Symplectic Structures and Quantum Mechanics

by

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Abstract

Canonical coordinates for the Schrödinger equation are introduced, making more transparent its Hamiltonian structure. It is shown that the Schrödinger equation, considered as a classical field theory, shares with Liouville completely integrable field theories the existence of a recursion operator which allows for the infinitely many conserved functionals pairwise commuting with respect to the corresponding Poisson bracket.

The approach may provide a good starting point to get a clear interpretation of Quantum Mechanics in the general setting, provided by Stone-von Neumann theorem, of Symplectic Mechanics. It may give new tools to solve in the general case the inverse problem of quantum mechanics whose solution is given up to now only for one-dimensional systems by the Gel’fand-Levitan-Marchenko formula.

1 Introduction.

In the past few years there has been a renewed interest in completely integrable Hamiltonian systems, specially in connection with the study of integrable quantum field theory, Yang-Baxter algebras and, more recently, quantum groups.

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Loosely speaking, completely integrable Hamiltonian systems are dynamical systems admitting a Hamiltonian description and possessing sufficiently many constants of motion so that they can be integrated by quadratures.

For two-dimensional field theories, a priori criteria of integrability, have been established only by methods more directly related to group theory and to familiar procedures of classical mechanics, looking at such systems as dynamics on (infinite-dimensional) phase manifold.

This point of view was also suggested by the occurrence in such models of a peculiar operator, the so called recursion operator, relevant for the effectiveness of the method, which naturally fits in this geometrical setting as a mixed tensor field on the phase manifold M.

In terms of such an operator the classical Liouville theorem on the integrability can be extended also to the infinite dimensional case. The same operator can be used to deal with Burgers equation.

Some years ago it was suggested the use of complex canonical coordinates in the formulation of a generalized dynamics including classical and quantum mechanics as special cases. In the same spirit a somehow dual viewpoint is proposed: rather than to complexify classical mechanics it is useful to give a formulation of quantum mechanics in terms of realified vector spaces.

By using the Stone-von Neumann theorem a quantum mechanical system is associated with a vector field on some Hilbert space (Schrödinger picture) or a vector field, i.e. a derivation, on the algebra of observables (Heisemberg picture).

In classical mechanics the analog infinitesimal generator of canonical transformations is a vector field on a symplectic manifold (the phase space).

Therefore, if we want to use similar procedures, we need to real off $L_2(Q, C)$, the Hilbert space of square integrable complex functions defined on the configuration space $Q$, as a symplectic manifold or, more specifically, as a cotangent bundle. We shall see that it can be considered as $T^*(L_2(Q, R))$, $L_2(Q, R)$ denoting the Hilbert space of square integrable real functions defined on $Q$.

This approach is different from previous ones also dealing with the integrability of quantum mechanical system in the Heisemberg and Schrödinger picture.
In order to make more transparent the geometrical and the physical content of the paper difficult technical aspects, which are however important in the context of infinite dimensional manifold, as, for instance, the distinction between weakly and strongly not degenerate bilinear forms, or the inverse of a Schrödinger operator and so on, will not be addressed. We shall limit ourselves to observe that no serious difficulties arise working on an infinite dimensional manifold whose local model is a Banach space, as in that case the implicit function theorem still holds true.

2 Complete Integrability and Recursion Operators

Complete integrability of Hamiltonian systems with finitely many degrees of freedom is exhaustively characterized by the Liouville-Arnold theorem. An alternative characterization which may apply also to systems with infinitely many degrees of freedom can be given as follows. Let \( M \) denote a smooth differentiable manifold, \( \mathcal{X}(M) \) and \( \Lambda(M) \) vector and covector fields on \( M \). With any \((1,1)\) tensor field \( T \) on \( M \), two endomorphisms

\[
\hat{T} : \mathcal{X}(M) \to \mathcal{X}(M) \quad \text{and} \quad \check{T} : \Lambda(M) \to \Lambda(M)
\]

are associated:

\[
T(a,X) = \langle \alpha, \hat{T}X \rangle = \langle \check{T}a, X \rangle,
\]

with \( X \) and \( \alpha \) belonging to \( \mathcal{X}(M) \) and \( \Lambda(M) \) respectively. The Nijenhuis tensor, or torsion, of \( T \) is the \((1,2)\) tensor field defined by:

\[
N_T(\alpha, X, Y) = \langle \alpha, H_T(X,Y) \rangle
\]

with the vector field \( H_T(X,Y) \) given by:

\[
H_T(X,Y) = [\mathcal{L}_X \hat{T}T - \hat{T} \mathcal{L}_X T] Y
\]

\( \mathcal{L}_X \) denoting the Lie’s derivative with respect to \( X \).

Integrability Criterion

A dynamical vector field \( \Delta \) which admits an invariant mixed tensor field \( T \), with vanishing Nijenhuis tensor \( N_T \) and bidimensional eigenspaces, completely separates

\footnote{The vector field \( \Delta \) is not supposed to be Hamiltonian. Its Hamiltonian structure is generated by the hypothesis of the bidimensionality of the eigenspaces of \( T \) and \( d\lambda \neq 0 \).}
in 1-degree of freedom dynamics. The ones associated with those degrees of freedom whose corresponding eigenvalues $\lambda$ are not stationary, are integrable and Hamiltonian $^4$.

An idea of the proof is given observing that the bidimensionality of eigenspaces of $T$ and the condition $N_T = 0$ imply the following form for $T$

$$T = \sum_i \lambda_i \left( \frac{\delta}{\delta \sigma^i} \otimes \delta \lambda^i + \frac{\delta}{\delta \sigma^i} \otimes \delta \phi^i + \frac{\delta}{\delta \sigma^i} \otimes \delta \phi^i \right) + \sum_{\ell=1}^2 \int_0^k dk \ k \frac{\delta}{\delta \psi^\ell_k} \otimes \delta \psi^\ell(k)$$

The invariance of $T \ (L_{\Delta} T = 0)$ implies for $\Delta$ the form

$$\Delta = \sum_{i=1}^n \Delta^i(\lambda^i) \frac{\delta}{\delta \phi^i} + \sum_{\ell=1}^2 \int dk \Delta^\ell(k) \left( \psi^1(k), \psi^2(k) \right) \frac{\delta}{\delta \psi^\ell(k)}$$

whose associated equations are:

$$\dot{\psi}^1(k) = \Delta^{1,k}(\psi^1(k), \psi^2(k))$$
$$\dot{\psi}^2(k) = \Delta^{2,k}(\psi^1(k), \psi^2(k))$$
$$\dot{\phi}^i = \Delta^i(\lambda^i)$$
$$\dot{\lambda}^i = 0$$

For the discrete part of the spectrum of $T$ a symplectic form $\omega_0$ can be defined $\omega_0 = \sum_i f_i(\lambda^i) \delta \lambda^i \wedge \delta \phi^i$ with respect to which the dynamics is a Hamiltonian one.

In next section the mentioned geometrical structures will be exhibited for the Schrödinger equation.

### 3 Canonical Coordinates for the Schrödinger equation

Although in an infinite dimensional symplectic manifold a Darboux’s chart, $a priori$ does not exist, for the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + U(r) \psi,$$  \hspace{1cm} (4)

natural canonical coordinates $p$ and $q$ can be introduced.

We introduce the real and the imaginary part of the wave function $\psi$:

$$\begin{align*}
\{ p(r, t) &= \text{Im} \psi(r, t) \\
q(r, t) &= \text{Re} \psi(r, t) \}
\end{align*}$$
and in this way $L_2(Q, C)$ is considered as the cotangent bundle of $L_2(Q, R)$.

In these new coordinates, equation (4) takes the form:

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta H_1 \\ \delta H_0 \end{pmatrix}$$  \hspace{1cm} (5)

where $H_1$ is defined by:

$$H_1[q, p] := \frac{1}{2} \int dr \left\{ \frac{\hbar^2}{m} [(\nabla p)^2 + (\nabla q)^2] + U(r)(p^2 + q^2) \right\}$$  \hspace{1cm} (6)

and $\frac{\delta H}{\delta q}, \frac{\delta H}{\delta p}$ denote the components of the gradient of $H[q, p]$ with respect to the real $L_2$ scalar product.

Our system is then a Hamiltonian dynamical system with respect to the Poisson bracket defined for any two functionals $F[q, p]$ and $G[q, p]$ by:

$$\Lambda_1(\delta F, \delta G) := \{F, G\}_1 := \frac{1}{\hbar} \int dr \left( \frac{\delta F}{\delta q} \cdot \frac{\delta G}{\delta p} - \frac{\delta F}{\delta p} \cdot \frac{\delta G}{\delta q} \right)$$  \hspace{1cm} (7)

What is less known is that the previous one is not the only possible Hamiltonian structure. As matter of fact the Schrödinger equation can also be written as:

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -\mathcal{H} \\ \mathcal{H} & 0 \end{pmatrix} \begin{pmatrix} \delta H_0 \\ \delta H_0 \end{pmatrix}$$  \hspace{1cm} (8)

where $H_0$ is defined by:

$$H_0[q, p] := \frac{1}{2} \int dr (p^2 + q^2)$$  \hspace{1cm} (9)

and $\mathcal{H}$ is the Schrödinger operator:

$$\mathcal{H} := -\frac{\hbar^2}{2m} \Delta + U(r)$$  \hspace{1cm} (10)

It is then again a Hamiltonian dynamical systems with a new Poisson bracket of any two functionals $F[q, p]$ and $G[q, p]$ given by:

$$\Lambda_0(\delta F, \delta G) := \{F, G\}_0 := \int dr \left( \frac{\delta F}{\delta q} \cdot \mathcal{H} \frac{\delta G}{\delta p} - \frac{\delta F}{\delta p} \cdot \mathcal{H} \frac{\delta G}{\delta q} \right)$$  \hspace{1cm} (11)

So, with the same vector field, we have two choices:
• A phase manifold with a universal symplectic structure:

\[ \omega_1 := \hbar \int d\mathbf{r} (\delta p \wedge \delta q) \] (12)

and a Hamiltonian functional depending on the classical potential.

• A phase manifold with a symplectic structure determined by the classical potential

\[ \omega_0 := \hbar \int d\mathbf{r} (\mathcal{H}^{-1} \delta p \wedge \delta q) \] (13)

and the universal Hamiltonian functional representing the quantum probability.

The two brackets satisfy the Jacobi Identity, as the associated 2-forms are closed for they do not depend on the point \((\psi \equiv (p, q))\) of the phase space.

We have then the relation:

\[ \frac{\delta H_1}{\delta u} = \tilde{T} \frac{\delta H_0}{\delta u} \] (14)

where:

\[ \tilde{T} := \Lambda_1^{-1} \circ \Lambda_0 = \begin{pmatrix} \mathcal{H} & 0 \\ 0 & \mathcal{H} \end{pmatrix} \] (15)

and

\[ \frac{\delta H}{\delta u} = \begin{pmatrix} \frac{\delta H}{\delta p} \\ \frac{\delta H}{\delta \psi} \end{pmatrix} \] (16)

As the tensor field \(T\) does not depend on the point \((\psi \equiv (p, q))\) of the phase space, its torsion is identically zero, so that the relation (14) can be iterated to:

\[ \frac{\delta H_n}{\delta u} = \tilde{T}^n \frac{\delta H_0}{\delta u} \] (17)

It turns out that the Schrödinger equation admits infinitely many conserved functionals defined by:

\[ H_n[q, p] := \frac{1}{2} \int d\mathbf{r} (p \mathcal{H}^n p + q \mathcal{H}^n q) \equiv \int d\mathbf{r} (\bar{\psi} \mathcal{H}^n \psi) \] (18)

They are all in involution with respect to the previous Poisson brackets:

\[ \{H_n, H_m\}_0 = \{H_n, H_m\}_1 = 0 \] (19)
This situation generalizes the one for finite dimensional Hamiltonian systems \(^4\). It is worth to stress that for smooth potentials \(U(x)\) in one space dimension, the eigenvalues of the Schrödinger operator \(\mathcal{H}\) are not degenerate and so the eigenvalues of \(T\) are double degenerate.

### 3.1 The eikonal transformation

The transformation:

\[
\begin{align*}
\{ p(r, t) &= A(r, t) \sin S(r, t) \hbar^{-1} \\
q(r, t) &= A(r, t) \cos S(r, t) \hbar^{-1} 
\end{align*}
\]  

(20)

is a canonical transformation between the \((p, q)\) coordinates and \((\pi = S(2\hbar)^{-1} J, \chi = A^2)\), as:

\[\delta p \wedge \delta q = \delta \left( \frac{S}{2\hbar} \right) \wedge \delta A^2 \]  

(21)

The Hamiltonian \(H_1\) becomes:

\[K_1[\chi, \pi] = \int dr \left\{ \frac{\hbar^2}{2m} \left( \frac{(\nabla \chi)^2}{4\chi} + 4\chi(\nabla \pi)^2 \right) + U\chi \right\} \]  

(22)

and Hamilton’s equations:

\[
\begin{cases}
\frac{\partial \pi}{\partial t} = -\frac{1}{\hbar} \frac{\delta K_1}{\delta \chi} \\
\frac{\partial \chi}{\partial t} = \frac{1}{\hbar} \frac{\delta K_1}{\delta \pi}
\end{cases}
\]  

(23)

give:

\[
\begin{cases}
\frac{\partial \pi}{\partial t} = \frac{\hbar}{2m} \frac{\Delta \sqrt{\chi}}{\sqrt{\chi}} - \frac{\hbar}{m} (\nabla \pi)^2 - U\hbar^{-1} \\
\frac{\partial \chi}{\partial t} = \frac{2\hbar}{m} \text{div}(\chi \nabla \pi)
\end{cases}
\]  

(24)

where \(P = \chi\) and \(J = \hbar \chi \frac{\nabla S}{m}\) represent the probability density and the current density respectively.

This transformation being nonlinear will transform previous biHamiltonian descriptions into a mutually compatible pair of nonlinear type. They are of \(C\)-type as introduced by Calogero \(^{17}\).
3.2 The quantum Lagrangians

Having considered equations of motion for a quantum system as equations for the integral curves of a vector field on a cotangent bundle, it is a natural question to ask if this vector field may be associated with a Lagrangian vector field on a tangent bundle.

This question for a Lagrangian Schrödinger Equation can be answered as follows: From equation (5) one gets Hamilton’s equations:

\[
\begin{align*}
\frac{\partial p}{\partial t} &= -\frac{i}{\hbar} \mathcal{H} q \\
\frac{\partial q}{\partial t} &= \frac{i}{\hbar} \mathcal{H} p
\end{align*}
\] (25)

from which we derive the second order equation:

\[
\frac{\partial^2 q}{\partial t^2} = -\frac{1}{\hbar^2} \mathcal{H}^2 q
\] (26)

The latter is the Euler-Lagrange equation associated with the Lagrangian functional:

\[
L_1[q] = \frac{1}{2} \int dr dt (q_t^2 - \frac{1}{\hbar^2} q^2 \mathcal{H}^2 q)
\] (27)

Of course the Legendre transformation

\[
\pi = \frac{\delta L_1}{\delta q_t}
\] (28)

does not give the Hamilton’s equation (25) but the related one:

\[
\begin{align*}
\frac{\partial \pi}{\partial t} &= -\frac{i}{\hbar} \mathcal{H}^2 q \\
\frac{\partial \pi}{\partial q} &= \pi
\end{align*}
\] (29)

Equations (25) follows straightforward from the Lagrangian \( L_0 \) given by:

\[
L_0[q] = \frac{1}{2} \int dr dt (q_t \mathcal{H}^{-1} q_t - \frac{1}{\hbar^2} q \mathcal{H} q)
\] (30)

Of course \( L_0 \) is the Lagrangian which gives rise to the \( \omega_0 \) symplectic form and that:

\[
\frac{\delta L_1}{\delta q} = \mathcal{H} \frac{\delta L_0}{\delta q} ; \quad \frac{\delta L_1}{\delta q_t} = \mathcal{H} \frac{\delta L_0}{\delta q_t}
\] (31)

or equivalently:
\[
\frac{\delta L_1}{\delta v} = \hat{T} \frac{\delta L_0}{\delta v}
\]  

(32)

where

\[
\frac{\delta L}{\delta v} := \left( \begin{array}{c} \frac{\delta L}{\delta q} \\ \frac{\delta L}{\delta q} \end{array} \right)
\]  

(33)

It is also clear that, as in the case of the Hamiltonian functionals, relation (32) can be iterated to give alternative Lagrangian descriptions.

4 Conclusions

It has been shown as the Schrödinger equation, considered as a vector field on an infinite dimensional vector space, admits more than one Hamiltonian formulation. Really it admits infinitely many alternative Hamiltonian descriptions in terms of

\[
H_n[q,p] := \frac{1}{2} \int d\mathbf{r} (p \hat{H}^n p + q \hat{H}^n q) \equiv \int d\mathbf{r} (\bar{\psi} \hat{H}^n \psi)
\]  

(34)

and

\[
\omega_n := \hbar \int d\mathbf{r} (\hat{H}^{n-1} \delta p \wedge \delta q).
\]  

(35)

providing us with the same vector field:

\[
\Delta := \frac{1}{\hbar} \int d\mathbf{r} (\hat{H} p \frac{\delta}{\delta q} - \hat{H} q \frac{\delta}{\delta p})
\]  

(36)

defined by:

\[
i_\Delta \omega_n := -\delta H_n,
\]  

(37)

These are associated with the Lagrangians

\[
L_n[q] = \frac{1}{2} \int d\mathbf{r} dt (q_t \hat{H}^{n-1} q_t - \frac{1}{\hbar^2} q \hat{H}^{n+1} q)
\]  

(38)

whose gradients are generated by the tensor field \( T \).

Even though our construction is a formal one, it is understood that the construction applies to any bounded, invertible operator \( \hat{\mathcal{H}} \).

Finally, it is worth to stress that the Schrödinger equation, in spite of its linearity, shows that the class of completely integrable field theories in higher dimensional
spaces is not empty. Moreover, previous analysis appears to be interesting also in the formulation of variational principles \(^{18}\) for stochastic mechanics.

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References


