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Generalized Gauge Invariants for Certain Nonlinear Schrödinger Equations

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In previous work, Doebner and I introduced a group of nonlinear gauge transformations for quantum mechanics, acting in a certain family of nonlinear Schrödinger equations. Here the idea for a further generalization is presented briefly. It makes possible the treatment of the logarithmic amplitude and the phase of the wave function on an equal footing, suggesting a more radical reinterpretation of these variables in linear and nonlinear quantum theory.

1 Background

Motivated by our desire to interpret a certain class of nonrelativistic current algebra representations as descriptive of quantum mechanical systems, H.-D. Doebner and I proposed a parameterized family of nonlinear Schrödinger equations (NLSEs) whose solutions would satisfy the appropriate equation of continuity [1, 2, 3]. It was then logically necessary to extend the usual gauge group for quantum mechanics to include transformations that could act nonlinearly [4, 5]. Writing the complex-valued wave function $\psi(\mathbf{x}, t)$, describing a single spinless particle in a pure state, as $\psi = R(\mathbf{x}, t)\exp[iS(\mathbf{x}, t)]$, where the amplitude R and the phase S are real, these nonlinear gauge trasnformations act by

$$R' = R, \qquad S' = \Lambda S + \gamma \ln R + \theta, \tag{1.1}$$

where Λ is a smooth, real-valued, nonzero function of t, γ is a smooth, real-valued function of t, and θ is a smooth, real-valued function of $\mathbf{x}$ and t. The transformations (1.1) map members of our family of NLSEs into each other, and have other desirable properties. In particular, they extend naturally to act on a hierarchy of N-particle wave functions $\psi_N(\mathbf{x}_1, \ldots, \mathbf{x}_N, t)$, defined on the (positional) configuration space, in a way that is strictly local and satisfies a separation condition for product states [6].

The justification for considering them to be gauge transformations is as follows. For all of the nonlinear quantum theories under discussion, we interpret $\rho = |\psi|^2 = R^2$ as the probability density in configuration space. We adopt as a working hypothesis the view (taken by many theorists) that all measurements in ordinary quantum mechanics can be regarded as a sequence of positional measurements, made at different times, where external fields exerting forces may be imposed on the system between measurements [7, 8]. Then for any wave function ψ obeying a Schrödinger equation (linear or nonlinear) in our family, the wave function ψ' transformed by (1.1) obeys a transformed Schrödinger equation, still in the family, with gauge-transformed external fields; while the outcomes of all physical measurements remain invariant.

To be explicit, with

$$\rho = \overline{\psi}\psi, \qquad \hat{\mathbf{j}} = \frac{1}{2i}\,[\,\overline{\psi}\nabla\psi - (\nabla\overline{\psi})\psi], \tag{1.2}$$

define the real, homogeneous nonlinear functionals

$$R_1 = \frac{\nabla \cdot \hat{\mathbf{j}}}{\rho}, \qquad R_2 = \frac{\nabla^2 \rho}{\rho}, \qquad R_3 = \frac{\hat{\mathbf{j}}^2}{\rho^2}, \qquad R_4 = \frac{\hat{\mathbf{j}} \cdot \nabla \rho}{\rho^2}, \qquad R_5 = \frac{(\nabla \rho)^2}{\rho^2}, \tag{1.3}$$

and consider the following family of one-particle NLSEs (where for mathematical convenience both sides have been divided by ψ):

$$\begin{aligned} i\frac{\dot{\psi}}{\psi} &= i\left[\sum_{j=1}^{2} \nu_j R_j[\psi] + \frac{\nabla \cdot (\mathcal{A}(\mathbf{x},t)\rho)}{\rho}\right] \\ &\quad + \left[\sum_{j=1}^{5} \mu_j R_j[\psi] + U(\mathbf{x},t) + \frac{\nabla \cdot (\mathcal{A}_1(\mathbf{x},t)\rho)}{\rho} + \frac{\mathcal{A}_2(\mathbf{x},t) \cdot \hat{\mathbf{j}}}{\rho} + \alpha_1 \ln \rho + \alpha_2 S\right]. \end{aligned} \tag{1.4}$$

Here the coefficients ν_j $(j = 1,2)$, μ_j $(j = 1,\ldots,5)$, and α_j $(j = 1,2)$ are smooth, real-valued functions of t; U is an external real-valued, time-dependent scalar field; and $\mathcal{A}$, $\mathcal{A}_1$ and $\mathcal{A}_2$ are distinct, external real-valued, time-dependent vector fields. Using the fact that $\nabla^2\psi/\psi = iR_1[\psi] + (1/2)R_2[\psi] - R_3[\psi] - (1/4)R_5[\psi]$, it is straightforward that Eq.(1.4) reduces to the usual, time-dependent linear Schrödinger equation

$$i\hbar\dot{\psi} = \frac{[-i\hbar\nabla - (e/c)\mathbf{A}(\mathbf{x},t)]^2}{2m}\psi + e\Phi(\mathbf{x},t)\psi \tag{1.5}$$

with external electromagnetic potentials $\mathbf{A}$, Φ, when

$$\begin{aligned} &\nu_1 = -\frac{\hbar}{2m}, \qquad \nu_2 = 0, \qquad \mathcal{A} = \frac{e}{2mc}\mathbf{A}, \\ &\mu_1 = 0, \qquad \mu_2 = -\frac{\hbar}{4m}, \qquad \mu_3 = \frac{\hbar}{2m}, \qquad \mu_4 = 0, \qquad \mu_5 = \frac{\hbar}{8m}, \\ &U = \frac{e}{\hbar}\Phi + \frac{e^2}{2m\hbar c^2}\mathbf{A}^2, \qquad \mathcal{A}_1 = 0, \qquad \mathcal{A}_2 = -\frac{e}{mc}\mathbf{A}, \qquad \alpha_1 = \alpha_2 = 0. \end{aligned} \tag{1.6}$$

Eq.(1.4) generalizes the class of nonlinear equations that Doebner and I first derived, to include external electromagnetic potentials, two additional external vector fields that can act nonlinearly (one of which was studied some time ago by Haag and Bannier [9]), and terms of the type proposed by Kostin [10] and by Bialynicki–Birula and Micielski [11]. An exploration of the relation of some of these terms with the separation property was begun in joint work with Svetlichny [12]. Though obtained on fundamental grounds, Eq.(1.4) contains as special cases a remarkable variety of independently-proposed nonlinear terms [13–19].

Since $\mathrm{Re}\,[\dot{\psi}/\psi] = (1/2)[\dot{\rho}/\rho]$, we see from inspection of the imaginary part of the right-hand side of (1.4) that $\dot{\rho}$ is the divergence of a vector field. As long as this falls off sufficiently rapidly at infinity, we have that $(d/dt)\int \rho(\mathbf{x},t)\,d\mathbf{x}$ is zero – thus the interpretation of ρ as a conserved probability density makes sense.

When the gauge transformations (1.1) is applied, we have

$$\begin{aligned} &\rho' = \overline{\psi}'\psi' = \rho, \\ &\hat{\mathbf{j}}' = \frac{1}{2i}\left[\overline{\psi}'\nabla\psi' - (\nabla\overline{\psi}')\psi'\right] = \Lambda\hat{\mathbf{j}} + \frac{\gamma}{2}\nabla\rho + \rho\nabla\theta. \end{aligned} \tag{1.7}$$

Thus ρ is gauge-invariant, while $\hat{\mathbf{j}}$ is not. Furthermore, if ψ satisfies an equation in the family defined by (1.4), then ψ' satisfies a transformed equation, with gauge-transformed coefficients

ν_j', μ_j', α_j', and external fields $\mathcal{A}'$, U', $\mathcal{A}_j'$ that can be expressed in terms of the unprimed quantities. We have a gauge-invariant current (see below), and gauge-invariant expressions for the usual, observable electric and magnetic fields. We also have formulas for independent gauge-invariant combinations of the coefficients ν_j, μ_j, and α_j, and the external vector fields. Here "gauge invariant" refers to the group of nonlinear transformations specified by (1.1). Naturally it is the gauge-invariant quantitities that must encode the physical content of a quantum theory described by one of equations in our family. Details of these transformations, and discussions of the gauge-invariant combinations, are published elsewhere.

2 Generalization of the Gauge Group

Next I shall describe and justify the idea for further generalization of this framework. It begins with the observation that the combination

$$\mathbf{j}^{gi} = \nu_1 \hat{\mathbf{j}} + \nu_2 \nabla \rho + \rho \mathcal{A} \tag{2.1}$$

is invariant under the transformation (1.1), so that $\mathbf{J} = -2\mathbf{j}^{gi}$ is a gauge-invariant current obeying $\dot{\rho} = -\nabla \cdot \mathbf{J}$. This means that our original working hypothesis, that all observations could be expressed as a succession of positional measurements at different times – i.e., in terms of $\rho(\mathbf{x}, t)$ – together with the imposition of external physical fields, may be unnecessarily stringent. Measurement procedures that detect $\mathbf{J}(\mathbf{x}, t)$, whether or not they can be expressed exclusively in terms of ρ and external fields, are equally compatible with (i.e., invariant under) the nonlinear gauge transformations (1.1).

Note also that unlike the formula for ρ, the expression for $\mathbf{J}$ involving (2.1) depends explicitly on two of the coefficients and one of the fields in Eq.(1.4). Indeed, there is no *a priori* reason why the expression for ρ could not also depend on these quantities. The important properties of the functions ρ and $\mathbf{J}$ are that they are invariant under the action of the group of nonlinear gauge transformations, that ρ is positive definite, and that they are related by an equation of continuity. Thus we might entertain the possibility of replacing the equation $\rho = |\psi|^2$ by a more general expression, that would have to be gauge invariant and reduce to $\rho = |\psi|^2$ in the case of the linear Schrödinger equation.

Now in standard, linear nonrelativistic quantum mechanics, the amplitude R and phase S of the wave function describing a pure state have very different status. The former is gauge invariant, and considered as physically observable; the latter is gauge dependent, and not observable. Likewise in the nonlinear quantum mechanics discussed in the previous section, R is manifestly gauge invariant, while S is not. When one reflects on this asymmetry, it seems increasingly extraordinary that we write a Schrödinger equation (linear or nonlinear) for the time-evolution by relating the *gauge* fields S, U and $\mathcal{A}$ to the *physical* field R, via the complex combination $R \exp[iS]$. Why should we not be able to couple gauge fields to gauge fields, and correspondingly, physical fields to physical fields? The purpose of this paper is to suggest a way to do just that, using a natural generalization of the nonlinearity Doebner and I proposed. The analysis applies even when the underlying physics is that of linear quantum mechanics!

If we return to Eqs.(1.1)–(1.4), we see that everything can be written very naturally in terms of the variables $\ln R$ and S. In particular, setting $T = \ln R$, Eq.(1.1) becomes

$$\begin{pmatrix} S' \\ T' \end{pmatrix} = \begin{pmatrix} \Lambda & \gamma \\ 0 & 1 \end{pmatrix} \begin{pmatrix} S \\ T \end{pmatrix} + \begin{pmatrix} \theta \\ 0 \end{pmatrix}, \tag{2.2}$$

where Λ and γ depend on t and θ depends on $\mathbf{x}$ and t. The condition $\Lambda \neq 0$ is just the requirement that the determinant of the matrix be nonvanishing. If we like, we can also write $\ln \rho = 2T$ so that $\nabla\rho/\rho = 2\nabla T$, and $\hat{\mathbf{j}}/\rho = \nabla S$. Then we can re-express the nonlinear functionals in (1.3) in terms of $\nabla^2 S$, $\nabla^2 T$, $(\nabla S)^2$, $\nabla S \cdot \nabla T$, and $(\nabla T)^2$; for example, $R_1 = \nabla^2 S + 2\nabla S \cdot \nabla T$, while $R_3 = (\nabla S)^2$. Since $\dot{\psi}/\psi$ is just $\dot{T} + i\dot{S}$, Eq.(1.4) becomes a pair of coupled partial differential equations for S and T. These logarithmic variables are familiar from earlier hydrodynamical and stochastic versions of quantum theory [20, 21].

It is time to take the leap. Eq.(2.2) practically cries out to be generalized to affine transformations modeled on the general linear group $GL(2, \mathbf{R})$:

$$\begin{pmatrix} S' \\ T' \end{pmatrix} = \begin{pmatrix} \Lambda & \gamma \\ \lambda & \kappa \end{pmatrix} \begin{pmatrix} S \\ T \end{pmatrix} + \begin{pmatrix} \theta \\ \phi \end{pmatrix}, \tag{2.3}$$

where Λ, γ, λ and κ are smooth, real-valued functions of t, and θ, ϕ are smooth, real-valued functions of $\mathbf{x}$ and t. This is essentially equivalent to complexifying the coefficients in (1.1). We can permit $\Lambda = 0$, but require that $\Delta = \kappa\Lambda - \lambda\gamma \neq 0$.

Immediately it is evident that the family of NLSEs must also be generalized for it to remain invariant under (2.3). The necessary (and natural) generalization is to introduce into the imaginary part of the right-hand side the terms $\nu_3 R_3$, $\nu_4 R_4$ and $\nu_5 R_5$, as well as external scalar and vector fields, so that there is symmetry between the real and imaginary parts. Thus

$$\begin{aligned} i\frac{\dot{\psi}}{\psi} = i\dot{T} - \dot{S} = i&\left[\sum_{j=1}^{5} \nu_j R_j[\psi] + \mathcal{T}(\mathbf{x}, t) + \frac{\nabla\cdot(\mathcal{A}(\mathbf{x}, t)\rho)}{\rho} + \frac{\mathcal{D}(\mathbf{x}, t)\cdot\hat{\mathbf{j}}}{\rho} + \delta_1 \ln\rho + \delta_2 S\right] \\ &+ \left[\sum_{j=1}^{5} \mu_j R_j[\psi] + U(\mathbf{x}, t) + \frac{\nabla\cdot(\mathcal{A}_1(\mathbf{x}, t)\rho)}{\rho} + \frac{\mathcal{A}_2(\mathbf{x}, t)\cdot\hat{\mathbf{j}}}{\rho} + \alpha_1 \ln\rho + \alpha_2 S\right], \end{aligned} \tag{2.4}$$

where $\mathcal{T}$ is a new external scalar field, and $\mathcal{D}$ a new external vector field. Note that the heat equation and other interesting equations of mathematical physics fall within this family; as well as the linear Schrödinger equation, with $\nu_3 = \nu_4 = \nu_5 = \delta_1 = \delta_2 = 0$, $\mathcal{T} = 0$, $\mathcal{D} = 0$, and the other values as in Eq.(1.6). Some equations with soliton-like solutions are also included [22].

As with the smaller family of nonlinear equations (1.4) and the smaller group of nonlinear gauge transformations (1.1), if ψ solves an equation within the class (2.4), then the wave function transformed under (2.3), $\psi' = R' \exp iS'$ with $R' = \ln T'$, solves another equation in the same class, but with transformed coefficients and transformed external fields. The question now is whether we can identify appropriate invariants under the group of transformations (2.3), in terms of which all the quantum observables can be expressed. If so, we are justified in considering R (or, alternatively, T) and S both as gauge fields, obeying one or another NLSE from the class (2.4), and deriving the physical fields from them as invariants under the enlarged nonlinear gauge group. We will have succeeded in treating S and $\ln R$ on an equal footing. It will even be possible to entertain quantum mechanics in a (nonlinear) gauge where $\ln R$ and S have been exchanged.

3 Generalized Gauge Invariants

From this point on, it is more convenient to work using the variables S and T. Consider then the coupled pair of general second-order quadratic partial differential equations,

$$\begin{aligned} \dot{S} = a_1\nabla^2 S + a_2\nabla^2 T + a_3(\nabla S)^2 + a_4\nabla S\cdot\nabla T + a_5(\nabla T)^2 \\ + a_6 S + a_7 T + u_0 + \mathbf{u}_1\cdot\nabla S + \mathbf{u}_2\cdot\nabla T, \end{aligned}$$

$$\dot{T} = b_1\nabla^2 S + b_2\nabla^2 T + b_3(\nabla S)^2 + b_4\nabla S\cdot\nabla T + b_5(\nabla T)^2 \\ +b_6 S + b_7 T + v_0 + \mathbf{v}_1\cdot\nabla S + \mathbf{v}_2\cdot\nabla T, \tag{3.1}$$

where the relation between (3.1) and (2.4) is given by

$$\begin{aligned} &a_1 = -\mu_1, \quad a_2 = -2\mu_2, \quad a_3 = -\mu_3, \quad a_4 = -2\mu_1 - 2\mu_4, \quad a_5 = -4\mu_2 - 4\mu_5, \\ &a_6 = -\alpha_2, \quad a_7 = -2\alpha_1, \quad u_0 = -U - \nabla\cdot\mathcal{A}_1, \quad \mathbf{u}_1 = -\mathcal{A}_2, \quad \mathbf{u}_2 = -2\mathcal{A}_1, \\ &b_1 = \nu_1, \quad b_2 = 2\nu_2, \quad b_3 = \nu_3, \quad b_4 = 2\nu_1 + 2\nu_4, \quad b_5 = 4\nu_2 + 4\nu_5, \\ &b_6 = \delta_2, \quad b_7 = 2\delta_1, \quad v_0 = \mathcal{T} + \nabla\cdot\mathcal{A}, \quad \mathbf{v}_1 = \mathcal{D}, \quad \mathbf{v}_2 = 2\mathcal{A}. \end{aligned} \tag{3.2}$$

Now the coefficients a_j, b_j obey the following transformation laws under (2.3), with the determinant $\Delta = \kappa\Lambda - \lambda\gamma$:

$$\begin{bmatrix} a_1' \\ a_2' \\ b_1' \\ b_2' \end{bmatrix} = \Delta^{-1} \begin{bmatrix} \kappa\Lambda & -\lambda\Lambda & \kappa\gamma & -\lambda\gamma \\ -\gamma\Lambda & \Lambda^2 & -\gamma^2 & \gamma\Lambda \\ \kappa\lambda & \lambda^2 & \kappa^2 & -\kappa\lambda \\ -\lambda\gamma & \lambda\Lambda & -\kappa\gamma & \kappa\Lambda \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{bmatrix}, \tag{3.3}$$

$$\begin{bmatrix} a_3' \\ a_4' \\ a_5' \\ b_3' \\ b_4' \\ b_5' \end{bmatrix} = \Delta^{-2}\mathcal{M} \begin{bmatrix} a_3 \\ a_4 \\ a_5 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}, \tag{3.4}$$

where

$$\mathcal{M} = \begin{bmatrix} \kappa^2\Lambda & -\kappa\lambda\Lambda & \lambda^2\Lambda & \kappa^2\gamma & -\kappa\lambda\gamma & \lambda^2\gamma \\ -2\kappa\gamma\Lambda & \Lambda(\kappa\Lambda+\lambda\gamma) & -2\lambda\Lambda^2 & -2\kappa\gamma^2 & \gamma(\kappa\Lambda+\lambda\gamma) & -2\lambda\gamma\Lambda \\ \gamma^2\Lambda & -\gamma\Lambda^2 & \Lambda^3 & \gamma^3 & -\gamma^2\Lambda & \gamma\Lambda^2 \\ \kappa^2\lambda & -\kappa\lambda^2 & \lambda^3 & \kappa^3 & -\kappa^2\lambda & \kappa\lambda^2 \\ -2\kappa\lambda\gamma & \lambda(\kappa\Lambda+\lambda\gamma) & -2\lambda^2\Lambda & -2\kappa^2\gamma & \kappa(\kappa\Lambda+\lambda\gamma) & -2\kappa\lambda\Lambda \\ \lambda\gamma^2 & -\lambda\gamma\Lambda & -\lambda\Lambda^2 & \kappa\gamma^2 & -\kappa\gamma\Lambda & \kappa\Lambda^2 \end{bmatrix},$$

and

$$\begin{bmatrix} a_6' \\ a_7' \\ b_6' \\ b_7' \end{bmatrix} = \Delta^{-1} \begin{bmatrix} \kappa\Lambda & -\lambda\Lambda & \kappa\gamma & -\lambda\gamma \\ -\gamma\Lambda & \Lambda^2 & -\gamma^2 & \gamma\Lambda \\ \kappa\lambda & \lambda^2 & \kappa^2 & -\kappa\lambda \\ -\lambda\gamma & \lambda\Lambda & -\kappa\gamma & \kappa\Lambda \end{bmatrix} \begin{bmatrix} a_6 \\ a_7 \\ b_6 \\ b_7 \end{bmatrix} + \Delta^{-1} \begin{bmatrix} \kappa\dot{\Lambda} - \lambda\dot{\gamma} \\ \Lambda\dot{\gamma} - \gamma\dot{\Lambda} \\ \kappa\dot{\lambda} - \lambda\dot{\kappa} \\ \Lambda\dot{\kappa} - \gamma\dot{\lambda} \end{bmatrix}. \tag{3.5}$$

For brevity we omit the transformation laws for the external fields.

The final task for this paper is to suggest invariant combinations of S and T. For simplicity, we consider only the matrix part of the transformation (2.3), i.e., we take $\theta = \phi = 0$. First suppose that X and Y obey

$$\begin{pmatrix} X' \\ Y' \end{pmatrix} = \begin{pmatrix} \Lambda & \gamma \\ \lambda & \kappa \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = A \begin{pmatrix} X \\ Y \end{pmatrix}, \tag{3.6}$$

and c_1, c_2 are coefficients. Then $c_1X + c_2Y$ is invariant under A if and only if $[c_1\, c_2]A^{-1} = [c_1'\, c_2']$. But one can verify from (3.4) that with $d_1 = 2a_3 + b_4$ and $d_2 = a_4 + 2b_5$, we have

$[d_1\, d_2]A^{-1} = [d_1'\, d_2']$. Hence $d_1S + d_2T$ can serve as one of the desired invariant combinations. Next let $L_1 = a_1S + a_2T$ and $L_2 = b_1S + b_2T$. We have

$$\begin{pmatrix} L_1' \\ L_2' \end{pmatrix} = \begin{pmatrix} \Lambda & \gamma \\ \lambda & \kappa \end{pmatrix} \begin{pmatrix} L_1 \\ L_2 \end{pmatrix} = A \begin{pmatrix} L_1 \\ L_2 \end{pmatrix}. \tag{3.7}$$

Therefore $d_1L_1 + d_2L_2$ is also an invariant. In fact, we can consider $d_1(\sigma L_1 + \tau S) + d_2(\sigma L_2 + \tau T)$ as a general linear combination of the invariants we have found, where σ and τ are fully invariant combination of the coefficients. For example, it is straightforward to verify that $a_1 + b_2$ and $a_1b_2 - a_2b_1$, which were earlier identified as gauge invariants for (2.2), are also invariants under (2.3). In short the desired invariant combinations of S and T exist, and we even have some flexibility in our choice: we can choose combinations that reduce to the usual formulas in the case of the linear Schrödinger equation!

This permits us to obtain a positive definite, gauge-invariant probability density and gauge-invariant current. Finally, a large subfamily of the equations (2.4) have solutions for which the gauge-invariant density and current obey a continuity equation. Details of these results are to be presented elsewhere.

4 Conclusion

Consideration of nonlinear gauge transformations modeled on the general linear group $GL(2, \mathbf{R})$ leads to a beautiful, apparently unremarked symmetry or duality between the phase and the logarithm of the amplitude in quantum mechanics. Both can be treated as gauge fields, suggesting the possibility of a fundamental reappraisal of the meaning of the wave function (and of gauge transformation). In particular, the linear Schrödinger equation is embedded in a natural class of nonlinear time-evolution equations, invariant as a class under nonlinear gauge transformations, extending (necessarily) the family that I proposed earlier in joint work with H.-D. Doebner. Formulas for gauge-invariant probability density and flux exist that apply across the whole class of nonlinear equations. The usual expressions for these quantities, along with the Schrd̈inger equation, are recovered for linearizable theories in a particular gauge.

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