ISSN 1064-5624, Doklady Mathematics, 2015, Vol. 91, No. 1, pp. 68–71. © Pleiades Publishing, Ltd., 2015.
Original Russian Text © T.S. Ratiu, O.G. Smolyanov, 2015, published in Doklady Akademii Nauk, 2015, Vol. 460, No. 4, pp. 385–388.

MATHEMATICS

Hamiltonian Structures in the Quantum Theory of Hamilton–Dirac Systems

T. S. Ratiu[a] and O. G. Smolyanov[b]

Presented by Academician V.V. Kozlov November 14, 2013

Received December 4, 2013

DOI: 10.1134/S1064562415010214

This paper discusses the Hamiltonian aspects of the quantum theory of constrained Hamiltonian systems; in particular, we extend results of [9, 6] to such systems. In this paper, we usually refer to these systems as Hamilton–Dirac systems, because it was Dirac who first defined them (under the name of generalized Hamiltonian systems). Such systems arise in the application of the Legendre transform to unconstrained Lagrangian systems with singular Lagrange function (for which the Legendre transform is noninvertible). It should be emphasized that constrained Hamiltonian systems bear no relation to Lagrangian systems with holonomic constraints; however, them can be regarded as objects dual to Lagrangian systems with nonholonomic constraints. Namely, the Legendre transform turns Lagrangian systems with nonholonomic constraints into unconstrained Hamiltonian systems with singular Hamilton function (for which the Legendre transform is noninvertible).

We introduce two types of Hamiltonian structures on quantum versions of Hamilton–Dirac systems. One of them determines a usual (but infinite-dimensional) Hamiltonian system, and the other determines an infinite-dimensional Hamilton–Dirac system. The Hamiltonian equation generated by the first structure coincides with the Schrödinger-type equation considered in [1]; the second structure leads to a system of Hamilton(–Dirac) equations coinciding with the system of Schrödinger-type equations considered in [5]. The corresponding Liouville and Liouville–Dirac equations (see below) determine the evolution of the probability distributions describing the states of the quantum versions of Hamilton–Dirac systems. Hamiltonian structures on the quantum versions of Hamilton–Dirac systems make it also possible to define, in a natural way, the secondary quantization of Hamilton–Dirac systems (as the quantization of such Hamiltonian structures; see [9]). Such an approach can also be applied to Hamilton–Dirac systems with interaction.

We also mention that, for (finite-dimensional) Hamilton–Dirac systems, an analogue of the Wigner function can be defined; its evolution is described by the system of "Moyal–Dirac equations," which is simultaneously a generalization of the Liouville–Dirac system describing the evolution of a nonquantized Hamilton–Dirac system and the Moyal equation describing the evolution of the quantum version of the classical unconstrained Hamiltonian system (see [5, p. 41 of the Russian translation; 7, Section 8.5; 8, Section 10.5] concerning the Dirac brackets). In the case of infinite-dimensional Hamilton–Dirac systems, instead of the Wigner function, the "Wigner measure" should be used.

This paper considers the algebraic aspects of the theory, and analytical assumptions are omitted.

1. NOTATION AND TERMINOLOGY

All locally convex topological vector spaces (LCSs) under consideration are assumed to be Hausdorff and either real or complex.[1] Given LCSs E_1 and E_2, by $\mathscr{L}^n(E_1, E_2)$ we denote the space of all continuous n-linear mappings of E_1 to E_2 endowed, unless otherwise specified, with the topology of uniform convergence on compact sets; $\mathscr{L}(E_1, E_2) := \mathscr{L}^1(E_1, E_2)$. The topological dual of an LCS E is denoted by E'; it is assumed that the topology on E' is compatible with the duality between E' and E. For $T \in \mathscr{L}(E_1, E_2)$, by $T^* \in \mathscr{L}(E_2', E_1')$ we denote its dual; if E_1 and E_2 are LCSs and $V \subseteq E_1$ is an open set, then a mapping $f\colon V \to E_2$ is said to be smooth if it is everywhere infinitely Gâteaux

[a] *Mathematics Section and Bernoulli Center, École Polytechnique Fédérale de Lausanne, Station 8, Lausanne, CH-1015 Switzerland*
e-mail: tudor.ratiu@epfl.ch

[b] *Mechanics and Mathematics Faculty, Moscow State University, Moscow, 119991 Russia*
e-mail: smolyanov@yandex.ru

[1] The definitions can largely be found in [1, 2].

differentiable (see, e.g., [3]) and, for any compact set $K \subset V$, the mapping $V \times K \times \ldots K \ni (x, h_1, h_2, ..., h_n) \mapsto f^{(n)}(x)(h_1, h_2, ..., h_n) \in E_2$ is continuous; here, $f^{(n)}(x) \in \mathscr{L}^n(E_1; E_2)$ denotes the nth Gâteaux derivative. We denote the set of all smooth mappings from an LCS E to an LCS G by $C^\infty(E, G)$.

An almost Poisson LCS is a pair $(E, \mathbb{J})$, where E is an LCS and $\mathbb{J}: E \to \mathscr{L}(E', E)$ is a smooth mapping such that $\mathbb{J}(x)^*(E') \subseteq E$ and $\mathbb{J}(x)^* = -\mathbb{J}(x)$ for all $x \in E$. If $f, g: E \to \mathbb{C}$ (or $E \to \mathbb{R}$, depending on whether E is a complex or real vector space) are smooth mappings, then the almost Poisson $\mathbb{J}$-bracket $\{f, g\}$ is defined as $\{f, g\}(x) := f'(x)(\mathbb{J}(x)g'(x))$. The $\mathbb{J}$-bracket $\{\cdot, \cdot\}$ is bilinear and skew-symmetric, and it satisfies the Leibniz rule with respect to each argument. For this bracket, the Jacobi identity holds if and only if $h_1[(\mathbb{J}'(x)\mathbb{J}(x)h_2)(h_3)] + h_2[(\mathbb{J}'(x)\mathbb{J}(x)h_3)(h_1)] + h_3[(\mathbb{J}'(x)\mathbb{J}(x)h_1)(h_2)] = 0$ for any $x \in E$ and $h_1, h_2, h_3 \in E'$. In this case, the $\mathbb{J}$-bracket is a Poisson bracket, and $(E, \mathbb{J})$ is called a Poisson LCS. If the mapping $\mathbb{J}(x)$ is invertible for each $x \in E$, then the preceding relation holds if and only if the differential 2-form $x \mapsto [(v_1, v_2) \mapsto (\mathbb{J}(x)^{-1}v_1)v_2]$ on E is closed. In this case, $(E, \mathbb{J})$ is called a symplectic LCS.

It turns out that statements can be shortened by using Poisson brackets for functions taking values in multidimensional vector spaces. These brackets can be defined as follows.

Suppose that $(E, \mathbb{J})$ is a symplectic LCS, $\{\cdot, \cdot\}$ is the Poisson bracket defined above, G_1 and G_2 are LCSs, and F_1 and F_2 are subspaces in $C^\infty(E, \mathbb{C})$; given $a \in G_1$, $b \in G_2$, $f \in F_1$, and $g \in F_2$, we set $(a \otimes f)(x) := f(x)a \in G_1$ and $(b \otimes g)(x) := g(x)b \in G_2$, so that $(a \otimes f, b \otimes g) \in C^\infty(E, G_1) \times C^\infty(E, G_2)$. The Poisson bracket $\{a \otimes f, b \otimes g\}$ is the mapping from E to $G_1 \otimes G_2$ defined by $\{a \otimes f, b \otimes g\}(x) := \{f, g\}(x)(a \otimes b)$, where $\{f, g\}$ is the Poisson bracket of the scalar functions. If G_3 is yet another LCS, then, for $f \in C^\infty(E, G_1)$, $g \in C^\infty(E, G_2)$, and $h \in C^\infty(E, G_3)$, the Jacobi identity holds; this means that, for all $x \in E$, we have $\{f, \{g, h\}\}(x) + \{g, \{h, f\}\}(x) + \{h, \{f, g\}\}(x) = 0$ in $G_1 \otimes G_2 \otimes G_3$ (we use the "associativity" of tensor product). The product $f \cdot g$ is defined by $(f \cdot g)(x) := f(x) \otimes g(x)$, so that $f \cdot g \in C^\infty(E, G_1 \otimes G_2)$. Moreover, the Leibniz rule $\{f, g \cdot h\} = \{f, g\} \cdot h + g \cdot \{f, h\} \in C^\infty(E, G_1 \otimes G_2 \otimes G_3)$ holds (here, we use the "associativity" and "commutativity" of tensor product). Therefore, it is natural to refer to the function $\{f, g\}$ as the Poisson bracket of the vector-valued functions f and g.

2. THE HAMILTON–DIRAC AND LIOUVILLE–DIRAC EQUATIONS

Definition 1. A Hamilton–Dirac system is a set $(E, \mathbb{J}, \mathscr{H}, \psi)$, where $(E, \mathbb{J})$ is a symplectic LCS, called the phase space of the Hamilton–Dirac system, $\mathscr{H}$ is a real- or complex-valued function on E, called the Hamilton function of the system, and ψ is a smooth mapping of the space E to an auxiliary LCS Z_ψ (both the mapping ψ and the set $\mathfrak{m}_\psi := \{x \in E \mid \psi(x) = 0\}$ are called constraints). It is also assumed that if $\psi(x) = 0$, then $\{\psi, \psi\}(x) = 0$ and $\{\mathscr{H}, \psi\}(x) = 0$ and that zero is a regular value of ψ.

Remark 1. This definition is a formalization of Dirac's definition of generalized Hamiltonian systems with constraints of the first class. These constraints may be primary or secondary, but this difference does not matter in the further considerations.

In what follows, we assume that $\mathbb{J}(x)$ does not depend on x, so that $\mathbb{J}(x) = \mathbb{J} \in \mathscr{L}(E', E)$ for all $x \in E$, where $\mathbb{J}^* = -\mathbb{J}$. Since $\mathbb{J}'(x) = 0$ for each $x \in E$, it follows that the $\mathbb{J}$-bracket is a Poisson bracket. Therefore, $(E, \mathbb{J})$ is a Poisson LCS and $C^\infty(E, \mathbb{C})$ is a Poisson algebra.

Definition 2. The Hamilton–Dirac equation for a Hamilton–Dirac system $(E, \mathbb{J}, \mathscr{H}, \psi)$ is the equation $f'(t) = \mathbb{J}((\mathscr{H}_E(t))'(f(t)))$ with respect to a function f: $\mathbb{R} \to \{x \in E \mid \psi(x) = 0\}$, where $\mathscr{H}_E(t) := \mathscr{H} + t\lambda(t)\psi$ (the function $\mathscr{H}_E(\cdot)$ is called the generalized Hamiltonian in [5]); the notation $(\mathscr{H}_E(t))'$ is used for the derivative of the function $\mathscr{H}_E(t)$: $E \to R$, and it is assumed that λ is an arbitrary function of t taking values in the space Z'_ψ.

Definition 3. The Liouville–Dirac system of equations is the system of equations $F(t) = \{\mathscr{H}_E, F(t)\}$, $\{\psi, F(t)\} = 0$ for a function $F(\cdot)$ of a real variable t taking values in the set of smooth functions on E; a solution of the Liouville–Dirac system is a function $F(\cdot)$ satisfying the equations of this system on the set m.

Proposition 1. *The Hamilton–Dirac equation is equivalent to the system of equations*

$$g'(t) = \mathbb{J}((\mathscr{H}_E(t))'(g(t))), \quad \psi(g(t)) = 0.$$

Remark 2. The relationship between the last system of equations and the Liouville–Dirac system is similar to that between an ordinary differential equation and the equation for its first integrals.

3. QUANTIZATION OF HAMILTON–DIRAC SYSTEMS

In this section, we define Schrödinger quantization of Hamilton–Dirac systems and describe a relationship between the quantum system thus obtained and Hamiltonian structures. First, we define pseudodifferential operators on the function spaces generated by the constraint $\mathfrak{m}_\psi$. We assume that E is the orthogonal sum $E = Q \oplus P$ of copies of $\mathbb{R}^n$ and $\mathrm{pr}_Q: E \to Q$ is the canonical projection. Let $S \subset E$ be a submanifold whose projection $\mathrm{pr}_Q(S)$ is a submanifold without boundary in Q, and let $\mathscr{F}_S$ be the vector space of Borel functions on S defined as follows: $\psi \in \mathscr{F}_S$ if and only if there exists a function $f_\psi \in L_2(\mathrm{pr}_Q(S))$ such that $\psi(q, p) = f_\psi(q)$ for all $(q, p) \in S$. We also assume that $\mathscr{F}_S$ is endowed with the Hilbert norm defined by $\|\psi\| :=$

$\|f_\psi\|_{L_2(\mathrm{pr}_Q(S))}$. Given a continuous function h on E and $\tau \in [0, 1]$, by $\mathcal{F}^h_S \subset \mathcal{F}_S$ we denote the vector space of all functions $\mathcal{F}_S$ for which the function $S \ni (q_1, p_1) \mapsto h((1-\tau)q + \tau q_1, p_1) e^{\mathrm{i}p_1(q-q_1)} \psi(q_1, p_1) \in \mathbb{C}$ is integrable over S at almost all $q \in \mathrm{pr}_Q(S)$ and the function $(q, p) \mapsto \int_S h((1-\tau)q + \tau q_1, p_1) e^{\mathrm{i}p_1(q-q_1)} \psi(q_1, p_1) dq_1 dp_1$ belongs to the space $\mathcal{F}_S$.

A pseudodifferential operator $\hat{h}^S_\tau$ on $\mathcal{F}^h_S$ with τ-symbol h is defined as follows: its domain is $D(\hat{h}^S_\tau) = \mathcal{F}^h_S$, and for $(q, p) \in S$, we set $(\hat{h}^S_\tau \psi)(q, p) := \int_S h((1-\tau)q + \tau q_1, p_1) e^{\mathrm{i}p_1(q-q_1)} (q_1, p_1) dq_1 dp_1$.

The mappings $h \mapsto \hat{h}^S_\tau$ can be called τ-quantizations; if $\tau = \frac{1}{2}$, then the corresponding τ-quantization is called a Weyl quantization, and we write $\hat{h}^S_W := \hat{h}^S_{1/2}$. This operator is symmetric, and in applications to quantum mechanics, its self-adjoint extensions are considered.

Remark 3. To the numerical Hamilton function h on the classical phase space (this function depends on $q \in Q$ and $p \in P$) the quantization operation assigns an operator being "the same" function of the noncommuting operators $\hat{q}$ and $\hat{p}$. Certainly, the function of noncommuting operators is determined nonuniquely, and the use of pseudodifferential operators is only one of the methods for constructing it. If $\tau = 0$, then $\hat{P}$ acts first; if $\tau = 1$, then $\hat{Q}$ acts first; in both cases, $\hat{h}_\tau$ may be nonsymmetric. One can say that, on $\hat{h}_W$, the operators $\hat{Q}$ and $\hat{P}$ act simultaneously, and this causes the operator $\hat{h}_W$ to be symmetric.

The pair $(E, \hat{\mathcal{H}})$ consisting of a Hilbert space E and a self-adjoint operator $\hat{\mathcal{H}} : E \to E$ is called a quantum system. Let $(E, \mathbb{J}, \mathcal{H}, \psi)$ be a Hamilton–Dirac system in which $E = Q \times P$, where Q and P are copies of $\mathbb{R}^n$, $\mathbb{J}$: $(\mathbf{p}, \mathbf{q}) \mapsto (\mathbf{q}, -\mathbf{p})$, and $\dim Z_\psi = k$, $2k < n$. Suppose that γ is another function on E taking values in an LCS and satisfying the following conditions (we can say that Z_γ determines a gauge):

(i) $\mathrm{Im}\,\psi'_2(\mathbf{q}, \mathbf{p}) = \mathbb{R}^k$ and $\mathrm{Im}\,\gamma'_1(\mathbf{q}, \mathbf{p}) = \mathbb{R}^k$ for all $\mathbf{q}$ and $\mathbf{p}$; the symbol ψ'_2 denotes the second partial derivative of ψ, and γ'_1 denotes the first partial derivative of γ;

(ii) $\mathrm{Rank}\{\gamma, \psi\}(x) = k$ for all $x \in E$; here, for each $x \in E$, $\{\gamma, \psi\}(x)$ denotes the Poisson bracket of vector-valued functions defined above.

Finally, we set $S(\gamma) := \{x \in E \mid \psi(x) = 0, \gamma(x) = 0\}$; we again assume that $S(\gamma)$ is a smooth manifold.

Definition 4 (cf. [1]). The quantum system $(\mathcal{F}_{S(\gamma)}, \hat{\mathcal{H}}^{S(\gamma)}_W)$ is called the Schrödinger γ-quantization of the Hamilton–Dirac system $(E, \mathbb{J}, \mathcal{H}, \gamma)$.

Remark 4. Sufficient conditions for the existence of the Schrödinger group $e^{\mathrm{i}t\hat{\mathcal{H}}^{S(\gamma)}_W}$ are given in [1].

Theorem 1. *For any functions γ_1 and γ_2 satisfying the above assumptions, there exists a unitary operator V_{γ_1, γ_2}: $\mathcal{F}_{S(\gamma_1)} \to \mathcal{F}_{S(\gamma_2)}$ such that $\hat{\mathcal{H}}^{S(\gamma_1)}_W = V^{-1}_{\gamma_1, \gamma_2} \hat{\mathcal{H}}^{S(\gamma_2)}_W V_{\gamma_1, \gamma_2}$.*

Since $\mathcal{F}_{S(\gamma)}$ is a complex Hilbert space, it follows that the imaginary part or inner product with the minus sign determines a symplectic structure on $\mathcal{F}_{S(\gamma)}$ (see, e.g., [4, 6, 7, 9]), which then generates the corresponding Hamiltonian equations and Liouville equations with respect to probability measures on $\mathcal{F}_{S(\gamma)}$. The following theorem describes the role of the choice of the function γ.

Theorem 2. *Let ν_{γ_1} and ν_{γ_2} be solutions of the Liouville equations with respect to time-dependent probabilities on $\mathcal{F}_{S(\gamma_1)}$ and $\mathcal{F}_{S(\gamma_2)}$, respectively. Suppose that there exists a unitary transformation V_{γ_1, γ_2}: $\mathcal{F}_{S(\gamma_1)} \to \mathcal{F}_{S(\gamma_2)}$ for which $(V_{\gamma_1, \gamma_2})_* \nu_{\gamma_1}(0) = \nu_{\gamma_2}(0)$ ($V_*\mu$ denotes the image of a measure μ under the transformation V).*

Then $(V_{\gamma_1, \gamma_2})_* \nu_{\gamma_1}(t) = \nu_{\gamma_2}(t)$ for all t.

4. SECONDARY QUANTIZATION OF HAMILTON–DIRAC SYSTEMS

The secondary quantization of Hamilton–Dirac systems (without interaction) can be defined by analogy with the case of classical Hamiltonian systems (without interaction) as the quantization of the Hamiltonian system $(\mathcal{F}_{S(\gamma)}, \mathbb{J}_{S(\gamma)}, \mathcal{H}^{S(\gamma)}_W)$, where $\mathbb{J}_{S(\gamma)}$ and $\mathcal{H}^{S(\gamma)}_W$ are, respectively, the symplectic structure and the Hamilton function defined as in [9].

However, the secondary quantization of Hamilton–Dirac systems with interaction has some special features. As in the classical case, a family of n identical finite-dimensional (the finite-dimensionality assumption is inessential) Hamilton–Dirac systems $(E, \mathbb{J}, \mathcal{H}, \psi)$ with $E = Q \times P$ is considered, and it is assumed that the interaction is described by a real-valued function h defined on the Cartesian product of n copies of E. It is also assumed that, for any $n - 1$ fixed elements $x_1, x_2, \ldots, x_{k-1}, x_{k+1}, \ldots \ldots, x_n \in E$,

$$\{h(x_1, x_2, \ldots, x_{k-1}, \cdot, x_{k+1}, \ldots, x_n), \psi\} = 0.$$

After that, we proceed as in the classical case studied in [9].

The quantization of Hamilton–Dirac systems described above differs from the quantization suggested by Dirac himself. We briefly describe Dirac's approach below. Let $(E, \mathbb{J}, \mathcal{H}, \psi)$ be a Hamilton–Dirac system (as above, we assume that $E = Q \oplus P$, where Q and P are copies of $\mathbb{R}^n$). We endow the space $E_D := L_2(Q, \mathbb{C})$ with a Hamiltonian structure for which the Hamiltonian equation is the Schrödinger equation with Hamiltonian $\hat{\mathcal{H}}_W$ (so that the corresponding Hamilton function is defined by $\mathcal{H}_D(g) := -\frac{i}{2}(\hat{\mathcal{H}}_W(g), g)$, where $g \in E_D$). We also assume that Z'_ψ is reflexive and, for each $k \in Z'_\psi$, the function Ψ^k is defined by $E_D \ni g \mapsto ((\widehat{k \circ \Psi})_W g, g)$. Then there exists a function Ψ_W: $E_D \to Z_\psi$ such that, for any $g \in E_D$ and $k \in Z'_\psi$, we have $k(\Psi_W(g)) = \Psi^k(g)$. Moreover, the quadruple $(E_D, \mathbb{J}_D, \mathcal{H}_D, \Psi_W)$ is an (infinite-dimensional) Hamilton–Dirac system.

Theorem 3. *The Hamilton–Dirac system of equations for the system* $(E_D, \mathbb{J}_D, \mathcal{H}_D, \Psi_W)$ *is equivalent to the following system of equations from* [5]:

$$i\frac{\partial f}{\partial t} = \hat{\mathcal{H}}_D f(t); \quad (\widehat{k \circ \Psi})_W f(t) = 0$$

for each $k \in Z'_\psi$.

Remark 5. It would be interesting to give a detailed proof of the equivalence (in an appropriate sense) of the last system of equations and the Schrödinger equation for the quantum system specified in Definition 4.

ACKNOWLEDGMENTS

This work was supported by the Government of Russian Federation, decree no. 220 (contract no. 11.G34.31.0054 between the Ministry of Education and Science of Russian Federation and Lomonosov Moscow State University). T.S. Ratiu acknowledges the support of Swiss National Science Foundation, grant no. 200021–140238. O.G. Smolyanov acknowledges the support of the Bernoulli Center, Federal Polytechnic School of Lausanne, where a major part of the work was completed, and the Russian Foundation for Basic Research (project no. 14-01-00516).

REFERENCES

1. S. Albeverio and O. G. Smolyanov, Dokl. Math. **67**, 411–415 (2003).
2. S. Albeverio, O. G. Smolyanov, and A. Yu. Khrennikov, Dokl. Math. **64**, 321–325 (2001).
3. V. I. Bogachev and O. G. Smolyanov, *Real and Functional Analysis* (Izhevsk, 2011) [in Russian].
4. P. R. Chernoff and J. E. Marsden, *Some Basic Properties of Infinite Dimensional Hamiltonian Systems* (Springer-Verlag, Berlin, 1974).
5. P. A. M. Dirac, *Lectures on Quantum Mechanics* (Yeshiva Univ., New York, 1964; Mir, Moscow, 1968).
6. V. V. Kozlov and O. G. Smolyanov, Dokl. Math. **85**, 416–420 (2012).
7. J. E. Marsden and T. S. Ratiu, *Introduction to Mechanics and Symmetry* (Springer-Verlag, Berlin, 1994).
8. J.-P. Ortega and T. S. Ratiu, *Momentum Maps and Hamiltonian Reduction* (Birkhäuser, Boston, Mass., 2004).
9. T. S. Ratiu and O. G. Smolyanov, Dokl. Math. **87**, 289–292 (2013).

Translated by O. Sipacheva