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A nonlinear N-Particle Model

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Abstract

An N-particle model with fourth order energy term is considered. For nonlinear Schrödinger equations the notion of selfconsistent potential is presented in a differential geometric invariant way. It is demonstrated that in nonlinear models selfconsistent potentials also contain antilinear terms and that for nonlinear N-particle models the gauge of the joint wave function can be decomposed into an abelian sum of symmetry generators of the dynamics of the joint wave function.

1 The basic Model

A mathematical investigation of nonlinear Schrödinger equations often is of interest (see [9]) because such equations play a role in the search of valid descriptions of interaction between particles (take for example Yukawas model for nucleon meson interaction). Surprisingly, usually no formal specification of the notion *particle* is to be found in the literature, at least not in a differential geometric invariant way. To give such an invariant approach is the aim of this paper.

As an example we start with a simple model. We consider N particles in $\mathbb{R}^3$ with equal mass m. Their Schrödinger wave functions are denoted by $\varphi_1, \ldots, \varphi_N$, the composite wave function is denoted by $\vec{\varphi} = (\varphi_1, \varphi_2, \ldots, \varphi_N)$. We assume that the particles have internal energies and that these energies can be considered as potential energies in selfinduced potentials.

By E_0 we denote the internal energy of the motionless single particle. In order that the particle is stable we must have $E_0 < 0$. We introduce the *joint wave* function

$$\psi = \sum_{l=1}^{N} \varphi_l. \tag{1.1}$$

The energy of the N-particle system is assumed to be

$$\mathcal{E}(\psi) = \mathcal{E}_{kin}(\psi) + \mathcal{E}_{pot}(\psi) = \frac{\hbar}{2m} \langle \nabla\psi, \nabla\psi \rangle + \gamma \int_{\mathbb{R}^3} V(\psi, \bar{\psi}) dx. \tag{1.2}$$

In order to have short-range attractive forces between the particles, later on our *basic assumption* is that expectation of potential energy is

$$\mathcal{E}_{pot}(\psi) = -\frac{1}{2} \int_{\mathbb{R}^3} |\psi|^4 dx. \tag{1.3}$$

Observe that this quantity is gauge invariant, were a quantity $\mathcal{F}(\psi)$ is said to be *gauge invariant* if ψ can be multiplied with any number of modulus 1 without changing the value of $\mathcal{F}$.

We measure time in units of $\hbar$ and we scale physical units and space variables such that $\hbar = 2m, \gamma = 1$. Hence the usual Schrödinger equation has the form

$$i\frac{\partial}{\partial t}\Phi = -\Delta\Phi + U\Phi, \tag{1.4}$$

with potential energy U.

Now consider the gauge group of each particle φ_k. Its infinitesimal transformation is $\varphi_k \to \varphi_k + \delta i \varphi_k$, where δ is inifintesimal. Hence the generator of that group is given by $i\varphi_k$.

Asymptotically, in case when the particles are almost free, that is when the overlap of the different wave functions φ_l, φ_k is almost equal to zero, then the dynamics for the infinitesimal generator of each gauge group shall be given by the Schrödinger equation

$$i\frac{\partial}{\partial t}(i\varphi_l) = -\Delta(i\varphi_l) + U(i\varphi_l) \tag{1.5}$$

for some suitable selfconsistent potential U (which yet has to be determined). At this point taking instead of φ_k the infinitesimal generator $i\varphi_k$ of its gauge group seems completely irrelevant, but at least it emphasizes that we consider tangent structures.

To determine this potential energy operator we observe that we know the expectation of U

$$\mathcal{E}_{pot}(\psi) = \langle \vec{\varphi}, U\vec{\varphi} \rangle$$

where $\vec{\varphi} = (\varphi_1, \varphi_2, \ldots, \varphi_N)$. In the linear case operator representations for observables $\mathcal{E}$ are easily recovered from their expectation $\mathcal{E}(\phi)$ if that is known as a function for general wave functions ϕ. We then find

$$2\langle \phi_b, \mathcal{E}\ \phi_a \rangle = \mathcal{E}''[i\phi_a, i\phi_b] - i\mathcal{E}''[i\phi_a, \phi_b] \tag{1.6}$$

where $\mathcal{E}''$ denotes the second variational derivative

$$\mathcal{E}''[\phi_a, \phi_b] := \frac{\partial}{\partial\lambda_2}\frac{\partial}{\partial\lambda_1}\mathcal{E}(\phi + \lambda_1\phi_a + \lambda_2\phi_b)_{|\lambda_1=\lambda_2=0}\ . \tag{1.7}$$

This formula is obtained only for the situation where the operator representation for the observable does not depend on the vector ϕ which represents the state of the system (*linear* *case*). Later on, we see that we may consider the matrix element $\langle \phi_b, \mathcal{E}\ \phi_a \rangle$ as the application of a two times covariant tensor (on the manifold of all possible ϕ) to a pair of tangent vectors. This leads to a differential geometric invariant generalisation of that formula (even for cases where the scalar expectation does not depend bilinearly on $\phi, \bar{\phi}$).

Definition 1: *Given a gauge invariant scalar quantity $\mathcal{F}(\phi)$, with $\mathcal{F} = 0$ when $\phi = 0$, and given two vectors ϕ_a, ϕ_b then the application to ϕ_a, ϕ_b of the selfconsistent operator F assigned to $\mathcal{F}(\phi)$ is defined to be*

$$\langle \phi_b, F\ \phi_a \rangle := \frac{1}{2} \left\{ \mathcal{F}(\phi)''[i\phi_a, i\phi_b] - i\mathcal{F}(\phi)''[i\phi_a, \phi_b] \right\} \tag{1.8}$$

Observe that $F = F(\phi)$ may depend on ϕ. Its expectation is defined to be

$$\mathit{expct}(F) := 2 \int_0^1 \lambda \langle \phi, F(\lambda\phi)\phi \rangle d\lambda$$

The integration is taken in order to assign to each power of ϕ a suitable scaling factor. Of course this definition only makes sense if $\mathit{expct}(F) = \mathcal{F}(\phi)$. To see this we observe that gauge invariance implies for the variational derivative in direction of $i\phi$ that $\mathcal{F}'(\phi)[i\phi] = 0$. Second derivatives in direction of ϕ and $i\phi$ then yield

$$\begin{aligned} \mathcal{F}''(\phi)[\phi, i\phi] &= 0 & (1.9) \\ \mathcal{F}''(\phi)[i\phi, i\phi] &= \mathcal{F}'(\phi)[\phi] & (1.10) \end{aligned}$$

By (1.9) and (1.8) we obtain

$$\begin{aligned} 2\int_0^1 \lambda \langle \phi, F(\lambda\phi)\phi \rangle &= \int_0^1 \lambda \mathcal{F}(\lambda\phi)''[i\phi, i\phi] d\lambda \\ &= \int_0^1 \mathcal{F}(\lambda\phi)'[\phi] d\lambda \\ &= \mathcal{F}(\phi) \end{aligned}$$

In this computation the second-last line followed from (1.10) and the last line from the fact that in the second-last line the integrand was a complete derivative with respect to λ.

Observe that the selfconsistent operator coming from a scalar quantity is by definition an operator which acts on tangent vectors, therefore it made sense to consider the asymptotic Schrödinger equation (1.5) as an equation acting on the generator of the gauge group instead on the wave function itself. That this also leads to different computational results will be seen from the following example.

We compute the selfconsistent potential U for the potential energy

$$\mathcal{E}_{pot}(\psi) = -\frac{1}{2} \int_{\mathbb{R}^3} |\psi|^4 dx.$$

We obtain

$$\langle \phi_b, U \phi_a \rangle = -\langle \phi_b, \psi^2 \bar{\phi_a} + 2|\psi|^2 \phi_a \rangle$$

which indeed has the prescribed expectation

$$expct(U) = -\frac{1}{2}\int_{\mathbb{R}^3} |\psi|^4 dx.$$

Observe that $U : \phi_a \to \psi^2\bar{\phi}_a + 2|\psi|^2\phi_a$ has an *antilinear* part, therefore it makes a difference wether this operator is applied to the generator of the gauge group instead to the wave function itself. Observe that by the same coputation the selfconsistent operator assigned to the energy is $-\Delta + U$.

Writing down equation (1.5) for the single particle we obtain

$$i\frac{\partial}{\partial t}(i\varphi_l) = -\Delta(i\varphi_l) - \left(\psi^2\,\overline{(i\varphi_l)} + 2|\psi|^2(i\varphi_l)\right). \tag{1.11}$$

This yields for the wave functions

$$i\frac{\partial}{\partial t}\varphi_l = -\Delta\varphi_l + \psi^2\bar{\varphi}_l - 2|\psi|^2\varphi_l.$$

By assumption, this only is the dynamics for the case when the particles are far apart. However, since our construction of the selfconsistent potential can be understood as the construction of a two times covariant tensor (by use of Lie derivatives) it really must represent the dynamics for arbitrary time, a fact which can be seen by parametrizing the manifold by help of the data of the emerging particles.

Now going over to the joint wave we obtain by summation

$$i\frac{\partial}{\partial t}\psi = -\Delta\psi - |\psi|^2\psi, \tag{1.12}$$

the well known nonlinear Schrödinger equation (NLS), which is known to be completely integrable in one dimension.

An important observation seems that this is the only dynamics which we have to know in order to analyze also the dynamics of individual particles. This because equation (1.11) is the equation of a symmetry group generator for the equation of the joint wave (see [4] or [5] for a general introduction of the symmetry concept in nonlinear dynamics). Summarizing we find

Observation: *The dynamics of the gauge group generators $i\varphi_1, ..., i\varphi_N$ of the individual particles is that of a symmetry group generator of the dynamics of the joint wave function. Furthermore the vector fields given by these gauge group generators $i\varphi_1, ..., i\varphi_N$ are commuting with each other (in the vector field Lie algbra).*

Indeed, the last statement about the abelian nature of the gauge group generators we did not yet prove, however it follows automatically from the generalisations presented in the next section.

2 Generalisation

Surprisingly, in most texts on interacting fields a differential geometric invariant definition of the notion *particle* is missing. Therefore in this section we shall concentrate on the question how a particle can be defined for interacting fields. We shall give a group theoretical justification that the results of the last section were no coincidence.

Heuristically we adopt the viewpoint that those parts of a joint field are called particles which have the property that small changes of their states have only negligible effects on the other particles. Out of this heuristic definition we shall make a precise one.

First, in order to be in a differential geometric correct setup, we shall change the definition of scalar products to

$$\langle\!\langle \phi_a, \phi_b \rangle\!\rangle := \textit{Real part of } \langle \phi_a, \phi_b \rangle$$

where $\langle \phi_a, \phi_b \rangle$ is the usual complex-Hilbert space scalar product. This change in scalar products we even consider in case of the usual linear Schrödinger theory. The reason for this unusual product is the following:
Rewrite the usual Schrödinger equation by splitting up complex functions in real and imaginary parts, i.e. $\Phi = v_1 + iv_2,\ v_1, v_2\ real$. Then the dynamics for Φ as given by equation (1.4) is represented by a dynamics for the two component quantity $\vec{v} := (v_1, v_2)^T$ in the following way

$$\vec{v}_t = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} grad \frac{1}{2} \{ < \nabla\vec{v}, \nabla\vec{v} > + < \vec{v}, U\vec{v} > \} \tag{2.1}$$

where $<\ ,\ >$ denotes the usual product in the direct sum of two real Hilbert spaces. This is a hamiltonion system where the symplectic structure is given the usual symplectic form

$$\Theta := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} .$$

Therefore we can make use of Emmy Noethers result which maps gradients of conserved quantities onto symmetry group generators. To be precise, the map $\Theta \times$ grad defines a Lie algebra homomorphism from the Poisson brackets onto the Lie algebra given by vector fields (Noether homomorphism). For this procedure Poisson brackets between two scalar quantities $F(\vec{v}), G(\vec{v})$ have to be defined as

$$\{F(\vec{v}), G(\vec{v})\} :=< \mathrm{grad}F(\vec{v}), \Theta \times \mathrm{grad}G(\vec{v}) > \tag{2.2}$$

Rewriting this in terms of complex quanties we find that the corresponding Poisson brackets are

$$\{F(\Psi), G(\Psi)\} := \langle\!\langle \mathrm{grad}F(\Psi), i\ \mathrm{grad}G(\Psi) \rangle\!\rangle \tag{2.3}$$

and that i grad is the corresponding Lie algebra homomorphism. This shows that the scalar product $\langle\!\langle\ ,\ \rangle\!\rangle$ is the natural product for defining Poisson brackets.

After having fixed our symplectic structure, setting up suitable dynamic laws is simple since the dynamics of the total field is the symmetry generator which corresponds via the Noether homomorphism to the energy function. So, assume that for an N-particle system $(\varphi_1, \cdots, \varphi_N)$ the energy is given by a gauge invariant expression $\mathcal{E}(\psi)$ in the joint wave function $\psi = \varphi_1 + \cdots + \varphi_N$ then the dynamics of the joint wave function must be

$$\psi_t = i\ \mathrm{grad}\ \mathcal{E}(\psi) \tag{2.4}$$

because dynamical laws are given as images of the energy function under the Noether homomorphism. For the case considered in the last section this is exactly the dynamics found in (1.12). Since the φ_l are probability wave functions we find the conserved quantities

$$W_l := \langle \varphi_l, \varphi_l \rangle = \langle\!\langle \varphi_l, \varphi_l \rangle\!\rangle = 1.$$

Hence

$$i\ \varphi_l = i \text{ grad } \frac{1}{2} \langle \varphi_l, \varphi_l \rangle$$

must be a symmetry generator whose dynamics is given by the linearisation of (2.4)

$$i\ \varphi_{lt} = i\ \{\text{grad } \mathcal{E}(\psi)\}'[i\varphi_l] \tag{2.5}$$

This is indeeed, by definition, the same as the Schrödinger equation with the selfconsistent energy operator. In order to see that the symmetry generators $i\ \varphi_l$ are commuting we consider the Poisson brackets

$$\{W_l, W_k\} := \langle\!\langle \text{grad} W_l, i \text{ grad} W_k \rangle\!\rangle.$$

As scalar products between gardients of conservation laws and symmetry generators these quantities must be time independent. Furthermore, since asymptotically the particles are free, i.e. the overlap between different wave functions is going to zero for $t \to \infty$ these Poisson brackets go to zero for $t \to \infty$, hence must be identically zero for reasons of time independence. Now mapping these brackets with the Noether homomorphism i grad onto vector fields we obtain that the corresponding vector fields commute. Hence the set of gauge generators must be an abelian subalgbera of the vector field Lie algbera. From there follows easily that indeed small changes in the gauge of one of the particles has negligible effects on the other particles. So we may summarize our considerations to:

Definition 2: *A field ψ with gauge invariant energy function $\mathcal{E}(\psi)$ is an N-particle system if there is a decomposition*

$$\psi = \varphi_1 + \cdots + \varphi_N$$

such that the different gauges $i\ \varphi_k$ are an abelian set of symmetry group generators for the dynamics

$$\psi_t = i \text{ grad } \mathcal{E}(\psi)$$

of the wave function ψ.

One should observe that this definition does not necessarily imply that asymptotically free particles emerge. So, the definiton also covers the case of bound particles.

3 The one-dimensional model

In this section we briefly come back to the one-dimensional case, which, although different approaches were chosen, has been used with success for a computational descriptions of nonlinear phenomena in nuclear models (see [6] [7]).

We consider the case of only one space variable where equation (1.12)

$$i \frac{\partial}{\partial t} \psi = -\psi_{xx} - |\psi|^2 \psi \tag{3.1}$$

is solvable. Observe that this equation is of the form

$$\psi_t = \Psi(\psi)^2(i\psi) = \Psi(\psi)\psi_x$$

where

$$\Psi(\psi) = iD + 2i\psi D^{-1}Re(\bar{\psi}\bullet)$$

is a hereditary operator (see [2], [4]) and where $Re(\bar{\psi}\bullet)$ is the map

$$\phi \to Real\ part\ of\ (\bar{\psi}\phi).$$

As a consequence of the hereditary property of $\Psi(\psi)$ we have [4] that the

$$\{K(\psi)_n \mid K(\psi)_n = \Psi(\psi)^n(i\psi)\ n \in \mathbb{N}\}$$

are an abelian set of symmetry group generators for (3.1). In case we have only one particle

$$\psi(x,t) = \psi(x+ct)\exp(-iE_0 t)$$

with (negative) internal energy E_0 and speed c this means

$$-i\ E_0\psi + c\psi_x = \Psi(\psi)^2(i\ \psi)$$

or, since $\psi_x = \Psi(\psi)(i\ \psi)$, that

$$\left\{\Psi(\psi)^2 - c\Psi(\psi) + E_0\right\}(i\ \psi) = 0\ .$$

If

$$\frac{c^2}{4} + E_0 \leq 0$$

we may write equivalently

$$(\Psi - \lambda_c)\left(\Psi - \bar{\lambda}_c\right)(i\ \psi) = 0$$

where

$$\lambda_c := \frac{c}{2} + i\ \sqrt{\frac{c^2}{4} + |E_0|}\ \ .$$

Hence for N emerging particles with asymptotic speeds $c_1, \cdots, c_n$ we must have asymptotically

$$\left\{\prod_{k=1}^{N}(\Psi - \lambda_{c_k})\left(\Psi - \bar{\lambda}_{c_k}\right)\right\}(i\ \psi) = 0\ . \tag{3.2}$$

However, since the left hand side of this expression is a sum of symmetry generators, this must be an invariant vector field, hence must be zero at all times. Furthermore, since this equation is of the form

$$\alpha i\ \psi = \alpha K(\psi)_0 = \sum_{n=1}^{2N}\alpha_n K(\psi)_n$$

it fulfills definition 2. Therefore this invariant reduction must describe the N-particle state of the NLS. Thus for one space dimension the N-particle state is a special multisoliton solution of the integrable cubic Schrödinger equation. Observe that the multisolitons, and for them a complete action-angle representation, for this equation is easily computed (see [8]). Furthermore, one should observe that in case of a single particle and due to the fact that the Schrödinger operator defines an isospectral formulation for the Korteweg de Vries equation (KdV) $u = |\psi|^2$ must be a single soliton of the KdV. Hence in case of a single particle the linear part of the selfconsistent potential must be a Bargmann potential, i.e. a reflectionless potential (see [1], [10]).

Observe that (3.2) is equivalent to the fact that $(i\ \psi)$ may be decomposed into eigenvectors of Ψ with eigenvalues $\lambda_{c_k}, \bar{\lambda}_{c_k}$. Therefore another notable point seems that in case of the reduction (3.2) the eigenvectors of Ψ with eigenvalues λ_{c_k}, which describe the single particles, are easily computed and that their dynamics is represented by another integrable equation where only self energy terms occur (see [3]).

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