LIE–NAMBU AND LIE–POISSON STRUCTURES IN LINEAR AND NONLINEAR QUANTUM MECHANICS*

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Space of density matrices in quantum mechanics can be regarded as a Poisson manifold with the dynamics given by certain Lie-Poisson bracket corresponding to an infinite dimensional Lie algebra. The metric structure associated with this Lie algebra is given by a metric tensor which is not equivalent to the Cartan-Killing metric. The Lie-Poisson bracket can be written in a form involving a generalized (Lie-)Nambu bracket. This bracket can be used to generate a generalized, nonlinear and completely integrable dynamics of density matrices.

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1. Introduction

The generalized quantum mechanics presented below is based on the idea of rewriting the Liouville-von Neumann equation in a triple bracket form, introduced by Białynicki-Birula and Morrison [2]. The triple bracket is an infinite dimensional analog of the Nambu bracket [3] where, as opposed to the structure constants ϵ_{klm} of the rotation Lie algebra appearing in the original Nambu bracket, the structure constants correspond to some infinite-dimensional Lie algebra. In the original Nambu paper an evolution of a physical system is generated by two "Hamiltonian functions", the energy H and J, where the latter is the Casimir invariant of $so(3)$ (squared angular momentum). The metric tensor used for constructing the invariant is, as usual, the one related to the Killing form [4]. In the triple bracket formulation of QM the analog of J is the Casimir invariant $S = 1/2\mathrm{Tr}(\rho^2)$

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which also can be written as $g^{ab}\rho_a\rho_b$ although the metric g^{ab} is no longer given by the Killing-Cartan tensor.

2. Lie–Poisson and Lie–Nambu structures in quantum mechanics

Let us start with the Dirac equation which can be written in a form of classical Hamilton equations

$$\frac{d}{d\tau}\phi_X(x) = -2in_{XX'}\frac{\delta H}{\delta\bar{\phi}_{X'}(x)}\,, \tag{1}$$

$$\frac{d}{d\tau}\chi^{X'}(x) = -2in^{XX'}\frac{\delta H}{\delta\bar{\chi}^{X}(x)}\,, \tag{2}$$

$$\frac{d}{d\tau}\bar{\phi}_{X'}(x) = 2in_{XX'}\frac{\delta H}{\delta\phi_X(x)}\,, \tag{3}$$

$$\frac{d}{d\tau}\bar{\chi}^{X}(x) = 2in^{XX'}\frac{\delta H}{\delta\chi^{X'}(x)}\,, \tag{4}$$

where $n_{XX'}$ is a 4-vector normal to a spacelike hyperplane in the Minkowski space and $d/d\tau$ is a derivative in the direction of $n_{XX'}$. Bispinorially the equation is

$$\frac{d}{d\tau}\phi_\alpha(x) = I_{\alpha\beta}\frac{\delta H}{\delta\phi^*_\beta(x)}\,, \tag{5}$$

$$\frac{d}{d\tau}\phi^*_\alpha(x) = -I_{\alpha\beta}\frac{\delta H}{\delta\phi_\beta(x)}\,, \tag{6}$$

where $I_{\alpha\beta}$ is the Poisson tensor, or

$$\omega^{\alpha\beta}\frac{d}{d\tau}\phi_\beta(x) = \frac{\delta H}{\delta\phi^*_\alpha(x)}\,, \tag{7}$$

$$-\omega^{\alpha\beta}\frac{d}{d\tau}\phi^*_\beta(x) = \frac{\delta H}{\delta\phi_\alpha(x)}\,, \tag{8}$$

where $\omega^{\alpha\beta}$ is the symplectic form. Let us denote the continuous arguments of the wave function by $\boldsymbol{a}$, $\boldsymbol{a}'$, *etc.* This allows us to introduce the following convention for the density matrices:

$$\rho_{\alpha,\alpha'}(\boldsymbol{a},\boldsymbol{a}') = \rho_a\,, \tag{9}$$

with the summation convention where two repeated lowercase Roman indices mean simultaneous summing over the Greek indices and integration over the Roman ones.

The Liouville–von Neumann equation for the density matrix can be written in a form involving the Lie-Poisson bracket [2]

$$\frac{d}{d\tau}\rho_a = \{\rho_a, H\}\,, \tag{10}$$

where

$$\{F, G\} = \rho_a \Omega^a{}_{bc} \frac{\delta F}{\delta \rho_b}\frac{\delta G}{\delta \rho_c}\,, \tag{11}$$

and the structure kernels $\Omega^a{}_{bc}$ satisfy conditions characteristic for Lie-algebraic structure constants

$$\Omega^a{}_{cb} = -\Omega^a{}_{bc}\,, \tag{12}$$

$$\Omega^a{}_{bc}\Omega^c{}_{de} + \Omega^a{}_{ec}\Omega^c{}_{bd} + \Omega^a{}_{dc}\Omega^c{}_{eb} = 0\,. \tag{13}$$

These two conditions imply the Jacobi identity. The explicit form of the structure constants is given below.

In order to convert the Lie–Poisson bracket into a Lie–Nambu bracket we first have to define a metric tensor to lower the upper index in the structure kernels. The apparently natural guess (the Killing–Cartan metric) $g_{ab} = \Omega^c{}_{ad}\Omega^d{}_{bc}$ is incorrect as it involves expressions like $\delta(0)$ which are not distributions in the Schwartz sense and such a metric cannot be invertible.

The correct definitions are

$$g^{ab} = \frac{1}{2}\frac{\delta^2 \mathrm{Tr}(\rho^2)}{\delta\rho_a \delta\rho_b}\,, \tag{14}$$

and its inverse. Equivalent definition can be given in terms of the symplectic and Poisson structures:

$$g_{ab} = -I_{\alpha\beta'} I_{\beta\alpha'} \delta(\boldsymbol{a} - \boldsymbol{b}')\delta(\boldsymbol{b} - \boldsymbol{a}')\,, \tag{15}$$

$$g^{ab} = -\omega^{\alpha\beta'}\omega^{\beta\alpha'}\delta(\boldsymbol{a} - \boldsymbol{b}')\delta(\boldsymbol{b} - \boldsymbol{a}')\,. \tag{16}$$

The metric tensor is symmetric

$$g_{ab} = g_{ba}\,, \tag{17}$$

and satisfies the invertibility conditions

$$g^{ab} g_{bc} = \delta^\alpha_\gamma \delta^{\alpha'}_{\gamma'} \delta(\boldsymbol{a} - \boldsymbol{c})\delta(\boldsymbol{a}' - \boldsymbol{c}') =: \delta^a_c\,, \tag{18}$$

where the delta functions correspond to a foliation of spacetime defining the time derivative.

In the same way one can define higher order tensors

$$g^{a_1\dots a_n} = \frac{1}{n!}\frac{\delta^n \mathrm{Tr}(\rho^n)}{\delta\rho_{a_1}\dots\delta\rho_{a_n}} \tag{19}$$

which are related to higher order Casimir invariants of the theory as we shall see later. The metric structure is identical to this used occasionally in quantum optics [6] and is interesting in itself as an infinite dimensional substitute for the Cartan–Killing metric.

The functional

$$S_2 = \tfrac{1}{2}g^{ab}\rho_a\rho_b = \tfrac{1}{2}\mathrm{Tr}\,(\rho^2)\,, \tag{20}$$

is related to Rényi's 2-entropy [5].

The Lie–Poisson bracket can be turned into the following Lie–Nambu triple bracket

$$\{F,G\} = [F,G,S_2] = \Omega_{abc}\frac{\delta F}{\delta\rho_a}\frac{\delta G}{\delta\rho_b}\frac{\delta S_2}{\delta\rho_c}\,, \tag{21}$$

where

$$\begin{aligned}\Omega_{abc} =& I_{\alpha\gamma'}I_{\beta\alpha'}I_{\gamma\beta'}\delta(\boldsymbol{a}-\boldsymbol{c}')\delta(\boldsymbol{b}-\boldsymbol{a}')\delta(\boldsymbol{c}-\boldsymbol{b}')\\ &- I_{\alpha\beta'}I_{\gamma\alpha'}I_{\beta\gamma'}\delta(\boldsymbol{a}-\boldsymbol{c}')\delta(\boldsymbol{c}-\boldsymbol{a}')\delta(\boldsymbol{b}-\boldsymbol{c}')\,.\end{aligned} \tag{22}$$

The antisymmetry of the triple bracket means that S_2 is a Casimir invariant of a Lie algebra of observables. Another Casimir invariant is $\mathrm{Tr}\,\rho$ since $\{\mathrm{Tr}\,\rho, F\} = 0$ for *any* differentiable F (hence not only those linear in ρ).

The triple bracket form of the Liouville–von Neumann equation shows that the time evolution in linear QM has *two* generators: the average energy (Hamiltonian function) and the invariant S, which measures Rényi's $\alpha = 2$ entropy. It is natural to ask what will be changed in the theory if, instead of generalizing the class of admissible Hamiltonian functions (which is typical of all the standard nonlinear generalizations of QM), we shall extend the class of entropies. The extended theory has a well defined probability interpretation, because the observables are represented by linear operators, provided the scaling by a constant, $\rho \to \lambda\rho$, is a symmetry of the dynamics. This imposes on the generalized entropies the 2-homogeneity condition: $S(\lambda\rho) = \lambda^2 S(\rho)$.

Only for $S[\rho] = 1/2\mathrm{Tr}(\rho^2)$ the linear observables are closed under the action of the bracket $\{\cdot,\cdot\}_S := [\cdot,\cdot,S]$. If we extend the class of acceptable S, we have to accept also a somewhat stronger form of the complementarity principle than in linear QM: Observables are always complementary to their (nonvanishing) time derivatives.

3. Jacobi identity

Consider the expression

$$J = \{\{F,G\}_S, H\}_S + \{\{H,F\}_S, G\}_S + \{\{G,H\}_S, F\}_S$$
$$= \frac{\delta F}{\delta\rho_d}\frac{\delta G}{\delta\rho_e}\frac{\delta^2 S}{\delta\rho_a\delta\rho_f}\frac{\delta H}{\delta\rho_b}\frac{\delta S}{\delta\rho_c}\left(\Omega_{def}\Omega_{abc} + \Omega_{bdf}\Omega_{aec} + \Omega_{ebf}\Omega_{adc}\right) \quad (23)$$

$\frac{\delta^2 S}{\delta\rho_a\delta\rho_f} = g^{af}$ for $S = S_2$ and (23) vanishes in virtue of the properties of the structure constants. For more general $S = S(f_2[\rho])$ we find

$$\frac{\delta S}{\delta\rho_c} = 2\frac{\partial S}{\partial f_2}\rho^c$$
$$\frac{\delta^2 S}{\delta\rho_a\delta\rho_f} = 4\frac{\partial^2 S}{\partial f_2^2}\rho^a\rho^f + 2\frac{\partial S}{\partial f_2}g^{af}. \quad (25)$$

Inserting these expressions into (23) we obtain

$$J = 8\frac{\delta F}{\delta\rho_d}\frac{\delta G}{\delta\rho_e}\frac{\partial^2 S}{\partial f_2^2}\rho^a\rho^f\frac{\delta H}{\delta\rho_b}\frac{\partial S}{\partial f_2}\rho^c\left(\Omega_{def}\Omega_{abc} + \Omega_{bdf}\Omega_{aec} + \Omega_{ebf}\Omega_{adc}\right) = 0 \quad (26)$$

since $\Omega_{abc}\rho^a\rho^c = 0$. This shows that there exists at least a class of extensions of the linear formalism which conserves the Poissonian structure of the dynamics. With this choice of S we obtain the dynamics given by

$$\frac{d}{dt}\rho_a = \{\rho_a, H\}_{S_2}C[\rho], \quad (27)$$

where $C[\rho] = 2\frac{\partial S}{\partial f_2} = C(f_2[\rho])$ is an integral of motion, as we shall see later. The only difference with respect to ordinary QM would be in a ρ-dependent rescaling of time.

4. Density matrix interpretation of solutions of the generalized evolution equation

It is essential to clarify the density matrix interpretation of the solutions of the generalized Liouville–von Neumann equation

$$\frac{d}{d\tau}\rho_a = [\rho_a, H, S]. \quad (28)$$

A priori, there is no general guarantee that the generalized dynamics will conserve positivity of ρ. The following theorems partially address this issue.

Consider a functional S (differentiable in f_k)

$$S[\rho] = S\big(f_1[\rho], \ldots, f_n[\rho], \ldots\big)\,, \tag{29}$$

where $f_k[\rho] = \mathrm{Tr}\,(\rho^k)$.

Theorem 1. For any $m \in N$, and any G, if S satisfies (29) then

$$[f_m, G, S] = 0\,. \tag{30}$$

Proof:

$$\begin{aligned}[\mathrm{Tr}\,(\rho^m), G, S] &= \sum_n [\mathrm{Tr}\,(\rho^m), G, f_n] \frac{\partial S}{\partial f_n} \\ &= -im \sum_n n \mathrm{Tr}\,\big(\hat{G}[\rho^{m-1}, \rho^{n-1}]\big) \frac{\partial S}{\partial f_n} = 0\,. \end{aligned} \tag{31}$$

This result covers many nontrivial generalizations of S_2. The particular case $m = 1$ implies that $\mathrm{Tr}\,\rho$ is conserved by all evolutions, a fact important for a definition of averages. For pure states $\mathrm{Tr}\,(\rho^m) = (\mathrm{Tr}\,\rho)^m$ so that the integrals f_m are not necessarily independent, but for all m, n f_m and f_n are in involution with respect to $[\cdot, \cdot, S]$. Jordan proved in [7] by an explicit calculation that in his formulation of nonlinear QM $\mathrm{Tr}\,\rho$ and $\mathrm{Tr}\,\rho^2$ are conserved — our theorem considerably generalizes this result.

Theorem 2. Let S satisfy (29) and ρ_t be a self-adjoint solution of (28). If ρ_0 is positive and has a finite number of nonvanishing eigenvalues $p_k(0)$, $0 < p_k(0) \leq 1$, then the eigenvalues of ρ_t are integrals of motion, and the evolution conserves positivity of ρ_t.

Proof: Since the nonvanishing eigenvalues of ρ_0 satisfy $0 < p_k(0) \leq 1 < 2$, it follows that for any α $p_k(0)^\alpha$ can be written in the form of a convergent Taylor series. By virtue of the spectral theorem the same is true for ρ_0^α and $\mathrm{Tr}\,(\rho_0^\alpha)$. Each term of the Taylor expansion of $\mathrm{Tr}\,(\rho_0^\alpha)$ is proportional to $f_n[\rho_0]$, for some n. But $f_n[\rho_0] = f_n[\rho_t]$ hence

$$\mathrm{Tr}\,(\rho_0^\alpha) = \mathrm{Tr}\,(\rho_t^\alpha) = \sum_k p_k(0)^\alpha = \sum_k p_k(t)^\alpha \tag{32}$$

for all real α. Since all $p_k(0)$ are assumed to be known (the initial condition), we know also $\sum_k p_k(0)^\alpha = \sum_k p_k(t)^\alpha$ for any α. We can now apply the result from information theory [5] that the knowledge of

$$\sum_{k=1}^{n<\infty} p_k(t)^\alpha \tag{33}$$

for all α *uniquely* determines $p_k(t)$. The continuity in t implies that $p_k(t) = p_k(0)$. □

The assumption that initially the density matrix has a *finite* number of nonvanishing eigenvalues $p_k(0)$ is necessary since the theorem we use in the proof is formulated in [5] for sums (33) with finite n.

The spectral decomposition of the density matrix

$$\rho_t = \sum_k p_k |k,t\rangle\langle k,t| \,, \tag{34}$$

(where $t \mapsto |k,t\rangle$ defines a one-parameter continuous family of orthonormal vectors) leads to the unitary (although ρ-dependent) transformation $|k,t\rangle = U(\rho_t,\rho_0)|k,0\rangle$. The density matrix then evolves as follows

$$\rho_t = U(\rho_t,\rho_0)\rho_0 U(\rho_t,\rho_0)^{-1} \,. \tag{35}$$

Let us remark finally that the Nambu-type dynamics of the density matrices induces the corresponding dynamics of various (linear or nonlinear) functions of ρ_a in a unique way. This concerns, in particular, partial traces which occur in decomposing systems into subsystems. It means that the operations of taking a partial trace over a subsystem and letting the system evolve commute. This property is, in general, non-evident if the dynamics is nonlinear [8].

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