Liouville Integrability of the Schrödinger Equation

by

Gaetano Vilasi

Dipartimento di Fisica Teorica e smsa, Università di Salerno, Via S. Allende, I-84081 Baronissi (SA), Italy. (vilasi@salerno.infn.it)
Istituto Nazionale di Fisica Nucleare, Sezione di Napoli, Italy. medskip
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Abstract

Canonical coordinates for both the Schrödinger and the nonlinear Schrödinger equations are introduced, making more transparent their Hamiltonian structures. It is shown that the Schrödinger equation, considered as a classical field theory, shares with the nonlinear Schrödinger, and more generally with Liouville completely integrable field theories, the existence of a recursion operator which allows for the construction of 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.
Introduction

Last two decades have shown the exciting prospects of tackling nonlinear field theories in two space-time dimensions nonperturbatively by exploiting their complete integrability properties [15, 9].

Relevant progresses in the analysis of these systems were the introduction of the Lax Representation [22], the Zakharov-Shabat scheme [19] and AKNS method [20, 5].

Lax Representation played an important role in formulating the inverse scattering method [29] which allows for the solution of the Cauchy problem by means of the Gel’fand-Levitan-Marchenko formula [18, 27].

A universal feature of almost such systems is that they are Hamiltonian systems with infinitely many degrees of freedom [17]. The inverse scattering method was then read as a canonical transformation from generic coordinates (potentials) to action-angle variables [17].

This fact made it only natural a formulation of a priori criteria of integrability, by methods more directly related to Group Theory [32, 29] and to familiar procedures of Classical Mechanics, looking at such systems as dynamics on (infinite-dimensional) phase manifold [30, 25, 26].

This point of view was also suggested by the occurrence in such models of a peculiar operator, the so-called recursion operator [22], 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 [11].

It will be shown that, in complete analogy with the case of the nonlinear Schrödinger equation, such an invariant tensor field exists for the Schrödinger equation too.

Some years ago it was suggested [33] the use of complex canonical coordinates in the formulation of a generalised dynamics including classical and quantum mechanics as special cases. In the same spirit a somehow dual viewpoint is proposed: to formulate 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 (Heisenberg picture).

In Classical Mechanics the analogous infinitesimal generator of canonical transformations is a vector field on a symplectic manifold (the phase space).

In order to use the familiar procedures of Classical mechanics, 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 $T^*(L_2(Q, R))$. 
$L_2(Q, \mathbb{R})$ denoting the Hilbert space of square integrable real functions defined on $Q$.

The approach is different from previous ones [21, 2, 8, 6] also dealing with the integrability of quantum mechanical systems in the Heisenberg 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. First section deals with Liouville integrability, the second one with the Schrödinger equation and last with the nonlinear one.

1 Complete Integrability and Recursion Operators

Complete integrability of Hamiltonian systems with finitely many degrees of freedom is exhaustively characterised by the Liouville-Arnold theorem [23, 31, 1]. An alternative characterisation 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 $\hat{T}$: $\mathcal{X}(M) \rightarrow \mathcal{X}(M)$ and $\check{T}$: $\Lambda(M) \rightarrow \Lambda(M)$ are associated:

$$T(\alpha, X) = <\alpha, \hat{T}X > = <\check{T}\alpha, X > \tag{1}$$

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:

$$N_T(\alpha, X, Y) = <\alpha, H_T(X, Y) > \tag{2}$$

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

$$H_T(X, Y) = [\mathcal{L}_X \hat{T} - \hat{T} \mathcal{L}_X]Y \tag{3}$$

$\mathcal{L}_X$ 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 in 1-degree of freedom dynamics. The ones associated with $\Delta$ are not supposed to be Hamiltonian. Its Hamiltonian structure is generated by the hypothesis of the bidimensionality of the eigenspaces of $T$ and $d\lambda \neq 0$. 

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those degrees of freedom whose corresponding eigenvalues $\lambda$ are not stationary, are integrable and Hamiltonian \[10, 12, 13, 24\].

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 $T$

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

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

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

whose associated equations are:

$\dot{\psi}^1(k) = \Delta_1^1(k) (\psi^1(k), \psi^2(k))$

$\dot{\psi}^2(k) = \Delta_2^1(k) (\psi^1(k), \psi^2(k))$

$\dot{\phi}^i = \Delta_i^i(\lambda^i)$

$\dot{\lambda}^i = 0$

In other words the eigenvalues of $T$ define a privileged coordinates frame reducing to quadratures all its automorphisms, i.e. all dynamics that leave it invariant.

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

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

## 2 Canonical Coordinates for the Schrödinger Equation

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

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

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:

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta H_p \\ \delta H_q \end{pmatrix} \quad (5)$$
where $H_1$ is defined by:

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

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -\mathcal{H} \\ \mathcal{H} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H_0}{\delta p} \\ \frac{\delta H_0}{\delta q} \end{pmatrix}$$  \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 $H$ is the Schrödinger operator:

$$\mathcal{H} := -\frac{\hbar^2}{2m} \triangle + U(r)$$  \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:

$$\omega_1 := \hbar \int dr (\delta p \wedge \delta q)$$  \hspace{1cm} (12)$$

and a Hamiltonian functional depending on the classical potential.

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

$$\omega_0 := \hbar \int dr (\mathcal{H}^{-1} \delta p \wedge \delta q)$$  \hspace{1cm} (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:

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

where:

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

(15)

and

\[
\frac{\delta H}{\delta u} = \begin{pmatrix} \frac{\delta H}{\delta q} \\ \frac{\delta H}{\delta p} \end{pmatrix}
\]

(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:

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

(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)

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.

### 2.1 The eikonal transformation

The transformation:

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

(20)

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

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

(21)

The Hamiltonian \( H_1 \) becomes:

\[
\tilde{H}_1[\chi, \pi] = \int \text{d}r \frac{h^2}{2m} \left( \frac{(\nabla \chi)^2}{4\chi} + 4\chi (\nabla \pi)^2 \right) + U \chi
\]

(22)
and Hamilton’s equations:
\[
\begin{align*}
\frac{\partial \pi}{\partial t} &= -\frac{i}{\hbar} \delta \tilde{H} \frac{\delta \chi}{\delta \pi}, \\
\frac{\partial \chi}{\partial t} &= \frac{i}{\hbar} \delta \tilde{H} \frac{\delta \chi}{\delta \pi},
\end{align*}
\]
(23)
give:
\[
\begin{align*}
\frac{\partial \pi}{\partial t} &= \frac{\hbar}{2m} \frac{\Delta \sqrt{\chi}}{\sqrt{\chi}} - \frac{\hbar}{m} (\nabla \pi)^2 - U \hbar^{-1} \\
\frac{\partial \chi}{\partial t} &= -\frac{2\hbar}{m} \text{div}(\chi \nabla \pi)
\end{align*}
\]
(24)
where \( P = \chi \) and \( J = \hbar \chi \frac{\nabla \Sigma}{m} \) 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 [4].

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.

3 The nonlinear Schrödinger equation

The two-dimensional nonlinear Schrödinger equation:
\[
i \hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \psi_{xx} + b |\psi|^2 \psi,
\]
(25)
in the canonical coordinates
\[
\begin{align*}
\{ p(x, t) = \text{Im} \psi(x, t) \\
q(x, t) = \text{Re} \psi(x, t)
\end{align*}
\]
takes the form:
\[
\begin{pmatrix}
p \\
q
\end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta K_1 \\ \delta \pi \end{pmatrix}
\]
(26)
where \( K_1 \) is defined by:
\[
K_1[q, p] := \frac{1}{2} \int dx \left\{ \frac{\hbar^2}{2m} [(\partial_x p)^2 + b(\partial_x q)^2] + (p^2 + q^2) \right\}
\]
(27)
It is then a Hamiltonian dynamical system with respect to the canonical Poisson bracket \( \Lambda_1 \) defined in [5]:
\[
\Lambda_1(\delta F, \delta G) := \{ F, G \}_1 := \frac{1}{\hbar} \int dx \left( \frac{\delta F}{\delta q} \cdot \frac{\delta G}{\delta p} - \frac{\delta F}{\delta p} \cdot \frac{\delta G}{\delta q} \right)
\]
(28)
The previous one is not the only possible Hamiltonian structure. As matter of fact the nonlinear Schrödinger equation can also be written as:
\[ \frac{d}{dt} \left( \begin{array}{c} q \\ p \end{array} \right) = \mathcal{H}_N \left( \begin{array}{c} \delta K_0 \\ \delta p \end{array} \right) \] (29)

where \( \mathcal{H}_N \) is the Poisson operator:

\[
\mathcal{H}_N = \frac{1}{\hbar} \begin{pmatrix}
-\frac{2 \alpha q D^{-1} p}{\sqrt{2m}} & -2 \alpha p D^{-1} q \\
-2 \alpha q D^{-1} p & -\frac{2 \alpha p D^{-1} q}{\sqrt{2m}}
\end{pmatrix}
\] (30)

with \( \alpha = b \sqrt{2m} \), and

\[ D^{-1} := \frac{1}{2} \left( \int_{-\infty}^{\infty} - \int_{x}^{\infty} \right) ; \quad K_0[q, p] := \frac{\hbar}{\sqrt{2m}} \int dx(qp_x) \] (31)

It is then again a Hamiltonian dynamical system with a new Poisson bracket \( \{ \} \) of any two functionals \( F[q, p] \) and \( G[q, p] \) given by:

\[
\Lambda_2(\delta F, \delta G) := \{ F, G \}_2 := \int dx \left( \frac{\delta F}{\delta q} \cdot \mathcal{H}_N \frac{\delta G}{\delta p} - \frac{\delta F}{\delta p} \cdot \mathcal{H}_N \frac{\delta G}{\delta q} \right)
\] (32)

Once again, with the same vector field, we have two choices:

- A phase manifold with the canonical symplectic structure:

\[ \omega_1 \equiv \Lambda_1^{-1} := \hbar \int dx (\delta p \wedge \delta q) \] (33)

and a Hamiltonian functional accounting for the interaction.

- A phase manifold with a symplectic structure determined by the interaction

\[ \omega_2 \equiv \Lambda_2^{-1} := \hbar \int dx (\mathcal{H}_N^{-1} \delta p \wedge \delta q) \] (34)

and a free Hamiltonian functional given by the mean value of the momentum \( \hat{p} = -i\hbar \partial_x \).

We have then the relation:

\[ \frac{\delta K_1}{\delta u} = \hat{T}_N \frac{\delta K_0}{\delta u} \] (35)

where:

\[
\hat{T} := \Lambda_1^{-1} \circ \Lambda_2 = \begin{pmatrix}
-\frac{2 \alpha q D^{-1} p}{\sqrt{2m}} & -2 \alpha p D^{-1} q \\
-2 \alpha q D^{-1} p & -\frac{2 \alpha p D^{-1} q}{\sqrt{2m}}
\end{pmatrix}
\] (36)

\[ ^4 \text{For simplicity the proof that } \Lambda_2 \text{ satisfy the Jacobi Identity is omitted.} \]
It can be shown that the sum $\Lambda_2 + \Lambda_1$ is again a Poisson bracket. This is equivalent to the vanishing of the torsion of the tensor field $T_N$, so that the relation (35) can be iterated to:

$$\frac{\delta K_n}{\delta u} = \dot{T}_N \frac{\delta K_0}{\delta u}$$

(37)

It turns out that the nonlinear Schrödinger equation admits infinitely many conserved functionals.

First three functionals are:

$$K_{-1}[q,p] := \frac{1}{2} \int dx (p^2 + q^2) \equiv \int dx (\bar{\psi} \psi)$$

$$K_0[q,p] := \int dx (qp_x) \equiv 2i \int dx (\bar{\psi} \psi_x)$$

$$K_1[q,p] := \frac{1}{2} \int dx \left\{ \frac{\hbar^2}{2m} \left[ (\partial_x p)^2 + (\partial_x q)^2 \right] + (p^2 + q^2)^2 \right\}$$

(38)

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

$$\{K_n, K_m\}_0 = \{K_n, K_m\}_1 = 0$$

(39)

Observing that

$$\frac{\delta K_0}{\delta u} = \dot{T}_N \frac{\delta K_{-1}}{\delta u}$$

(40)

the recursion relation (37) can be completed to:

$$\frac{\delta K_n}{\delta u} = \dot{T}_N^{n+1} \frac{\delta K_{-1}}{\delta u}$$

(41)

Turning back to the complex notation, with $\hbar = 2m = \alpha = 1$, we have the general scheme of the next page.
Schrödinger Hierarchy

\[ \dot{\psi} = -i \hat{\mathcal{H}}^2 \psi \]

s-Gordon Hierarchy ← \( \hat{T}_G \) \( \psi = \psi_x \) \( \rightarrow \hat{T}_K \) KdV Hierarchy

\[ \dot{\psi} = i(\psi_{xx} + |\psi|^2 \psi) \]

\[ \dot{\psi} = -(\psi_{xxx} + 3|\psi|^2 \psi_x) \]

\[ \dot{\psi} = -i(\psi_{xxxx} + 4|\psi|^2 \psi_{xx} + 3\psi \psi_x^2 + 2\psi |\psi_x|^2 + \psi^2 \psi_{xx} + \frac{3}{2} |\psi|^4 \psi) \]

Nonlinear Schrödinger Hierarchy

\[ \hat{T} \bullet := -\Delta \bullet + U \bullet \equiv \hat{\mathcal{H}} \bullet \]
\[ \hat{T}_G \bullet := \partial_{xx} \bullet + \psi_x D^{-1} \psi_x \bullet \]
\[ \hat{T}_K \bullet := \partial_{xx} \bullet + \frac{2}{3} \psi \bullet + \frac{1}{3} \psi_x D^{-1} \bullet \]
\[ \hat{T}_N \bullet := i(\partial_x \bullet + \psi D^{-1}[\psi(\bullet) + \bar{\psi}(\bullet)]) \]
4 Concluding Remarks

It is interesting to observe that $K_{-1}$ is a conserved functional both for the Schrödinger and the nonlinear Schrödinger equations. The same is not true for $K_0$. This is due the fact that Schrödinger equation is not invariant under space translations and $K_0$ corresponds to the mean value $<\hat{p}>$ of the linear momentum $\hat{p} = -i\hbar\partial_x$. In other words the vector field associated to $K_0$ via the canonical Poisson bracket $\Lambda_1$ is invariant for translation.

It is worth finally to compare the recursion operators of the Schrödinger, with vanishing potential $U(x)$, and Nonlinear Schrödinger, with $\alpha = 0$, hierarchies. It turns out that $T = T_2^2$.

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