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Infinite-Order Symmetries for Quantum Separable Systems

A B S T R A C T

We develop a calculus to describe the (in general) infinite-order differential operator symmetries of a nonrelativistic Schrödinger eigenvalue equation that admits an orthogonal separation of variables in Riemannian n-space. The infinite-order calculus exhibits structure not apparent when one studies only finite-order symmetries. The search for finite-order symmetries can then be reposed as one of looking for solutions of a coupled system of PDEs that are polynomial in certain parameters. Among the simple consequences of the calculus is that one can generate algorithmically a canonical basis for the space. Similarly we can develop a calculus for conformal symmetries of the time-dependent Schrödinger equation if it admits R-separation in some coordinate system. This leads to energy-shifting symmetries.

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1 Introduction

The main point we want to get across in this paper is that if a Schrödinger equation on a pseudo-Riemannian manifold (real or complex)

$$(\Delta_n + V(x))\,\Psi = E\Psi, \qquad \text{or} \qquad (\Delta_n + V(x))\,\Theta = \Theta_t$$

admits an orthogonal separation (or R-separation) of variables, then the differential symmetry operators for the system, *including those of infinite order*, can be obtained by solving a strictly finite system of PDEs with parameters. The finite order symmetry (or conformal symmetry) operators correspond to solutions that are polynomial in the parameters. This point of view exhibits

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a structure in the space of symmetries that is not apparent when one looks for finite order symmetries alone. Understanding this structure is of particular importance for superintegrable systems [1, 2, 3, 4, 5, 6, 7] where there exist differential symmetries that are not obvious from the separation of the systems in a single coordinate system.

We will describe the basic ideas by first reviewing the simplest example, the time-dependent Schrödinger equation (with potential) in two-dimensional space time [8]. There we can easily produce infinite-order conformal symmetries and show their relevance to finding energy shifting operators for the time-independent Schrödinger equation. However, the system is so simple that one might not appreciate the vital role of variable separation in the results. This is clarified when we take up the study of the time-independent Schrödinger equation (with potential) on a two-dimensional pseudo Riemannian space. The approach extends to any number of space variables.

2 Infinite order conformal symmetries for the time-dependent Schrödinger equation in one spatial dimension

The basic equation is the heat or time-dependent Schrödinger equation

$$(\partial_t - \partial_{xx} - V(x))\,\Psi(x,t) = 0. \tag{1}$$

Here V and Ψ are complex analytic functions of the complex variables x, t. Recall that an operator L, acting on the solution space of (1), is a **(conformal) symmetry** if

$$[\partial_t - H, L] \equiv \partial_t L - [H, L] = R(\partial_t - H)$$

for some linear operator R. Here $H = \partial_{xx} + V(x)$.

We have separation of variables for (1), in the coordinates $\{x, t\}$. Indeed the potential $V(x,t) = V_1(x) + V_2(t)$ also permits separation, but a gauge

transformation $\Psi(x,t) = e^{T(t)}\Theta(x,t)$ with $T'(t) = V_2(x)$ leads to equation (1) again for Θ.

It should not be thought that (1) refers only to Cartesian coordinates. Indeed, there are 3 R-separable coordinate systems for this equation:

1. Cartesian coordinates (x,t), $\quad \Psi_{xx} + V(x)\Psi = \Psi_t$

2. heat coordinates (u,τ), $\quad u = x/\sqrt{t}, \quad \tau = \ln t$. If we set $\Psi = e^{-u^2/4}\Theta(u,\tau)$, then (1) becomes

$$\Theta_{uu} + \left(-\frac{u^2}{4} - \frac{1}{2} + e^{\tau}V\right)\Theta = \Theta_{\tau}$$

   separable if $e^{\tau}V = \tilde{V}(u)$.

3. Airy coordinates (u,τ), $\quad u = x - t^2/2, \quad \tau = t$. If we set $\Psi = e^{-\tau^3/12 - u\tau/2}\Theta(u,\tau)$, then (1) becomes

$$\Theta_{uu} + \left(\frac{1}{2}u + V\right)\Theta = \Theta_{\tau}$$

   separable if $V = \tilde{V}(u)$.

This means that the symmetry analysis below applies to potentials of the form

$$V = f(x), \qquad V = \frac{f(\frac{x}{\sqrt{t}})}{t}, \qquad \text{or} \qquad V = f(x - \frac{t^2}{2}),$$

We will only consider the action of $L(t)$ on the solution space of (1). Then each term ∂_x^2 in the formal expansion of the (possibly infinite-order) conformal symmetry

$$L(t) = \sum_{n,m=0}^{\infty} \ell(x,t)_{n,m}\partial_x^n\partial_t^m$$

can be replaced successively by $\partial_t - V(x)$, if at each stage the terms in the expansion are reordered so that the derivative terms act directly on the solution space. Thus $L(t)$ can be placed in the **canonical form**

$$L(t) = a(x,t,\lambda)\partial_x + b(x,t,\lambda). \tag{2}$$

Here we consider

$$a(x,t,\lambda) = \sum_{m=0}^{\infty} a_m(x,t)\partial_t^m, \qquad \lambda = \partial_t$$

with a similar interpretation for b. (We could also expand a in a power series in $\lambda - \lambda_0$ so it is only necessary for a to be analytic in λ about some complex number λ_0. We have chosen $\lambda_0 = 0$ for clarity of exposition.) The action of $L(t)$ on constant energy solutions

$$\Psi(x,t) = e^{Et}\phi(x), \qquad H\phi = E\phi$$

can be made rigorous, even if a, b aren't analytic:

$$L\Psi = e^{Et}\{a(x,t,E)\partial_x + b(x,t,E)\}\phi(x).$$

Now let us determine the conditions on a and b so that $L(t)$, is a symmetry. The conditions are

$$\begin{aligned} b_x &= \frac{1}{2}a_t - \frac{1}{2}a_{xx} \\ b_t &= \frac{1}{2}a_{tx} - \frac{1}{2}a_{xxx} + 2a_x\lambda - 2a_xV - aV_x. \end{aligned}$$

The integrability condition for these equations is

$$a_{tt} - 2a_{xxt} + a_{xxxx} + 4a_{xx}(V-\lambda) + 6a_xV_x + 2aV_{xx} = 0. \tag{3}$$

Theorem: Condition (3) is necessary and sufficient for $L(t) = a(x,t,\lambda)\partial_x + b(x,t,\lambda)$ to be a symmetry.

It is not difficult to find all solutions of (3) which are of the form

$$a = \exp(t\kappa(\lambda))f(x,\lambda).$$

We obtain the 4th-order ordinary differential equation:

$$f_{xxxx} + (4V - 4\lambda - 2\kappa)f_{xx} + 6V_xf_x + (2V_{xx} + \kappa^2)f = 0. \tag{4}$$

It is easy to show that these solutions occur in raising operator/ lowering operator pairs [8].

To solve equation (4) we make use of Whittaker's theorem: Let $u(x)$ and $v(x)$ be solutions of the differential equations $u^{''} - p(x)u = 0$, $v^{''} - q(x)v = 0$. Then $y(x) = u(x)v(x)$ satisfies

$$(p-q)y^{''''} - (p'-q')y''' - 2(p^2-q^2)y'' + (-pp' + qq' + 5p'q - 5pq')y'$$

$$+(p'^2 - q'^2 - (p-q)(p''+q'') + (p-q)^3)y = 0.$$

Now consider the equations

$$i)\ u'' + Vu = (\lambda+\kappa)u, \qquad ii)\ v'' + Vv = \lambda v,$$

i.e., $p = \lambda + \kappa - V$, $q = \lambda - V$. Then we get (4) with $f = uv$. Similarly, we can find structure results for the basic equation (3).

Although our theorems exhibit clearly the structure of the generalized symmetries, other methods for computing the recurrences may be simpler.

Example: (pseudo-Coulomb potential) We compute the possible solutions of (4) of the form $f(x,\lambda) = x$. We find the pseudo-Coulomb potential

$$V(v) = \frac{a^2}{x^2} - b^2x^2, \qquad \kappa = \pm 4b.$$

Here the raising and lowering operators are of finite order, and they raise and lower by a fixed energy. The raising and lowering operators and H generate the Lie algebra $s\ell(2)$ and a standard weight vector argument yields the bound state energy levels for the hydrogen atom.

Example: (Morse potential) We compute the solutions of (4) of the form $f(x,\lambda) = \exp(\mu(\lambda)x)$. We find that μ is independent of λ and

$$V(x) = D[2\exp(-\mu x) - \exp(-2\mu x)]$$

where D, μ are positive parameters. The Schrödinger equation admits the generalized (infinite-order) symmetries

$$L^{\pm} = e^{t\kappa^{\pm}}\left[e^{\mu x}\partial_x + (\frac{\kappa^{\pm}}{2\mu} - \frac{\mu}{2})e^{\mu x} - \frac{2\mu D}{\kappa^{\pm}}\right].$$

where $\kappa^{\pm}(\lambda) = \mu^2 \pm 2\mu\sqrt{\lambda}$. Since $\kappa^+(\lambda) + \kappa^-(\lambda + \kappa^+(\lambda)) = 0$ for $\sqrt{\lambda} + \mu \geq 0$ and $\kappa^-(\lambda) + \kappa^+(\lambda + \kappa^-(\lambda)) = 0$ for $\sqrt{\lambda} - \mu \geq 0$, we can easily verify that

$$L^+L^- \sim D - \frac{4D^2}{(\mu - 2\sqrt{\lambda})^2}, L^-L^+ \sim D - \frac{4D^2}{(\mu + 2\sqrt{\lambda})^2}$$

where equality is meant in the sense that the two sides agree when applied to a solution of (1). Thus we have the commutation relations

$$[L^+, L^-] \sim \frac{-32D^2\mu\sqrt{\lambda}}{(\mu^2 - 4\lambda)^2}$$

$$[\lambda, L^+] \sim (\mu^2 + 2\mu\sqrt{\lambda})L^+, \qquad [\lambda, L^-] \sim (\mu^2 - 2\mu\sqrt{\lambda})L^-,$$

an analog of the commutation relations for the Lie algebra $s\ell(2)$.

Even though L^+, L^-, λ don't generate a finite dimensional Lie algebra, one can easily mimic the (weight vector) approach to the representation theory of $s\ell(2)$ to determine the irreducible representations of the associative algebra generated by these three operators. Note the "Casimir operator" C acting on the solution space of (1):

$$C = L^+L^- + \frac{4D^2}{(\mu - 2\sqrt{\lambda})^2} \sim L^-L^+ + \frac{4D^2}{(\mu + 2\sqrt{\lambda})^2} \sim D.$$

We look for a "lowest weight vector" Ψ_0 for λ, i.e., a nonzero solution of the equations

$$(\lambda - H)\Psi_0 = 0, \qquad \lambda\Psi_0 = E_0\Psi_0, \qquad L^-\Psi_0 = 0.$$

Evaluating $C\Psi_0 = D\Psi_0$ we find $4D^2/(\mu - 2\sqrt{E_0})^2 = D$ or

$$E_0 = \mu^2(\frac{\sqrt{D}}{\mu} - \frac{1}{2})^2,$$

assuming $\mu - 2\sqrt{E_0} \geq 0$. Recursively applying L^+ to get $\Psi_n = (L^+)^n\Psi_0$ with eigenvalues E_n satisfying the recurrence $E_{n+1} = E_n + \kappa^+(E_n) = (\mu + \sqrt{E_n})^2$, we find the spectrum

$$E_n = \mu^2[\frac{\sqrt{D}}{\mu} - (n + \frac{1}{2})]^2, \qquad n = 0, 1, 2, \cdots.$$

As an application of the determining equations

$$a_{tt} - 2a_{xxt} + a_{xxxx} + 4a_{xx}(V - \lambda) + 6a_x V_x + 2aV_{xx} = 0, \tag{5}$$

let us consider the problem of finding those potentials that admit third order invariants,

$$L(t) = a(x, t\lambda)\partial_x + b(x, t, \lambda)$$

where we consider λ as a second order invariant. Thus we look for solutions of (5) of the form

$$a(x, t, \lambda) = A(x, t)\lambda + B(x, t)$$

where $A(x, t) \neq 0$. Substituting this expression into (5) and equating powers of λ we find

$$A_{xx} = 0 \Longrightarrow A = \alpha(t) + \beta(t)x \tag{6}$$

$$A_{tt} - 4B_{xx} + 6A_x V_x + 2AV_{xx} = 0 \tag{7}$$

$$B_{tt} - 2B_{xxt} + B_{xxxx} + 4B_{xx}V + 6B_x V_{xx} = 0. \tag{8}$$

Substituting (6) into (7) and integrating we find

$$B(x,t) = \ddot{\alpha}(t)\frac{x^2}{8} + \ddot{\beta}(t)\frac{x^3}{24} + \beta(t)W(x) + \frac{1}{2}\left(\alpha(t) + \beta(t)x\right)W'(x) + \gamma(t)x + \delta(t),$$

where $V(x) = W'(x)$.

Substituting this result into (8) we find the functional equation for the potential:

$$\begin{aligned}
&\alpha^{(4)}(t)[\frac{x^2}{8}] + \alpha^{(3)}(t)[-\frac{1}{2}] + \ddot{\alpha}(t)[\frac{3}{2}W' + \frac{3x}{2}W'' + \frac{x^2}{4}W'''] + \dot{\alpha}(t)[-W'''] \\
&+\alpha(t)[3W'W''' + \frac{1}{2}W''''' + 3(W'')^2] + \beta^{(4)}(t)[\frac{x^3}{24}] + \beta^{(3)}(t)[-\frac{x}{2}] \\
&+\ddot{\beta}(t)[\frac{x^3}{12}W''' + \frac{3x^2}{4}W'' + \frac{3x}{2}W' + \frac{1}{2}W] + \dot{\beta}(t)[-3W'' - W'''x] \\
&+\beta(t)[\frac{x}{2}W''''' + 3xW'W''' + WW''' + 3(W'')^2x + 12W'W'' + \frac{5}{2}W'''] \\
&+\ddot{\gamma}(t)[x] + \gamma(t)[6W'' + 2W'''x] + \ddot{\delta}(t) + \delta(t)[2W'''] = 0.
\end{aligned} \tag{9}$$

To find all solutions W we would need to study this functional equation in detail. However, many solutions are obvious. Indeed if we choose

$$\alpha(t) \equiv \alpha_0, \quad \beta(t) \equiv \beta_0, \quad \gamma(t) \equiv \gamma_0, \quad \delta(t) \equiv \delta_0,$$

i.e., constants, then (9) becomes a nonlinear ODE for the potential $W(x)$, and every solution yields a potential with a third-order differential symmetry operator.

Another very important case is obtained by setting

$$\alpha(t) = \alpha_0 e^{\kappa t}, \quad \beta(t) = \beta_0 e^{\kappa t}, \quad \gamma(t) = \gamma_0 e^{\kappa t}, \quad \delta(t) = \delta_0 e^{\kappa t},$$

where κ is a constant. Then we can factor $e^{\kappa t}$ from (9) and the result is an ODE for W again. For these potentials $L(t)$ becomes a third order energy raising operator, increasing the energy from H to $H + \kappa$. Every third order raising operator is associated with a third order lowering operator, so all these cases permit ladders of bound state energy levels, subject to normalization requirements.

3 Two-dimensional separable systems for the time-independent Schrödinger equation $(\Delta_2 + V)\Psi = E\Psi$

If $\{x, y\}$ is an orthogonal separable coordinate system in a general Riemannian space, the corresponding Schrödinger operator has the form [9]

$$H = L_1 = \frac{1}{f_1(x) + f_2(y)} \left(\partial_x^2 + \partial_y^2 + v_1(x) + v_2(y) \right). \tag{10}$$

and, due to the separability, there is the second-order symmetry operator

$$L_2 = \frac{f_2(y)}{f_1(x) + f_2(y)} \left(\partial_x^2 + v_1(x) \right) - \frac{f_1(x)}{f_1(x) + f_2(y)} \left(\partial_y^2 + v_2(y) \right),$$

i.e., $[L_2, H] = 0$, and the operator identities

$$f_1(x)H + L_2 = \partial_x^2 + v_1(x), \qquad f_2(y)H - L_2 = \partial_y^2 + v_2(y). \tag{11}$$

We look for a partial differential operator $\tilde{L}(H, L_2, x, y)$ that satisfies

$$[H, \tilde{L}] = 0. \tag{12}$$

We require that the symmetry operator take the standard form

$$\tilde{L} = \sum_{j,k} \left(A_{j,k}(x,y)\partial_{xy} + B_{j,k}(x,y)\partial_x + C_{j,k}(x,y)\partial_y + D_{j,k}(x,y)\right) H^j L_2^k. \tag{13}$$

(Again, only for convenience do we expand about $(H_0, L_0) = (0, 0)$. We only require analyticity about some point (H_0, L_0).) Note that if the formal operators (13) contained partial derivatives in x and y of orders ≥ 2 we could use the identities (11), recursively, and rearrange terms to achieve the unique standard form (13).

Using operator identities

$$[\partial_x, H] = -\frac{f_1'}{f_1 + f_2}H + \frac{v_1'}{f_1 + f_2}, \quad [\partial_y, H] = -\frac{f_2'}{f_1 + f_2}H + \frac{v_2'}{f_1 + f_2},$$

$$[\partial_x, L_2] = -\frac{f_1' f_2}{f_1 + f_2}H + \frac{f_2 v_1'}{f_1 + f_2}, \quad [\partial_y, L_2] = \frac{f_1 f_2'}{f_1 + f_2}H - \frac{f_1 v_2'}{f_1 + f_2},$$

we see that

$$(f_1(x) + f_2(y))[H, A(x,y)\partial_{xy} + B(x,y)\partial_x + C(x,y)\partial_y + D(x,y)] =$$

$$(A_{xx} + A_{yy} + 2B_y + 2C_x)\partial_{xy} + (B_{xx} + B_{yy} - 2A_y v_2 + 2D_x - Av_2')\partial_x$$
$$+(2A_y f_2 + Af_2')\partial_x H - 2A_y\partial_x L_2 + (C_{xx} + C_{yy} - 2A_x v_1 + 2D_y - Av_1')\partial_y$$
$$+(2A_x f_1 + Af_1')\partial_y H + 2A_x\partial_y L_2$$
$$+(D_{xx} + D_{yy} - 2B_x v_1 - 2C_y v_2 - Bv_1' - Cv_2')$$
$$+(2B_x f_1 + 2C_y f_2 + Bf_1' + Cf_2')H + (2B_x - 2C_y)L_2.$$

The symmetry condition (12) is equivalent to the system of equations

$$\partial_{xx}A_{j,k} + \partial_{yy}A_{j,k} + 2\partial_y B_{j,k} + 2\partial_x C_{j,k} = 0, \tag{14}$$

$$\begin{aligned}\partial_{xx}B_{j,k} + \partial_{yy}B_{j,k} - 2\partial_y A_{j,k}v_2 + 2\partial_x D_{j,k} - A_{j,k}v_2' + \\ (2\partial_y A_{j-1,k}f_2 + A_{j-1,k}f_2') - 2\partial_y A_{j,k-1} = 0,\end{aligned} \tag{15}$$

$$\begin{aligned}\partial_{xx}C_{j,k} + \partial_{yy}C_{j,k} - 2\partial_x A_{j,k}v_1 + 2\partial_y D_{j,k} - A_{j,k}v_1' + \\ (2\partial_x A_{j-1,k}f_1 + A_{j-1,k}f_1') + 2\partial_x A_{j,k-1} = 0,\end{aligned} \tag{16}$$

$$\begin{aligned}\partial_{xx}D_{j,k} + \partial_{yy}D_{j,k} - 2\partial_x B_{j,k}v_1 - 2\partial_y C_{j,k}v_2 - B_{j,k}v_1' - C_{j,k}v_2' \\ +(2\partial_x B_{j-1,k}f_1 + 2\partial_y C_{j-1,k}f_2 + B_{j-1,k}f_1' + C_{j-1,k}f_2') + (2\partial_x B_{j,k-1} - 2\partial_y C_{j,k-1}) = 0.\end{aligned} \tag{17}$$

Note that condition (13) makes sense, at least formally, for infinite order differential equations. Indeed, one can consider H, L_2 as parameters in these equations. Then once $\tilde{L}$ is expanded as a power series in these parameters, the terms are reordered so that the powers of the parameters are on the right, before they are replaced by explicit differential operators. Alternatively one can consider the operator $\tilde{L}$ as acting on a simultaneous eigenbasis of the commuting operators H and L_2, in which case the parameters are the eigenvalues.

In this view we can write

$$\begin{aligned}\tilde{L}(H, L_2, x, y) &= A(x, y, H, L_2)\partial_{xy} + B(x, y, H, L_2)\partial_x \\ &+ C(x, y, H, L_2)\partial_y + D(x, y, H, L_2),\end{aligned} \tag{18}$$

and consider $\tilde{L}$ as an at most second-order order differential operator in x, y that is analytic in the parameters H, L_2. Then the above system of equations can be written in the more compact form

$$A_{xx} + A_{yy} + 2B_y + 2C_x = 0, \tag{19}$$

$$B_{xx} + B_{yy} - 2A_y v_2 + 2D_x - Av_2' + (2A_y f_2 + Af_2')H - 2A_y L_2 = 0, \tag{20}$$

$$C_{xx} + C_{yy} - 2A_x v_1 + 2D_y - Av_1' + (2A_x f_1 + Af_1')H + 2A_x L_2 = 0, \quad (21)$$

$$D_{xx} + D_{yy} - 2B_x v_1 - 2C_y v_2 - Bv_1' - Cv_2' \quad (22)$$

$$+(2B_x f_1 + 2C_y f_2 + Bf_1' + Cf_2')H + (2B_x - 2C_y)L_2 = 0.$$

and this system has many solutions.

We start with a very special case

$$A \equiv 0, \quad B = X(x, H, L_2), \quad C = Y(y, H, L_2), \quad D = \tilde{X}(x, H, L_2) + \tilde{Y}(y, H, L_2). \quad (23)$$

Then the above PDEs uncouple into ODEs for X and Y, whose structure we can easily analyse. We write

$$\tilde{L} = M(H, L_2, x, \partial_x) + N(H, L_2, y, \partial_y)$$

where

$$M(H, L_2, x, \partial_x) = \sum_{j,k} \left(X_{j,k}(x)\partial_x + \tilde{X}_{j,k}(x) \right) H^j L_2^k, \quad (24)$$

with a similar equation for N. We immediate obtain the system of equations

$$X_{j,k}'' + 2\tilde{X}_{j,k}' = 0, \quad (25)$$

$$\tilde{X}_{j,k}'' - v_1' X_{j,k} - 2v_1 X_{j,k}' + 2f_1 X_{j-1,k}' + f_1' X_{j-1,k} + 2X_{j,k-1}' = \alpha_{j,k}.$$

with a similar sytem for $Y_{j,k}$.

Equations (25) can be written in the more compact form

$$X''' + 4(v_1 - f_1 H - L_2)X' + 2(v_1' - f_1' H)X = -2P(H, L_2), \quad \tilde{X} = -\frac{1}{2}X', \quad (26)$$

where the arbitrary function $P(H, L_2)$ (a separation parameter that we frequently choose to be a polynomial) is common to the equations for X and for Y. The first equation (26) always has solutions for any f_1, v_1, say continuously differentiable. Thus we can always construct M and it will be analytic in the parameters H, L_2. (Of course, a basic question is for what choices of f_1, v_1, P do solutions X exist that are polynomials in the parameters H, L_2?)

Similarly, the equation for $Y(H, L_2, y)$ is

$$Y''' + 4(v_2 - f_2 H + L_2)Y' + 2(v_2' - f_2' H)Y = 2P(H, L_2), \quad \tilde{Y} = -\frac{1}{2}Y'. \quad (27)$$

Once we have obtained M and N, then we see that the operator $L_3 = M + N$ commutes with H:

$$[H, L_3] = \frac{1}{f_1 + f_2}P(H, L_2) - \frac{1}{f_1 + f_2}P(H, L_2) = 0.$$

Thus we can view L_3 as an infinite order differential symmetry operator for H. (In special cases this will be a finite order operator.)

Theorem: For any v_1, v_2, f_1, f_2 all solutions of the equations (26), (27) determine a separated symmetry operator of the form $L_3 = M(x) + N(y) = (X\partial_x + \tilde{X}) + (Y\partial_y + \tilde{Y})$.

A straightforward computation yields

$$[L_2, M] = \frac{f_2}{f_1 + f_2}P(H, L_2), \qquad [L_2, N] = \frac{f_1}{f_1 + f_2}P(H, L_2),$$

so $[L_2, L_3] = P(H, L_2) \neq 0$. Thus, L_3 is *not* a function of H and L_2.

An exactly analogous construction using the commutators

$$[H, \tilde{M}] = \frac{f_1}{f_1 + f_2}P(H, L_2), \qquad [H, \tilde{N}] = \frac{f_2}{f_1 + f_2}P(H, L_2)$$

yields the operator $L_4 = \tilde{M} + \tilde{N}$, not a symmetry, such that $H = L_1, L_2, L_3, L_4$ satisfy the commutation relations

$$[L_1, L_2] = [L_1, L_3] = [L_2, L_4] = [L_3, L_4] = 0,$$

$$[L_1, L_4] = [L_2, L_3] = P.$$

If we choose $P(H, L_2) = I$, the identity operator, these are just the canonical commutation relations.

Example: Let us consider the quantum Hamiltonian

$$H = \partial_x^2 + \partial_y^2 + x.$$

It is known to be associated with several symmetries, such as

$$\ell_0 = \partial_y, \quad \ell_1 = \{\partial_y, x\partial_y - y\partial_x\}_+ - \frac{1}{2}y^2, \quad \ell_2 = \partial_x\partial_y + \frac{1}{2}y,$$

where $\{A, B\}_+ = (AB + BA)$ is the anticommutator of two operators. The occurence of ℓ_0 is obvious, because y is an ignorable variable for the Hamiltonian. How can we obtain ℓ_1 and ℓ_2, which are associated with the separation of the Schrödinger equation in parabolic and shifted parabolic coordinates, from our cartesian coordinate construction? The obvious separation in cartesian coordinates yields the additional second order symmetry

$$L_2 = \frac{1}{2}(\partial_x^2 - \partial_y^2 + x).$$

Let us now consider the defining equations for a symmetry in the following form:

$$X''' + 4(x - \frac{1}{2}H - L_2)X' + 2X = (\frac{1}{2}H - L_2), \quad Y''' - 4(\frac{1}{2}H - L_2)Y' = -(\frac{1}{2}H - L_2).$$

These equations have the solutions

$$X = \frac{1}{2}(\frac{1}{2}H - L_2), \qquad Y = \frac{y}{4} - \frac{1}{8}.$$

The corresponding symmetry is thus finite and given by

$$L_3 = \frac{1}{2}(\partial_y^2\partial_x + \frac{1}{2}y\partial_y) - \frac{1}{4}\partial_y^2 = \{\ell_2, \partial_y\}_+ - \frac{1}{4}\partial_y^2 - \frac{1}{2}$$

We see that our construction yields reasonably easily the existence of ℓ_2 and thereby ℓ_1. Note also that $[\partial_y, \ell_1] = 2\ell_2$.

4 The general case in two dimensions

Up to now we have only considered the special case $A = 0, B = X(x), C = Y(y), D = \tilde{X}(x) + \tilde{Y}(y)$ of conditions (19,20,21,22). Let us now consider the case such that $A \equiv 0$, but otherwise, B, C, D are arbitrary. Then there

is a function $G(x, y, H, L_2)$ such that $B = -\partial_x G, \qquad C = \partial_y G$, and the determining conditions simplify to

$$1) \qquad G_{xxxy} + G_{xyyy} = 0,$$

$$2) \qquad \frac{1}{2}G_{xxxx} + 2G_{xx}v_1 + G_x v_1' - (2G_{xx}f_1 + G_x f_1')H - 2G_{xx}L_2 =$$

$$\frac{1}{2}G_{yyyy} + 2G_{yy}v_2 + G_y v_2' - (2G_{yy}f_2 + G_y f_2')H + 2G_{yy}L_2.$$

The first determining equation means that

$$G(x, y) = K(x, y) + F(x) + J(y)$$

where F, J are arbitrary and K is harmonic: $K_{xx} + K_{yy} = 0$. This representation is unique in K, F, J, up to the addition of the harmonic separable function $\tilde{K}(x, y) = \frac{a}{2}(x^2 - y^2) + bx + cy + d$. Alternatively, we can write

$$G(x, y) = z_1(x + iy) + z_2(x - iy) + F(x) + J(y)$$

where z_1, z_2 are arbitrary analytic functions. Then only condition 2) remains to be satisfied. Specific examples are readily apparent.

Example: If we make the ansatz $G = X(x, H, L_2)Y(y, H, L_2)$ then, in addition to the well known angular momentum invariant given earlier, we find the following polynomial invariants:

$$X = (\frac{1}{4} + L_2)\cos x + s(1 + \beta H),\ Y = (\frac{1}{4} + L_2)\cosh y + t(1 + \xi H), \quad (28)$$

$$v_1(x) = 2s\frac{\sin x}{\cos^2 x} + \frac{a_1}{\cos^2 x},\ f_1(x) = -2s\beta\frac{\sin x}{\cos^2 x} + \frac{a_2}{\cos^2 x},$$

$$v_2(y) = 2t\frac{\sinh y}{\cosh^2 y} + \frac{b_1}{\cosh^2 y},\ f_2(y) = -2t\xi\frac{\sinh y}{\cosh^2 y} + \frac{b_2}{\cosh^2 y},$$

$$D = -\frac{1}{2}(\frac{1}{4} + L_2)\left(t\cos x(1 + \xi H) + s\cosh y(1 + \beta H)\right).$$

$$\tilde{L} = -2x(y^2 + 4L_2)\partial_x + 2y(x^2 - 4L_2)\partial_y + x^2 - y^2, \quad (29)$$

$$v_1(x) = \frac{1}{8}x^2 + \frac{a_1}{x^2},\ f_1(x) = \frac{a_2}{x^2},\ v_2(y) = \frac{1}{8}y^2 + \frac{b_1}{y^2},\ f_2(y) = \frac{b_2}{y^2}.$$

Example: Again we consider the special case of conditions (19,20,21,22) such that $A \equiv 0$ where now we require

$$G(x,y) = -2\log(X(x) + Y(y)) + \mathcal{F}(x) + \mathcal{J}(y) = K(x,y) + F(x) + J(y)$$

where F, J are arbitrary and K is harmonic. Then the harmonic requirement on K implies that

$$K = -2\log(X + Y) + \tilde{F}(x) + \tilde{J}(y)$$

where

$$(X')^2 = \frac{\alpha}{12}X^4 + \frac{\beta}{3}X^3 + \gamma X^2 + 2\delta X + \phi,$$

$$(Y')^2 = -\frac{\alpha}{12}Y^4 + \frac{\beta}{3}Y^3 - \gamma Y^2 + 2\delta Y - \phi,$$

$$X'' = \frac{\alpha}{6}X^3 + \frac{\beta}{2}X^2 + \gamma X + \delta, \quad Y'' = -\frac{\alpha}{6}Y^3 + \frac{\beta}{2}Y^2 - \gamma Y + \delta.$$

Further,

$$\tilde{F}(x) = \frac{1}{3}\frac{X'''}{X'}, \qquad \tilde{J}(y) = \frac{1}{3}\frac{Y'''}{Y'},$$

and the metric and potential terms have the solution

$$v_1 - f_1 H = \frac{-\frac{a}{12}X^4 - \frac{b}{3}X^3 + \frac{b_1}{2}X^2 + \eta_1 X + \eta_2}{24(X')^2},$$

$$v_2 - f_2 H = \frac{\frac{a}{12}Y^4 - \frac{b}{3}Y^3 - \frac{b_1}{2}Y^2 + \eta_1 Y - \eta_2}{24(Y')^2}.$$

Here, $\alpha, \beta, \gamma, \delta, \phi$ and

$$a = a^{(1)} + a^{(2)}H, b = b^{(1)} + b^{(2)}H, b_1 = b_1^{(1)} + b_1^{(2)}H,$$

$$\eta_1 = \eta_1^{(1)} + \eta_1^{(2)}H, \eta_2 = \eta_2^{(1)} + \eta_2^{(2)}H$$

are parameters.

The remaining condition is

$$\frac{1}{2}F'''' + 2F''(v_1 - f_1H - L_2) + F'(v_1 - f_1'H) - \frac{1}{2}J''''$$
$$-2J''(v_2 - f_2H - L_2) - J'(v_2' - f_2'H) =$$
$$\frac{1}{36}\left(\frac{a}{2}X^2 + bX - \frac{a}{2}Y^2 + bY\right) + \frac{2}{3}\left(\frac{X'''}{X'}(v_1 - f_1H) - \frac{Y'''}{Y'}(v_2 - f_2H)\right)$$
$$+\tilde{F}'(v_1' - f_1'H) - \tilde{J}'(v_2' - f_2'H).$$

The simplest family of solutions is obtained by setting $F \equiv \tilde{F}, J \equiv \tilde{J}$ and $\alpha = \beta = a = b = 0$.

Now we consider the general case of conditions (19,20,21,22). Then there are two functions $F(x, y, H, L_2), G(x, y, H, L_2)$ such that

$$A = \partial_{xy}F, \qquad B = -\frac{1}{2}\partial_{xyy}F - \partial_x G, \qquad C = -\frac{1}{2}\partial_{xxy}F + \partial_y G,$$

and the determining conditions simplify to

$$1) \qquad 2G_{xyyy} + \frac{1}{2}F_{xyyyyy} + 2F_{xyyy}(v_2 - f_2H + L_2)$$
$$+3F_{xyy}(v_2' - f_2H) + F_{xy}(v_2'' - f_2''H) =$$
$$-2G_{xxxy} + \frac{1}{2}F_{xxxxxy} + 2F_{xxxy}(v_1 - f_1H - L_2)$$
$$+3F_{xxy}(v_1' - f_1'H) + F_{xy}(v_1'' - f_1''H),$$

$$2) \qquad \frac{1}{2}F_{xxxxyy} + 2F_{xxyy}(v_1 - f_1H) + F_{xxy}(v_2' - f_2'H) + \frac{1}{2}G_{xxxx} +$$
$$2G_{xx}(v_1 - f_1H - L_2) + G_x(v_1' - f_1'H) =$$
$$-\frac{1}{2}F_{xxyyyy} - 2F_{xxyy}(v_2 - f_2H) - F_{xyy}(v_1' - f_1'H) + \frac{1}{2}G_{yyyy} +$$
$$2G_{yy}(v_2 - f_2H + L_2) + G_y(v_2' - f_2'H).$$

Theorem: For any v_1, v_2, f_1, f_2 there are always solutions for the above equations in which $A \not\equiv 0$, $G \equiv 0$ and F factors as $F = \mathcal{X}(x, H, L_2)\mathcal{Y}(y, H, L_2)$ where $\mathcal{X}'\mathcal{Y}' \neq 0$.

Indeed, with $X = \mathcal{X}', Y = \mathcal{Y}'$ we have a solution of equations (19,20,21,22) whenever $X'Y' \neq 0$ and X and Y satisfy the ordinary differential equations

$$X''' + 4X'(v_1 - f_1 H - L_2) + 2X(v_1' - f_1' H) = 0 \tag{30}$$

$$Y''' + 4Y'(v_2 - f_2 H + L_2) + 2Y(v_2' - f_2' H) = 0. \tag{31}$$

5 Final remarks

The underlying structure of the solutions of the general equations (19,20,21,22) is fairly simple. Let $u_1(x, L_2) = u_1[L_2], u_2(x, L_2) = u_2[L_2]$ be a basis of solutions of the separated equation

$$\left(\frac{d^2}{dx^2} + v_1(x) - f_1(x)H - L_2\right) u = 0, \tag{32}$$

and let $w_1(y, L_2), w_2(y, L_2)$ be a basis of solutions of the separated equation

$$\left(\frac{d^2}{dy^2} + v_2(y) - f_2(y)H - L_2\right) w = 0. \tag{33}$$

Then for any parameter $\hat{L}_2$ the operator

$$S(\hat{L}_2) = w_2[\hat{L}_2]u_2[\hat{L}_2]\,(w_1[L_2]u_1[L_2]\partial_{xy} - w_1'[L_2]u_1[L_2]\partial_x$$

$$-w_1[L_2]u_1'[L_2]\partial_y + w_1'[L_2]u_1'[L_2]\,)$$

is a symmetry operator of L_1 that maps any eigenspace of L_2 into another (generally different) eigenspace. The point is that the Wronskian of any two solutions of (32) or of (33) is constant. It is not hard to characterize the space spanned by all linear combinations of functions $w_2[\hat{L}_2]u_2[\hat{L}_2]w_1[L_2]u_1[L_2]$ and this gives the equations for A. Similarly we can characterize B, C, and D. The details can be complicated, but the principle is simple.

All of these methods in this paper extend to n dimensions. If any of the equations

- $\sum_{i,j=1}^{n} g^{ij} p_1 p_j + V(x) = E$, $n \geq 2$

- $(\Delta_n + V(x))\,\Psi(x) = E\Psi(x),\ n \geq 2$
- $(\Delta_n + V(x))\,\Psi(x) = \partial_t \Psi(x),\ n \geq 1$
- $(\Delta_n + V(x))\,\Psi(x) = 0,\ n \geq 3$

on a pseudo-Riemannian manifold admits an orthogonal (in the space variables) separable or R-separable coordinate system then we can develop a similar calculus to describe all differential symmetries and conformal symmetries of the system, even those of infinite order. In the lowest dimensional cases we have verified the same statements for nonorthogonal separable systems. We will provide all these details in forthcoming papers.

References

[1] Friš, J., Smorodinskii, Ya.A., Uhlír, A.M., and Winternitz, P., Symmetry Groups in Classical and Quantum Mechanics. Sov.J.Nucl.Phys., 1967, Vol.4, p. 444.

[2] Makarov, A.A., Smorodinsky, Ya.A., Valiev, Kh., and Winternitz, P. A Systematic Search for Nonrelativistic Systems with Dynamical Symmetries, Nuovo Cimento, 1967, Vol.A 52, p. 1061.

[3] Hietarinta, J., Direct methods for the search of the second invariant. Physics Report, 1987, Vol.147, pp. 87-154.

[4] Kalnins, E.G., Miller, W., and Pogosyan, G.S., Superintegrability and associated polynomial solutions. Euclidean space and the sphere in two dimensions, J.Math.Phys., 1996, Vol.37, p. 6439.

[5] Kalnins, E.G., Kress, J., Miller, W., and Pogosyan, G.S., Completeness of superintegrability in two-dimensional constant curvature spaces; J. Phys. A: Math Gen., 2001, Vol.34, pp. 4705–4720.

[6] Kalnins, E.G., Kress, J., Miller, W., and Pogosyan, G.S., Complete sets of invariants for dynamical systems that admit a separation of variables, J. Math. Phys., 2002, Vol.43, pp. 3592–3609.

[7] Gravel S., and Winternitz, P., Superintegrability with third-order integrals in quantum and classical mechanics; CRM Preprint 2002.

[8] Kalnins, E.G., Levine, R.D., and Miller, W., Conformal symmetries and generalized recurrences for heat and Schrödinger equations in one spatial dimension; in "Mechanics, Analysis and Geometry: 200 years after Lagrange", M.Francaviglia, ed., North Holland, Amsterdam 1991, pp. 237-256.

[9] Eisenhart, L.P., Separable Systems of Stäckel, Annals of Math. (2), 1934, Vol.35, pp. 284-305.