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RECENT ADVANCES ON LIE SYSTEMS AND THEIR APPLICATIONS

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Abstract. After a quick presentation of the theory of Lie systems from a geometric perspective, recent progresses on their applications when compatible geometric structures exist will be described with a special emphasis in the particular case of admissible Kähler structures, and therefore with applications in Quantum Mechanics.

1. Introduction: Lie systems of differential equations. Solution of systems of differential equations appearing in many physical problems is not an easy task. In geometric terms they are represented by vector fields and their solutions are given by the flow of the associated vector fields. Symmetry and reduction techniques are generally used and many times a previous knowledge of particular solutions may be useful. The best situation is that of the so called Lie (or Lie–Scheffers) systems, for which there is a nonlinear superposition rule allowing us to write the general solution in terms of a generic finite family of particular solutions.

These systems appear very often in many problems in science and engineering. After a quick review of their properties we will fix our attention on the particular case of quantum mechanics, where they are useful in studying the time evolution of a quantum system and also in the solution of particular cases of time-independent Schrödinger equations.

Lie–Scheffers systems [32] are non-autonomous systems of first-order differential equations admitting a function $\Phi : \mathbb{R}^{n(m+1)} \to \mathbb{R}$, $x = \Phi(u_1, \ldots, u_m; k_1, \ldots, k_n)$, $u_a \in \mathbb{R}^n$, called *superposition rule*, such that the general solution is

$$x(t) = \Phi(x_{(1)}(t), \ldots, x_{(m)}(t); k_1, \ldots, k_n) \ , \qquad (1)$$

with $\{x_{(a)}(t)\,|\,a = 1, \ldots, m\}$ being a generic set of particular solutions of the system and where $k_1, \ldots, k_n$, are real numbers.

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They are a generalisation of linear superposition rules for homogeneous linear systems for which $m = n$ and $x = \Phi(x_{(1)}, \ldots, x_{(n)}; k_1, \ldots, k_n) = k_1 x_{(1)} + \ldots + k_n x_{(n)}$, but the number m may be different from the dimension n, and the function Φ is nonlinear in this more general case. For instance for inhomogeneous linear systems $m = n + 1$ and $x = \Phi(x_{(1)}, \ldots, x_{(n+1)}; k_1, \ldots, k_n) = x_{(n+1)} + k_1(x_{(1)} - x_{(n+1)}) + \ldots + k_n(x_{(n)} - x_{(n+1)})$.

These systems appear quite often in many different branches of science ranging from pure mathematics to classical and quantum physics, control theory, economy, etc., and are related with equations in Lie groups and in general connections in fibre bundles. Forgotten for a long time, they had a revival due to the work by Winternitz and coworkers (see e.g. [8, 12, 15, 38]). One particular example is Riccati equation [20], of a fundamental importance not only in physics (for instance factorisation of second order differential operators and shape invariance [23, 31], Darboux transformations [6, 26] and in general supersymmetry in quantum mechanics [27]), but also in mathematics (reduction of second order linear differential equations to first order ones [20], second variation methods in calculus of variations, Riccati hierarchy [29], etc.).

In the solution of such non-autonomous systems of first-order differential equations we can use techniques imported from group theory, for instance Wei–Norman method [20], and reduction techniques [9, 11] coming from the theory of connections. Recently proposed generalisations have also been shown to be useful for dealing with other systems of differential equations, as for instance Emden–Fowler [13] and Abel equations [16].

The geometric concept of superposition rule is the following: a superposition rule for a t-dependent vector field X in an n-dimensional manifold M is a map $\Phi : M^m \times M \to M$ such that if $\{x_{(1)}(t), \ldots, x_{(m)}(t)\}$ is a generic set of integral curves of X, then $x(t) = \Phi(x_{(1)}(t), \ldots, x_{(m)}(t), k)$, with $k \in M$, is an integral curve of X, and each integral curve is obtained in this way (see also [10] for a more geometric definition in terms of connections).

The result of Lie Theorem in modern terms is that a t-dependent vector field X admits a superposition rule if there exist r fields $X_1, \ldots, X_r$ in M and functions $b_1(t), \ldots, b_r(t)$ such that $X(x, t)$ be a linear combination

$$X(x,t) = \sum_{\alpha=1}^{r} b_\alpha(t)\, X_\alpha(x). \tag{2}$$

The t-dependent vector field can be seen as a family of vector fields $\{X_t \,|\, t \in \mathbb{R}\}$. Then a system X admits a superposition rule if and only if the minimal Lie algebra V^X containing the vector fields $\{X_t\}_{t\in\mathbb{R}}$, namely $V^X = \mathrm{Lie}(\{X_t \,|\, t \in \mathbb{R}\})$, is finite-dimensional.

The paradigmatic example is that of Lie–Scheffers systems on Lie groups [10, 11, 12, 24]: M is a Lie group G. Consider a basis of right-invariant vector fields X_α in G as corresponding to the opposite Lie algebra of $\mathfrak{g}$. If $\{a_1, \ldots, a_r\}$ is a basis for the tangent space T_eG and X^R_α, $\alpha = 1, \ldots, r$, denotes the right-invariant vector field in G such that $X^R_\alpha(e) = a_\alpha$, a Lie–Scheffers system is

$$\dot g(t) = -\sum_{\alpha=1}^{r} b_\alpha(t) X^R_\alpha(g(t)) \ . \tag{3}$$

When applying $(R_{g(t)^{-1}})_{*g(t)}$ to both sides we obtain the equation on T_eG

$$(R_{g(t)^{-1}})_{*g(t)}(\dot{g}(t)) = -\sum_{\alpha=1}^{r} b_\alpha(t)a_\alpha\ . \tag{4}$$

The motivation for the choice of the minus sign on the right hand side will be clear shortly. This equation is usually written with a slight abuse of notation as follows:

$$(\dot{g}\,g^{-1})(t) = -\sum_{\alpha=1}^{r} b_\alpha(t)a_\alpha\ . \tag{5}$$

Such an equation is right-invariant. Then, if $\bar{g}(t)$ is a solution of (5) with initial condition $\bar{g}(0) = e$, the solution $g(t)$ with initial conditions $g(0) = g_0$ is given by $\bar{g}(t)g_0$. This shows that there is a superposition rule $\Phi : G \times G \to G$ involving only one solution

$$\Phi(g, g_0) = gg_0.$$

This example is very useful because there are many other related examples. For instance, Lie–Scheffers systems on homogeneous spaces for G [11, 24]. Let H be a closed subgroup of G and consider the homogeneous space $M = G/H$. Then $\tau : G \to G/H$ is a principal bundle. The right-invariant vector fields X_α^R are τ-projectable and the τ-related vector fields in M are the fundamental vector fields $-X_\alpha = -X_{a_\alpha}$ corresponding to the natural left action of G on M, i.e. $\tau_{*g}X_\alpha^R(g) = -X_\alpha(gH)$, and we will have a Lie–Scheffers system on M associated to (4) given by (2). This is the reason for minus sign in (3). Then, as the vector field in G defined by the right-hand side of (3) is τ-projectable on the t-dependent vector field (2), a solution of this last system starting from $x_0 = [eH]$ will be of the form $x(t) = \Phi(g(t), x_0)$, with $g(t)$ being the solution of (4) such that $g(0) = e$. The converse property is true: given a Lie–Scheffers system defined by complete vector fields X_α on a homogeneous space M, with associated Lie algebra $\mathfrak{g}$, we can see these X_α as fundamental vector fields relative to an action to be found by integrating the vector fields. Recall that if $\Psi : G \times M \to M$ is a transitive action of the Lie group G on a manifold M, called a homogeneous space, then by choosing a fixed point $x_0 \in M$, M can be identified with the set G/G_{x_0} of left-cosets, with respect to the isotopy group $G_{x_0} = \{g \in G \,|\, \Psi(g, x_0) = x_0\}$. The map $F : G \to M$ given by $F(g) = \Psi(g, x_0)$ is epijective and such that the equivalence relation associated to F coincides with the equivalence relation defined by the subgroup G_{x_0}, and the induced bijection $\bar{F} : G/G_{x_0} \to M$ gives the mentioned identification.

1.1. Wei–Norman method. There is a method to solve directly equation (5) that is a generalisation of the one proposed by Wei and Norman [36, 37] for finding the time evolution operator for a linear systems of type

$$\frac{dU(t)}{dt} = H(t)U(t) \quad \text{with } U(0) = I.$$

PROPOSITION 1.1. *If $g(t)$, $g_1(t)$ and $g_2(t)$ are differentiable curves in G such that $g(t) = g_1(t)g_2(t)$ for every $t \in \mathbb{R}$, then*

$$R_{g(t)^{-1}\,*g(t)}(\dot{g}(t)) = R_{g_1(t)^{-1}\,*g_1(t)}(\dot{g}_1(t)) + \mathrm{Ad}(g_1(t))\big\{R_{g_2(t)^{-1}\,*g_2(t)}(\dot{g}_2(t))\big\}. \tag{6}$$

The generalisation to several factors is as follows: if $g(t) = g_1(t)g_2(t)\cdots g_l(t) = \prod_{i=1}^{l} g_i(t)$, then

$$R_{g(t)^{-1}*g(t)}(\dot{g}(t)) = \sum_{i=1}^{l}\Big(\prod_{j<i}\mathrm{Ad}(g_j(t))\Big)\{R_{g_i(t)^{-1}*g_i(t)}(\dot{g}_i(t))\},$$

where $g_0(t) = e$ for all t.

The generalised Wei–Norman method consists on writing $g(t)$ in terms of its second kind canonical coordinates,

$$g(t) = \prod_{\alpha=1}^{r}\exp(-v_\alpha(t)a_\alpha) = \exp(-v_1(t)a_1)\cdots\exp(-v_r(t)a_r),$$

and transforming the equation into a system of differential equations for the functions $v_\alpha(t)$, with initial conditions $v_\alpha(0) = 0$ for all $\alpha = 1,\dots,r$.

Then, using the expression of the above property, with $l = r = \dim G$ and $g_\alpha(t) = \exp(-v_\alpha(t)a_\alpha)$ for all α, we see that [11, 24]

$$\begin{aligned} R_{g(t)^{-1}*g(t)}(\dot{g}(t)) &= -\sum_{\alpha=1}^{r}\dot{v}_\alpha\Big(\prod_{\beta<\alpha}\mathrm{Ad}(\exp(-v_\beta(t)a_\beta))\Big)a_\alpha \\ &= -\sum_{\alpha=1}^{r}\dot{v}_\alpha\Big(\prod_{\beta<\alpha}\exp(-v_\beta(t)\mathrm{ad}(a_\beta))\Big)a_\alpha. \end{aligned}$$

Then the fundamental expression of the Wei–Norman method is

$$\sum_{\alpha=1}^{r}\dot{v}_\alpha\Big(\prod_{\beta<\alpha}\exp(-v_\beta(t)\mathrm{ad}\,(a_\beta))\Big)a_\alpha = \sum_{\alpha=1}^{r} b_\alpha(t)a_\alpha, \tag{7}$$

with $v_\alpha(0) = 0$, $\alpha = 1,\dots,r$.

This system of differential equations for the functions $v_\alpha(t)$ is integrable by quadratures if the Lie algebra is solvable, and in particular, for nilpotent Lie algebras.

1.2. The reduction method. Sometimes it may happen that the only nonvanishing coefficients in (2) are those corresponding to a subalgebra $\mathfrak{h}$ of $\mathfrak{g}$. Then the equation reduces to a simpler equation on a subgroup, involving less coordinates. The fundamental result is that if we know a particular solution of the problem associated in a homogeneous space, the original equation reduces to one on the isotopy subgroup.

The method is based on the following property: if $g'(t)$ is a curve in the group G, and the curve $\overline{g}(t)$ is defined by $\overline{g}(t) = g'(t)g(t)$, where $g(t)$ is a solution of (3), then the new curve in G, $\overline{g}(t)$, is a solution of a new Lie system in G. Indeed, [24]

$$R_{\overline{g}(t)^{-1}*\overline{g}(t)}(\dot{\overline{g}}(t)) = R_{g'^{-1}(t)*g'(t)}(\dot{g}'(t)) - \sum_{\alpha=1}^{r} b_\alpha(t)\mathrm{Ad}(g'(t))a_\alpha,$$

which is an equation similar to the original one but with a different right hand side. This defines an action of the group of curves in the Lie group G on the set of Lie systems on the group that can be used to reduce a given Lie system to a simpler one. Of course, if $g(0) = g'(0) = e$, then also $\overline{g}(0) = e$.

The aim is to choose the curve $g'(t)$ in such a way that the new equation be simpler. For instance, we can choose a subgroup H and look for a choice of $g'(t)$ such that the right hand side lies in T_eH, and hence $\overline{g}(t) \in H$ for all t.

If $\Psi : G \times M \to M$ is a transitive action of G on a homogeneous space M, the integral curves starting from the point $p \in M$ associated to both Lie systems are related by

$$\overline{x}(t) = \Psi(\overline{g}(t), p) = \Psi(g'(t)g(t), p) = \Psi(g'(t), x(t)),$$

because $\Psi(g(t), p) = x(t)$.

Therefore, this gives an action of the group of curves in G on the set of associated Lie systems in homogeneous spaces. More explicitly, a curve $g'(t)$ in the group, transforms the Lie system (2) in a homogeneous space M into a new one

$$\dot{\bar{x}} = \sum_{\alpha=1}^{r} \bar{b}_\alpha(t) X_\alpha(\bar{x}),$$

where (see e.g. [24])

$$\bar{b} = \mathrm{Ad}(g'(t))b(t) + \dot{g}'\, g'^{-1}. \tag{8}$$

The important result is that the knowledge of a particular solution $x_1(t)$ of the associated Lie system in G/H allows us to reduce the problem to one in the subgroup H.

Theorem 1.2. *Each solution of* (5) *on the group G can be written in the form $g(t) = g_0(t)h(t)$, where $g_0(t)$ is a curve on G projecting onto the given solution $x_p(t)$ for the left action λ on the homogeneous space G/H, i.e. $x_p(t) = \Psi(g_0(t), x_p(0))$, and $h(t)$ is a solution of an equation like* (5) *but for the subgroup H, given explicitly by*

$$(\dot{h}\, h^{-1})(t) = -\mathrm{Ad}(g_0^{-1}(t))\Big(\sum_{\alpha=1}^{r} b_\alpha(t)a_\alpha + (\dot{g}_0\, g_0^{-1})(t)\Big) \in T_eH. \tag{9}$$

In fact, if a particular solution $x_p(t)$ of the corresponding problem in a homogeneous space is known, there will be a curve $g_0(t)$ in G starting from $e \in G$ such that $x_p(t) = \Psi(g_0(t), x_p(0))$, and any other such curve will be of the form $g_0(t)h(t)$ where $h(t) \in G_{x_p(0)}$, which shows that if we take as $g'(t)$ in the factorization of $\overline{g}(t)$ the curve $g_0^{-1}(t)$, the curve $\overline{g}(t)$ is but $h(t) \in G_{x_p(0)} = H$, which will be simpler to determine. Moreover, if $x(t)$ is a solution of (2) and we define $y = \Psi(g_0^{-1}(t), x(t))$, then

$$\frac{dy}{dt} = \frac{d}{dt}\big(\Psi(g_0^{-1}(t), x(t))\big) = \frac{d}{dt}\big(\Psi(g_0^{-1}(t)\, g(t), x(0))\big) = \frac{d}{dt}(\Psi(h(t), x(0))),$$

and therefore $y(t) = \Psi(g_0^{-1}(t), x(t))$ is a solution of a Lie system with associated Lie group $H = G_{x_p(0)}$. Superposition rules are a consequence of iterated reductions when a sufficient number of solutions is known. Mixed superposition rules have also been introduced [17, 28] using particular solutions in different homogeneous spaces for the same group.

The theory can be extended to deal with second order differential equations of Lie type and interesting results have been found. For instance, 1-dim and 2-dim harmonic oscillator with time-dependent frequency [18], Pinney equation [14, 35], Ermakov system and its generalisations [17].

The existence of additional compatible geometric structures, like symplectic or Poisson structures [1, 2, 19, 25], or the more general case of Jacobi [30] and Dirac structures [7], and k-symplectic structures [33, 34], may be useful in the search for solutions. We restrict our exposition to the symplectic case, and we do not present here explicit results for more general cases, but we refer to the original papers because we are now interested in applications of Lie systems in quantum mechanics. Take now a symplectic manifold (M, Ω) and suppose that the vector fields arising in the expression of the t-dependent vector field describing a Lie system are Hamiltonian vector fields closing on a real finite-dimensional Lie algebra. When these vector fields are complete, they correspond to a symplectic action of the Lie group G on (M, Ω). The Hamiltonian functions h_α, defined by $i(X_\alpha)\Omega = -dh_\alpha$, do not close on the same Lie algebra when the Poisson bracket is considered, but we can only say that $d\big(\{h_\alpha, h_\beta\} - h_{[X_\alpha, X_\beta]}\big) = 0$, and then, when M is connected they span a Lie algebra extension of the original one. The important fact is that we can define a t-dependent Hamiltonian $h_t = \sum_\alpha b_\alpha(t) h_\alpha$, in such a way that $i(X_t)\Omega = -dh_t$.

As an example we can consider the system of differential equations of an n-dimensional Winternitz–Smorodinsky oscillator of the form

$$\begin{cases} \dot{x}_i = p_i, \\ \dot{p}_i = -\omega^2(t) x_i + \dfrac{k}{x_i^3}, \end{cases} \qquad i = 1, \dots, n, \; x_i \neq 0,$$

which describes the integral curves of the t-dependent vector field on $\mathrm{T}^*\mathbb{R}^n$

$$X_t = \sum_{i=1}^n \left[p_i \frac{\partial}{\partial x_i} + \left(-\omega^2(t) x_i + \frac{k}{x_i^3} \right) \frac{\partial}{\partial p_i} \right],$$

which can be written as $X_t = X_2 + \omega^2(t) X_1$ with X_1, X_2 and $X_3 = -[X_1, X_2]$ being

$$X_1 = -\sum_{i=1}^n x_i \frac{\partial}{\partial p_i}, \quad X_2 = \sum_{i=1}^n \left(p_i \frac{\partial}{\partial x_i} + \frac{k}{x_i^3} \frac{\partial}{\partial p_i} \right), \quad X_3 = \sum_{i=1}^n \left(x_i \frac{\partial}{\partial x_i} - p_i \frac{\partial}{\partial p_i} \right).$$

Note that X_t is a Lie system, because X_1, X_2 and X_3 close on a $\mathfrak{sl}(2, \mathbb{R})$ Lie algebra:

$$[X_1, X_2] = -X_3, \qquad [X_1, X_3] = X_1, \qquad [X_2, X_3] = -X_2.$$

Moreover, the preceding vector fields are Hamiltonian vector fields with respect to the usual symplectic form $\omega_0 = \sum_{i=1}^n dx^i \wedge dp_i$ with Hamiltonian functions

$$h_1 = \frac{1}{2} \sum_{i=1}^n x_i^2, \qquad h_2 = \frac{1}{2} \sum_{i=1}^n \left(p_i^2 + \frac{k}{x_i^2} \right), \qquad h_3 = \sum_{i=1}^n x_i p_i,$$

which obey the commutation relations

$$\{h_1, h_2\} = h_3, \qquad \{h_1, h_3\} = -h_1, \qquad \{h_2, h_3\} = h_2.$$

Consequently, every curve h_t that takes values in the real Lie algebra $(W, \{\cdot, \cdot\})$ spanned by h_1, h_2 and h_3 gives rise to a Lie system which is Hamiltonian in $\mathrm{T}^*\mathbb{R}^n$ with respect to the symplectic structure ω_0 in such a way that the t-dependent vector field is given by

$$X_t = X_2 + \omega^2(t) X_1 = \widehat{\omega}_0^{-1}(dh_2 + \omega^2(t) dh_1),$$

i.e. the Hamiltonian is $h_t = h_2 + \omega^2(t) h_1$.

2. Geometric approach to quantum mechanics. The Schrödinger picture of pure states in quantum mechanics admits a geometric interpretation similar to that of classical mechanics [3, 4, 5, 12]. A separable complex Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ can be considered as a real linear space, to be then denoted by $\mathcal{H}_\mathbb{R}$. The norm in $\mathcal{H}$ defines a norm in $\mathcal{H}_\mathbb{R}$, where $\|\psi\|_\mathbb{R} = \|\psi\|_\mathbb{C}$. Moreover, the linear space $\mathcal{H}_\mathbb{R}$ is endowed with a natural symplectic structure as follows:

$$\omega(\psi_1, \psi_2) = 2\,\mathrm{Im}\langle\psi_1, \psi_2\rangle, \tag{10}$$

and then $\mathcal{H}_\mathbb{R}$ is a real manifold modelled with a Banach space admitting a global chart.

The tangent space $T_\phi\mathcal{H}_\mathbb{R}$ at any point $\phi \in \mathcal{H}_\mathbb{R}$ can be identified with $\mathcal{H}_\mathbb{R}$ itself: the isomorphism associates $\psi \in \mathcal{H}_\mathbb{R}$ with the vector $\dot\psi \in T_\phi\mathcal{H}_\mathbb{R}$ given by

$$\dot\psi f(\phi) := \left(\frac{d}{dt} f(\phi + t\psi)\right)\bigg|_{t=0}, \quad \forall f \in C^\infty(\mathcal{H}_\mathbb{R}). \tag{11}$$

The real manifold can be endowed with a symplectic 2-form ω:

$$\omega_\phi(\dot\psi, \dot\psi') = 2\,\mathrm{Im}\langle\psi, \psi'\rangle. \tag{12}$$

One can see that the constant symplectic structure ω in $\mathcal{H}_\mathbb{R}$, considered as a Banach manifold, is exact, i.e., there exists a 1-form $\theta \in \bigwedge^1(\mathcal{H}_\mathbb{R})$ such that $\omega = -d\theta$. Such a 1-form $\theta \in \bigwedge^1(\mathcal{H})$ is, for instance, the one defined by

$$\theta(\psi_1)[\dot\psi_2] = -\,\mathrm{Im}\langle\psi_1, \psi_2\rangle. \tag{13}$$

This shows that the geometric framework for the usual Schrödinger picture of pure states is that of symplectic mechanics, as in the classical case. In order to avoid some topological technicalities relative to domain and composition of non-bounded operators, we restrict ourselves to the case of finite-dimensional Hilbert spaces.

A continuous vector field in $\mathcal{H}_\mathbb{R}$ is a continuous map $X : \mathcal{H}_\mathbb{R} \to \mathcal{H}_\mathbb{R}$. For instance for each $\phi \in \mathcal{H}$, the constant vector field X_ϕ defined by $X_\phi(\psi) = \dot\phi$ is the generator of the one-parameter subgroup of transformations of $\mathcal{H}_\mathbb{R}$ given by $\Phi(t, \psi) = \psi + t\phi$.

As another particular example of vector field consider the vector field X_A defined by the $\mathbb{C}$-linear map $A : \mathcal{H} \to \mathcal{H}$, and in particular when A is skew-selfadjoint.

With the natural identification natural of $T\mathcal{H}_\mathbb{R} \approx \mathcal{H}_\mathbb{R} \times \mathcal{H}_\mathbb{R}$, the vector field X_A is given by

$$X_A : \phi \mapsto (\phi, A\phi) \in \mathcal{H}_\mathbb{R} \times \mathcal{H}_\mathbb{R}. \tag{14}$$

When $A = I$, X_I is the Liouville vector field generator of dilations along the fibres, $\Delta = X_I$, given by $\Delta(\phi) = (\phi, \phi)$.

Given a selfadjoint operator A in $\mathcal{H}$, we can define a real function a (also denoted by f_A) in $\mathcal{H}_\mathbb{R}$ by

$$a(\phi) = f_A(\phi) = \langle\phi, A\phi\rangle. \tag{15}$$

Then

$$\begin{aligned} da_\phi(\dot\psi) &= \frac{d}{dt} a(\phi + t\psi)\big|_{t=0} = \frac{d}{dt}\big[\langle\phi + t\psi, A(\phi + t\psi)\rangle\big]\big|_{t=0} \\ &= 2\,\mathrm{Re}\langle\psi, A\phi\rangle = 2\,\mathrm{Im}\langle -\mathrm{i}\, A\phi, \psi\rangle = \omega(-\mathrm{i}\, A\phi, \psi). \end{aligned}$$

If we recall that the Hamiltonian vector field defined by the function a is such that for each $\psi \in T_\phi\mathcal{H} = \mathcal{H}$,

$$da_\phi(\dot{\psi}) = \omega(X_a(\phi), \psi),$$

we see that

$$X_a(\phi) = -\mathrm{i}\, A\phi. \tag{16}$$

Therefore if A is the Hamiltonian H of a quantum system, the Schrödinger equation describing time-evolution plays the rôle of 'Hamilton equations' for the Hamiltonian dynamical system $(\mathcal{H}, \omega, h)$, where $h(\phi) = \langle \phi, H\phi\rangle$: the integral curves of X_h satisfy

$$\dot{\phi} = X_h(\phi) = -\mathrm{i}\, H\phi. \tag{17}$$

The real functions $a(\phi) = \langle \phi, A\phi\rangle$ and $b(\phi) = \langle \phi, B\phi\rangle$ corresponding to two selfadjoint operators A and B satisfy

$$\{a, b\}(\phi) = -\mathrm{i}\, \langle \phi, [A, B]\phi\rangle, \tag{18}$$

i.e. $\{f_A, f_B\} = f_{-i\,[A,B]}$, because

$$\{a, b\}(\phi) = [\omega(X_a, X_b)](\phi) = \omega_\phi(X_a(\phi), X_b(\phi)) = 2\,\mathrm{Im}\langle A\phi, B\phi\rangle,$$

and taking into account that

$$2\,\mathrm{Im}\langle A\phi, B\phi\rangle = -\mathrm{i}\,[\langle A\phi, B\phi\rangle - \langle B\phi, A\phi\rangle] = -\mathrm{i}\,[\langle \phi, AB\phi\rangle - \langle \phi, BA\phi\rangle],$$

we find the above result.

In particular, on integral curves of the vector field X_h defined by a Hamiltonian H,

$$\dot{a}(\phi) = \{a, h\}(\phi) = -\mathrm{i}\, \langle \phi, [A, H]\phi\rangle,$$

which is usually known as Ehrenfest theorem:

$$\frac{d}{dt}\langle \phi, A\phi\rangle = -\mathrm{i}\, \langle \phi, [A, H]\phi\rangle. \tag{19}$$

There is another relevant symmetric $(0, 2)$ tensor field which is given by the real part of the inner product. It endows $\mathcal{H}_\mathbb{R}$ with a Riemann structure by

$$g(u, v) = 2\,\mathrm{Re}\langle u, v\rangle, \qquad u, v \in \mathcal{H}_\mathbb{R}. \tag{20}$$

in such a way that the Hermitean structure defining the Hilbert space structure can be recovered as

$$\langle u, v\rangle = \frac{1}{2}\,[g(u, v) + \mathrm{i}\,\omega(u, v)], \qquad u, v \in \mathcal{H}_\mathbb{R}.$$

We also have a complex structure J, corresponding to multiplication by i seen as a real linear map, such that

$$g(v_1, v_2) = -\omega(Jv_1, v_2), \qquad \omega(v_1, v_2) = g(Jv_1, v_2), \tag{21}$$

together with

$$g(Jv_1, Jv_2) = g(v_1, v_2), \qquad \omega(Jv_1, Jv_2) = \omega(v_1, v_2). \tag{22}$$

The triplet (g, J, ω) defines a Kähler structure on $\mathcal{H}_\mathbb{R}$ and the symmetry group of the theory must be the unitary group $U(\mathcal{H})$ whose elements preserve the inner product, or in an alternative but equivalent way (in the finite-dimensional case), by the intersection of the orthogonal group $O(2n, \mathbb{R})$ and the symplectic group $\mathrm{Sp}(2n, \mathbb{R})$.

The non-degeneracy of ω and g allows us to associate the corresponding contravariant tensor fields Λ and G, respectively. It is well-known that the first one defines a Poisson structure. The second one gives rise to a commutative composition law in the space of functions as

$$(f_1, f_2) = G(df_1, df_2). \tag{23}$$

In particular, if A and B are self-adjoint operators,

$$\begin{aligned}(a,b)(\phi) = G_\phi(df_A(\phi), df_B(\phi)) = g_\phi(X_a(\phi), X_b(\phi))\\ = 2\,\mathrm{Re}\langle A\phi, B\phi\rangle = \langle A\phi, B\phi\rangle + \langle B\phi, A\phi\rangle,\end{aligned}$$

i.e.

$$(a,b)(\phi) = \langle \phi, (AB+BA)\phi\rangle \Longleftrightarrow (f_A, f_B)(\phi) = \langle \phi, [A,B]_+\phi\rangle.$$

Important particular cases are:

$$(f_A, f_A) = G(df_A, df_A) = 2f_{A^2}, \quad (f_A, f_I) = G(df_A, df_I) = 2f_A, \tag{24}$$

where I is the identity.

On the other hand, the fundamental concept for measurements is the expectation value of observables,

$$e_A(\psi) = \frac{\langle \psi, A\psi\rangle}{\langle \psi, \psi\rangle}, \tag{25}$$

and note that two vectors ψ_1, ψ_2 such that $e_A(\psi_1) = e_A(\psi_2)$ for each observable A, i.e.

$$\frac{\langle \psi_2, A\psi_2\rangle}{\langle \psi_2, \psi_2\rangle} = \frac{\langle \psi_1, A\psi_1\rangle}{\langle \psi_1, \psi_1\rangle}, \quad \forall A \in \mathrm{Her}(\mathcal{H})$$

should be considered as indistinguishable. This is only possible when ψ_2 is proportional to ψ_1, and therefore the elements describing the quantum states must be rays rather than vectors, i.e. the space of states is not $\mathbb{C}^n$ but the projective space $\mathbb{CP}^{n-1}$.

It is possible to define a Kähler structure on $\mathbb{CP}^{n-1}$ and then to study Lie–Kähler systems leading to superposition rules for time evolution in this projective space.

On the other side, we can compute (e_A, e_A) for the expectation value function e_A of a self-adjoint operator A in a pure state ψ, and we see that, as $e_A = f_A/f_I$,

$$\|\psi\|^2(e_A, e_A)(\psi) = \frac{\langle \psi, A^2\psi\rangle}{\|\psi\|^2} - \left(\frac{\langle \psi, A\psi\rangle}{\|\psi\|^2}\right)^2 \Longleftrightarrow (e_A, e_A) = \frac{2}{f_I}(e_{A^2} - e_A^2),$$

where I is the identity in $\mathcal{H}$, because

$$e_A = \frac{f_A}{f_I} \Longrightarrow de_A = \frac{1}{f_I}\,df_A - \frac{f_A}{f_I^2}\,df_I, \tag{26}$$

and then, from

$$G(de_A, de_A) = G\left(\frac{1}{f_I}\,df_A - \frac{f_A}{f_I^2}\,df_I, \frac{1}{f_I}\,df_A - \frac{f_A}{f_I^2}\,df_I\right)$$

we see that

$$G(de_A, de_A) = \frac{1}{f_I^2}\,G(df_A, df_A) + \frac{f_A^2}{f_I^4}\,G(df_I, df_I) - 2\,\frac{f_A}{f_I^3}\,G(df_A, df_I),$$

and using relations (24) we obtain

$$(e_A, e_A) = G(de_A, de_A) = \frac{2}{f_I}\,(e_{A^2} - e_A^2).$$

This shows the physical meaning of the commutative product (23) as providing the dispersion of measurement results of an observable.

3. Lie systems and time evolution in quantum mechanics. Once the fundamental axioms of quantum mechanics in a fixed time have been translated to geometric terms we should analyse time evolution. The only assumption in this new framework is that it must be a symmetry. Then time evolution from time t_0 to time t is described in terms of the evolution operator $U(t, t_0)$:

$$\psi(t) = U(t, t_0)\psi(t_0), \tag{27}$$

which must be a symmetry of the theory, i.e. linearity, symplectic and Riemannian structure must be preserved, and then for each fixed t_0, $U(t, t_0)$ is a curve in the unitary group $U(\mathcal{H})$.

If we assume by simplicity that $\mathcal{H}$ is finite-dimensional, then as

$$\frac{dU(t, t_0)}{dt} \in T_{U(t,t_0)}U(\mathcal{H}) \Longrightarrow \frac{dU(t, t_0)}{dt}(U(t, t_0))^{-1} \in T_I U(\mathcal{H}) \approx \mathfrak{u}(\mathcal{H}),$$

and therefore, there exists a curve $H(t)$ in $\mathrm{Herm}(n, \mathbb{C})$ such that

$$\frac{dU(t, t_0)}{dt} = -\mathrm{i}\, H(t)U(t, t_0). \tag{28}$$

In this equation $H(t)$ does not depend on t_0 because of the relation

$$U(t, t_0) = U(t, t_1)U(t_1, t_0),$$

which implies

$$\frac{dU(t, t_0)}{dt}(U(t, t_0))^{-1} = \frac{dU(t, t_1)}{dt}(U(t, t_1))^{-1}.$$

The evolution equation (28) shows that the evolution operator for a time-dependent Schrödinger equation is a Lie system in the unitary group $U(\mathcal{H})$ with associated Lie algebra $\mathfrak{u}(\mathcal{H})$ in the most general case. Sometimes however we can deal with some of its subalgebras.

Every curve $H(t)$ in $\mathfrak{u}(\mathcal{H})$ can be written as a linear combination of at most n^2 elements, those of a basis of $\mathfrak{u}(\mathcal{H})$, and therefore these (finite-dimensional) quantum systems are Lie systems.

As the elements of the Vessiot–Guldberg Lie algebra are skew-Hermitians, all of them define simultaneously Hamiltonian vector fields and Killing vector fields, and the system is a Lie–Kähler system.

As an example consider a Hamiltonian operator $H(t)$ that can be written as a linear combination, with some t-dependent real coefficients $b_1(t), \ldots, b_r(t)$, of some Hermitian operators,

$$H(t) = \sum_{k=1}^{r} b_k(t)H_k, \tag{29}$$

where the H_k's form a basis of a real finite-dimensional Lie algebra V relative to the Lie bracket of observables, i.e. $[H_j, H_k] = \sum_{l=1}^r \mathrm{i}\, c_{jkl}\, H_l$, with $c_{jkl} \in \mathbb{R}$ and $j, k, l = 1, \ldots, r$. Using (27) and (28) we see that $H(t)$ determines a t-dependent Schrödinger equation

$$\frac{d\psi}{dt} = -\mathrm{i}\, H(t)\psi = -\mathrm{i} \sum_{k=1}^r b_k(t) H_k \psi.$$

The vector fields X_k such that $X_k(\psi) = -\mathrm{i}\, H_k\, \psi$ are such that the t-dependent vector field X corresponding to the equation is $X = \sum_{k=1}^r b_k(t) X_k$ and

$$[X_j, X_k] = -\sum_{l=1}^r c_{jkl} X_l, \qquad j, k = 1, \ldots, r.$$

As an instance, if $\mathcal{H} = \mathbb{C}^2$, the time evolution is described by a curve $-\mathrm{i}\, H(t) := \dot{U}_t U_t^{-1}$ in the Lie algebra $\mathfrak{u}(2)$ of $U(2)$. By using the basis

$$I_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and defining $\mathbf{S} := (\sigma_1, \sigma_2, \sigma_3)/2$ and $\mathbf{B} := (B_1, B_2, B_3)$, the Hamiltonian can be written as

$$H(t) := B_0(t) I_0 + \mathbf{B}(t) \cdot \mathbf{S}.$$

By using the identification of $\mathbb{C}^2$ with $\mathbb{R}^4$, the Schrödinger equation is

$$\begin{pmatrix} \dot{q}_1 \\ \dot{p}_1 \\ \dot{q}_2 \\ \dot{p}_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 2B_0(t) + B_3(t) & -B_2(t) & B_1(t) \\ -2B_0(t) - B_3(t) & 0 & -B_1(t) & -B_2(t) \\ B_2(t) & B_1(t) & 0 & 2B_0(t) - B_3(t) \\ -B_1(t) & B_2(t) & B_3(t) - 2B_0(t) & 0 \end{pmatrix} \begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \end{pmatrix},$$

while the vector fields are now

$$\begin{aligned} X_0 &= -\Gamma = p_1 \frac{\partial}{\partial q_1} - q_1 \frac{\partial}{\partial p_1} + p_2 \frac{\partial}{\partial q_2} - q_2 \frac{\partial}{\partial p_2}, \\ X_1 &= \frac{1}{2}\left(p_2 \frac{\partial}{\partial q_1} - q_2 \frac{\partial}{\partial p_1} + p_1 \frac{\partial}{\partial q_2} - q_1 \frac{\partial}{\partial p_2} \right), \\ X_2 &= \frac{1}{2}\left(-q_2 \frac{\partial}{\partial q_1} - p_2 \frac{\partial}{\partial p_1} + q_1 \frac{\partial}{\partial q_2} + p_1 \frac{\partial}{\partial p_2} \right), \\ X_3 &= \frac{1}{2}\left(p_1 \frac{\partial}{\partial q_1} - q_1 \frac{\partial}{\partial p_1} - p_2 \frac{\partial}{\partial q_2} + q_2 \frac{\partial}{\partial p_2} \right), \end{aligned}$$

satisfying

$$[X_0, \cdot\,] = 0, \qquad [X_1, X_2] = -X_3, \qquad [X_2, X_3] = -X_1, \qquad [X_3, X_1] = -X_2.$$

The vector fields X_0, X_1, X_2, X_3 are Hamiltonian with Hamiltonian functions

$$\begin{aligned} h_0(\psi) &= \frac{1}{2}\langle \psi, \psi \rangle = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2), & h_1(\psi) &= \frac{1}{2}\langle \psi, S_1\psi \rangle = \frac{1}{2}(q_1 q_2 + p_1 p_2), \\ h_2(\psi) &= \frac{1}{2}\langle \psi, S_2\psi \rangle = \frac{1}{2}(q_1 p_2 - p_1 q_2), & h_3(\psi) &= \frac{1}{2}\langle \psi, S_3\psi \rangle = \frac{1}{4}(q_1^2 + p_1^2 - q_2^2 - p_2^2), \end{aligned}$$

which are not functionally independent, but $h_0^2 = 4(h_1^2 + h_2^2 + h_3^2)$. Another example can be found in [25].

When $\mathcal{H}$ is not finite-dimensional, Lie system theory also applies if the t-dependent Hamiltonian can be written as a linear combination with t-dependent coefficients of Hamiltonians H_i closing, under the commutator bracket, on a real finite-dimensional Lie algebra.

Note however that this Lie algebra does not necessarily coincide with the corresponding classical one, but it is, in general, a Lie algebra extension.

4. Lie systems and time-independent Schrödinger equation. A linear SODE in normal form $\phi'' = b_1(x)\phi + b_2(x)\phi'$ can be written in the form of a system of two first-order differential equations in the variables (v_ϕ, ϕ):

$$\begin{cases} v'_\phi = b_2(x)v_\phi + b_1(x)\phi \\ \phi' = v_\phi. \end{cases} \tag{30}$$

By identifying $\mathbb{R}^2$ with $T\mathbb{R}$, (v_ϕ, ϕ) are bundle coordinates, the preceding system determines the integral curves of the x-dependent vector field

$$X = v_\phi \frac{\partial}{\partial\phi} + (b_1(x)\phi + b_2(x)v_\phi)\frac{\partial}{\partial v_\phi}, \tag{31}$$

which is said to be a SODE vector field because of the coefficient of $\partial/\partial\phi$.

The linear system determining its integral curves is

$$\begin{pmatrix} v'_\phi \\ \phi' \end{pmatrix} = \begin{pmatrix} b_2(x) & b_1(x) \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_\phi \\ \phi \end{pmatrix}. \tag{32}$$

The projection onto $\mathbb{R}$ of such curves are solutions of the equation $\phi'' = b_2(x)\phi' + b_1(x)\phi$.

We are mainly interested in equations of Schrödinger type, those with $b_2(x) \equiv 0$. The corresponding vector field is then a linear combination $X = b_1(x)X_1 - X_3$ where

$$X_1 = \phi\frac{\partial}{\partial v_\phi}, \qquad X_3 = -v_\phi\frac{\partial}{\partial\phi}, \tag{33}$$

which together with

$$X_2 = \frac{1}{2}\left(v_\phi\frac{\partial}{\partial v_\phi} - \phi\frac{\partial}{\partial\phi}\right), \tag{34}$$

close on a Lie algebra isomorphic to $\mathfrak{sl}(2,\mathbb{R})$:

$$[X_1, X_3] = 2\,X_2, \qquad [X_1, X_2] = X_1, \qquad [X_3, X_2] = -X_3\,. \tag{35}$$

Therefore Schrödinger type equations and the corresponding linear systems are Lie systems with Vessiot–Lie algebra $\mathfrak{sl}(2,\mathbb{R})$. Vector fields X_1, X_2 and X_3 are fundamental vector fields corresponding to the linear action of $SL(2,\mathbb{R})$ on $\mathbb{R}^2$.

If $\mathbb{R}^2_* = \mathbb{R}^2 - \{(0,0)\}$, the map $F : \mathbb{R}^2_* \to \mathbb{R}$ defined by $F(x,y) = x/y$, if $y \neq 0$, and $F(x,0) = \infty$, is equivariant with respect to the restriction of the linear action Φ of $SL(2,\mathbb{R})$ on $\mathbb{R}^2_*$ and the action Ψ of $SL(2,\mathbb{R})$ on $\mathbb{R}$, or even better on the real projective line

$\mathbb{R}P^1 = \overline{\mathbb{R}} = \mathbb{R}\cup\{\infty\}$, by linear fractional transformations, i.e. $\Psi : SL(2,\mathbb{R})\times\mathbb{R}P^1 \to \mathbb{R}P^1$, is defined by

$$\Psi(A,u) = \frac{\alpha u+\beta}{\gamma u+\delta} \qquad \text{if } u \neq -\frac{\delta}{\gamma}\,,$$
$$\Psi(A,\infty) = \frac{\alpha}{\gamma}\,, \qquad \Psi\left(A,-\frac{\delta}{\gamma}\right) = \infty,$$
$$A = \begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix} \in SL(2,\mathbb{R}).$$

Equivariance means that $F\circ\Phi_A = \Psi_A\circ F$. The corresponding fundamental vector fields of the action Ψ are now

$$\overline{X}_1 = \frac{\partial}{\partial u}\,, \qquad \overline{X}_2 = u\frac{\partial}{\partial u}\,, \qquad \overline{X}_3 = u^2\frac{\partial}{\partial u}\,,$$

and as F is equivariant, the fundamental vector fields associated to Φ and Ψ are F-related [11, 12], i.e. $\overline{X}_i = F_*(X_i)$, $i=1,2,3$, and then a system defined by the vector fields $\overline{X}_i$ is a Lie system corresponding to a Riccati equation.

The image under F of an integral curve of the x-dependent vector field $X = b_1(x)X_1 + b_2(x)X_2 + b_3(x)X_3$, which is a linear system, is an integral curve of $\bar{X} = \bar{b}_1(x)X_1 + \bar{b}_2(x)X_2 + \bar{b}_3(x)X_3$, i.e. a solution of the corresponding Riccati equation.

We can also introduce a new vector field

$$X_4 = \frac{1}{2}\left(v_\phi\,\frac{\partial}{\partial v_\phi} + \phi\,\frac{\partial}{\partial\phi}\right), \tag{36}$$

which commutes with X_1, X_2 and X_3 and together with them generate the Lie algebra $\mathfrak{gl}(2,\mathbb{R})$, which corresponds to the Lie group $\mathrm{GL}(2,\mathbb{R})$. Any Lie system with such a group is $X = b_1(x)X_1 + b_2(x)X_2 + b_3(x)X_3 + b_4(x)X_4$, whose integral curves are determined by the system

$$\begin{pmatrix} v'_\phi\\ \phi'\end{pmatrix} = \begin{pmatrix}\frac{1}{2}(b_2(x)+b_4(x)) & b_1(x)\\ -b_3(x) & \frac{1}{2}(b_2(x)-b_4(x))\end{pmatrix}\begin{pmatrix} v_\phi\\ \phi\end{pmatrix}. \tag{37}$$

Note also that $\overline{X}_4 = F_*(X_4) = 0$. The vector field (31) can be considered as a particular case of (37) corresponding to the choice $b_3 = -1$ and $b_2 = b_4$.

Recall also that the group of curves in a Lie group G acts on the set of Lie systems with associated Vessiot–Lie algebra $\mathfrak{g}$, and this property can be used to reduce a given Lie system to another one of the same type or, in our case, to relate Schrödinger type equations with different potentials by means of curves in $GL(2,\mathbb{R})$. This is the essence of Darboux transformation method as shown in [26]. The advantage to see Schrödinger equations as Lie systems with Vessiot–Lie algebra $\mathfrak{gl}(2,\mathbb{R})$ instead of $\mathfrak{sl}(2,\mathbb{R})$ is that we can transform by curves which are in $GL(2,\mathbb{R})$ but not in $SL(2,\mathbb{R})$ (see [6]).

Coming back to the mentioned action of the group of curves in $GL(2,\mathbb{R})$, we see that if we are interested in taking into account the tangent bundle character of $T\mathbb{R}$, we should consider transformations induced from those of the base manifold. So, given a strictly positive function φ_0 we can consider the invertible map associating the function ϕ with the new function $\bar\phi$ by means of $\phi = \varphi_0\,\bar\phi$. This induces a transformation

$$\begin{pmatrix} v_\phi \\ \phi \end{pmatrix} = \begin{pmatrix} \varphi_0(x) & \varphi_0'(x) \\ 0 & \varphi_0(x) \end{pmatrix} \begin{pmatrix} v_{\bar\phi} \\ \bar\phi \end{pmatrix}. \tag{38}$$

If ϕ is a solution of $\phi'' = b_1(x)\phi + b_2(x)\phi'$, then $\bar\phi$ satisfies

$$\varphi_0(x)\bar\phi'' + (2\varphi_0'(x) - b_2(x)\varphi_0(x))\bar\phi' + (\varphi_0'' - b_1(x)\varphi_0 - b_2(x)\varphi_0')\bar\phi = 0,$$

and then if for instance $\varphi_0(x)$ is a particular solution of the given equation, we deduce that the given equation reduces to $\varphi_0(x)\,\bar\phi'' + (2\varphi_0'(x) - b_2\varphi_0(x))\bar\phi' = 0$, in which the dependent variable $\bar\phi$ is absent, which is quickly integrated by order reduction. This is an explicit example of reduction procedure for Lie system when a particular solution is known.

The usefulness of the transformation $\phi = \varphi_0\,\bar\phi$ in factorisation problems has recently been proved in [21, 22], the differential operator $\partial/\partial x$ becoming a ladder-like operator $\partial/\partial x - \varphi_0'/\varphi_0$. This allows us to introduce factorisable Hamiltonians, their partners leading to supersymmetric quantum mechanics and interesting relations among their spectra, in particular special methods for introducing or removing eigenvalues and eigenstates.

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