how one deals with the process of quantisation.

There is a question about the relevance of the solutions of the Schrödinger Equations obtained from the use of I_2 and I_3 since they do not seem to have any connection with the physically accepted solution obtained using I_1. Nevertheless their Schrödinger Equations have the same algebraic structure as that of the equation corresponding to I_1. Consequently one should expect a point transformation to relate the three equations pairwise. This is a task still to be performed!

The question of the application of these transformations to higher-dimensional systems is raised in [7]. (See also [8] in which the expression "quantum Arnold transformation" is introduced to describe this class of transformation.) It was in such an application in 1976 that it was realised for the classical case that it was simply a point transformation of one Hamiltonian to another. Admittedly the problem under consideration was the three-dimensional time-dependent linear oscillator, which could be considered to be rather special. One recalls the Jauch-Hill-Fradkin Tensor of the corresponding two- and three-dimensional simple harmonic oscillator and its interpretation in terms of the derivation of the orbital properties of the system [9,10]. Similar properties were found for the corresponding time-dependent tensor [11] . While it would seem that the solutions of the Schrödinger Equations obtained from the use of I_2 and I_3 appear to serve no purpose, it may be that there is some way of relating the quantal operators to the properties of the quantal oscillator in higher dimensions.

In considering multidimensional systems it is equally important that the algebraic properties of the system being investigated and the target system be reconcilable. If one is considering point transformations, then the number of point symmetries of both systems needs to be the same and not just the numbers for there needs to be algebraic consistency. This is the only type of symmetry considered in this paper, but there are applications in which the transformations may be more generalised and so one would not expect the conservation of point symmetry. A case in point is the reduction of the Kepler Problem to a simple harmonic oscillator plus a conservation law [12].

A final word of caution appears to be necessary. When one is using a transformation from one space to another, it is advised to make the transformation one-to-one. This then preserves the quantisation properties such as a discrete spectrum.

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