On Energy Functions for String-Like Continuous Curves, Discrete Chains, and Space-Filling One Dimensional Structures

Shuangwei Hu, Ying Jiang, and Antti J. Niemi

1Department of Physics and Astronomy, Uppsala University, P.O. Box 803, S-75108, Uppsala, Sweden
2Department of Physics, Shanghai University, Shangda Rd. 99, 200444 Shanghai, P.R. China
3Laboratoire de Mathematiques et Physique Theorique CNRS UMR 6083, Federation Denis Poisson, Universite de Tours, Parc de Grandmont, F37200, Tours, France
4Department of Physics, Beijing Institute of Technology, Haidian District, Beijing 100081, P. R. China

Abstract

The theory of string-like continuous curves and discrete chains have numerous important physical applications. Here we develop a general geometrical approach, to systematically derive Hamiltonian energy functions for these objects. In the case of continuous curves, we demand that the energy function must be invariant under local frame rotations, and it should also transform covariantly under reparametrizations of the curve. This leads us to consider energy functions that are constructed from the conserved quantities in the hierarchy of the integrable nonlinear Schrödinger equation (NLSE). We point out the existence of a Weyl transformation that we utilize to introduce a dual hierarchy to the standard NLSE hierarchy. We propose that the dual hierarchy is also integrable, and we confirm this to the first non-trivial order. In the discrete case the requirement of reparametrization invariance is void. But the demand of invariance under local frame rotations prevails, and we utilize it to introduce a discrete variant of the Zakharov-Shabat recursion relation. We use this relation to derive frame independent quantities that we propose are the essentially unique and as such natural candidates for constructing energy functions for piecewise linear polygonal chains. We also investigate the discrete version of the Weyl duality transformation. We confirm that in the continuum limit the discrete energy functions go over to their continuum counterparts, including the perfect derivative contributions.

∗Electronic address: hushuangwei@gmail.com
†Electronic address: yjiang@shu.edu.cn
‡Electronic address: Antti.Niemi@physics.uu.se
I. INTRODUCTION

The theory of continuous curves in three dimensional space \cite{1} is one of the pillars of differential geometry \cite{2}. The study of string-like objects and their properties, both continuous and discrete, is similarly pivotal to several apparently disparate subfields of physics. Examples include polymers \cite{3}, \cite{4}, Kirchoff-type elastic rods \cite{5}-\cite{7}, vortices in fluid dynamics, \cite{8}, \cite{9}, \cite{10}, turbulence \cite{11}, superconductors \cite{12}, \cite{13}, superfluids \cite{14}, plasmas \cite{15}, metallic hydrogen \cite{16}, and confining \cite{17}, cosmic \cite{18} and fundamental \cite{19} strings in high energy physics, and numerous other applications. Strings can display intricate geometry including knots \cite{20}, strings can proceed by leapfrogging \cite{21}, \cite{10}, and strings might even realize exotic exchange statistics in three dimensions \cite{22}. Among the several general level theoretical contributions, we in addition draw attention to \cite{23} and to \cite{24} as particularly notable ones.

In the present article we shall be mainly interested in deriving geometric energy functions for discretized curves, or more precisely piecewise linear polygonal chains in three space dimensions. The motivation comes from a recently proposed approach to the physics of proteins \cite{25}-\cite{29}. A protein is a biologically relevant example of a piecewise linear polygonal chain, with vertices identified as the central C$\alpha$ carbons of the amino acids. A biologically active protein is also particularly interesting from the point of view of physics of string-like structures in three space dimensions. It is an object that despite an inherent one dimensional character, has physical properties that causes it to collapse into a space filling construct. We propose that the study of space filling, collapsed string-like objects can have several important ramifications also in other areas of physics, from understanding turbulent flows in fluid dynamics to potentially new forms of matter in high energy physics.

Our approach is based on the observation, first made by Hasimoto \cite{30}, \cite{31}, \cite{8}, \cite{9} in the context of fluid dynamics, that the one dimensional nonlinear Schrödinger equation (NLSE) describes string-like objects such as vortex filaments. For this he introduced a change of variables that relates the wave function of the NLSE to the Frenet frame representation of a space curve. The NLSE is a widely studied example of an integrable model \cite{32}-\cite{34} both due to its stature as a universal theoretical construct, and due to the abundance of both theoretical \cite{32}, \cite{33} and practical \cite{34} applications. Among the remarkable properties of the NLSE is the ability to support solitons as classical solutions. In the case of continuous curves, when the energy is computed by the canonical Hamiltonian of the NLSE and the ensuing configuration is related to the geometry of a curve by the Hasimoto transformation, the soliton describes the buckling of the curve.

A properly discretized version of the NLSE preserves the integrability \cite{35}, \cite{36}. It also supports soliton solutions that can be utilized to model the buckling of piecewise linear polygonal chains, via a discretized version of the Hasimoto transformation. This has been applied in \cite{27}, \cite{37} to propose that the loop structures that are the characteristic geometric features of folded proteins, could be modeled using a properly discretized version of the NLSE energy function. In the case of proteins, the loops are solitons that cause the string-like C$\alpha$ backbone to buckle and collapse into a space filling configuration. As a consequence, from a general point of view, chains that support solitons with geometric interpretation are truly curiosity arousing: Despite its inherently one dimensional character, a discrete string-like chain that supports solitons at that cause it to buckle, appears like a localized space filling, particle-like extended object.

In the following, we shall first outline how energy functions of continuous curves are
derived from purely geometric considerations, by demanding both invariance under local frame rotations and covariance under curve reparametrizations. We show how the NLSE together with its integrable hierarchy emerges naturally, when we demand that the energy function of a curve can not depend on the choice of framing along the curve. We scrutinize the properties of the Zakharov-Shabat recursion relation between the conserved quantities in the NLSE hierarchy, from the point of view of frame independence. We observe that there is the possibility to introduce a dual hierarchy, which is related to the original NLSE hierarchy by a Weyl scaling transformation. It turns out that the dual hierarchy has some quite attractive features. In particular, it embraces two of the conserved quantities of the NLSE hierarchy, the length and the helicity (Chern-Simons), that have no place in the standard NLSE recursion relations. We confirm by explicit computation that the leading order terms of the dual hierarchy are mutually in involution, suggesting that the dual hierarchy gives rise to a novel integrable set of conserved quantities. But at the moment we still lack a general proof that the dual hierarchy is fully integrable i.e. that all the infinitely many quantities that form this hierarchy are indeed in involution.

We then proceed to the discrete case, of potentially space-filling chains. We first review the discrete generalization of the Frenet equations. We show by an explicit computation, that the two known integrable discretizations introduced in and coincide, by devising an explicit change of variables that maps these models to each other. We then proceed to a discretization of the Zakharov-Shabat recursion relation. For this we adopt a geometric principle, that the discrete version of the recursion relation should be formulated by demanding invariance under local frame rotation. We introduce the ensuing discretizations of the conserved quantities, both in the case of the standard NLSE hierarchy and in the case of its Weyl dual hierarchy. We confirm that in the continuum limit where the distance between the vertices in the discrete case vanishes, the discretized versions of the conserved quantities indeed go smoothly over to their continuum versions, including the perfect derivative contributions which are necessary for the consistency of the higher order Zakharov-Shabat recursion relations. We conclude with a discussion on the discrete energy functions that can be utilized for example in numerical studies, to describe the physical properties of piecewise linear polygonal chains, their buckling, and the ensuing space-filling capacity.

II. FRAMING AND REPARAMETRIZING CONTINUOUS CURVES

We consider a general, filamental, space curve $\gamma$ in $\mathbb{R}^3$ that can be described by a class $C^3$ differentiable map $x(z)$. Here $z \in [0, L]$ is a generic parametrization and $L$ is the length of the curve,

$$H_{-1} \equiv L = \int_0^L dz \sqrt{x_z \cdot x_z} \equiv \int_0^L dz \left\| \frac{dx}{dz} \right\|$$

We note that this is essentially the standard time independent Nambu-Goto action of a string. For simplicity we shall assume that there are no inflection points along $\gamma$, so that $\|x_z\| \neq 0$. But a generalization to include inflection points is straightforward.

In the absence of inflection points, the curve $\gamma$ can be globally framed as follows. The unit length tangent vector is

$$t = \frac{1}{\|x_z\|} x_z$$

(2)
It is orthogonal to the unit length bi-normal vector
\[ b = \frac{x_z \times x_{zz}}{||x_z \times x_{zz}||} \]

The unit length normal vector is
\[ n = b \times t \]

The three vectors \((n, b, t)\) form the right-handed orthonormal Frenet frame, at each point of the curve \(\gamma\).

The Frenet equation relates the frames at different points along \(\gamma\). Explicitely, the Frenet equation is [1], [2]
\[
\frac{d}{dz} \begin{pmatrix} n \\ b \\ t \end{pmatrix} = \sqrt{g} \begin{pmatrix} 0 & \tau & -\kappa \\ -\tau & 0 & 0 \\ \kappa & 0 & 0 \end{pmatrix} \begin{pmatrix} n \\ b \\ t \end{pmatrix}
\]

Here
\[
\sqrt{g} = \frac{ds}{dz} = \sqrt{x_z(z) \cdot x_z(z)} = ||x_z|| = \sqrt{g_{zz}}
\]

Since \(\gamma\) is one dimensional, the metric on \(\gamma\) has only one component that we denote \(g_{zz}\). This determines the local scale of curve parametrization vis-à-vis the metric in \(\mathbb{R}^3\). Further,
\[
\kappa(z) = \frac{||x_z \times x_{zz}||}{||x_z||^3}
\]
is the (Frenet) curvature of \(\gamma\) on the osculating plane that is spanned by \(t\) and \(n\), and
\[
\tau(z) = \frac{(x_z \times x_{zz}) \cdot x_{zzz}}{||x_z \times x_{zz}||^2}
\]
is the torsion of \(\gamma\).

If the metric, curvature and torsion are known we can construct the frames by solving (3), and then proceed to construct the curve by solving (2). The solution is unique, up to rigid translations and rotations of the curve. In this manner the Frenet equation proposes us to construct energy functions for curves in \(\mathbb{R}^3\), in terms of the curvature and the torsion and the way how the curve is parametrized.

In the following we shall denote by \(s \in [0, L]\) the arc-length parameter, while \(z\) denotes generic parametrization. The arc-length parameter \(s\) measures the length along \(\gamma\) in terms of the distance scale of the three dimensional ambient space. The change of variables from a generic parameter \(z\) to the arc-length parameter \(s\) is
\[
s(z) = \int_0^z ||x_z(z')|| dz'
\]

Accordingly, we consider the effects of infinitesimal local diffeomorphisms along \(\gamma\), obtained by deforming \(s\) as follows
\[
s \rightarrow z = s + \epsilon(s)
\]
Here \(\epsilon(s)\) is an arbitrary infinitesimally small function such that
\[
\epsilon(0) = \epsilon(L) = 0 = \epsilon_s(0) = \epsilon_s(L)
\]
The Lie algebra of diffeomorphisms \( \mathfrak{g} \) of a line segment in \( \mathbb{R}^1 \) is the classical Virasoro (Witt) algebra. This proposes us to define a function \( f(s) \) on \( \gamma \) to have a weight \( h \) akin the conformal weight, if \( f(s) \) transforms according to

\[
\delta f(s) = -\left( \epsilon \frac{d}{ds} + h \epsilon_s \right) f(s)
\]

(8)

under the infinitesimal diffeomorphism \( \mathfrak{g} \). If \( f \) has weight \( h_1 \) and \( g \) has weight \( h_2 \) then the product \( fg \) has weight \( h_1 + h_2 \). We also note the finite version of (8),

\[
f(s) \rightarrow \tilde{f}(z) = \left( \frac{dt}{ds} \right)^{-h} f(s)
\]

Since the three dimensional geometric shape of the curve \( \gamma \) in \( \mathbb{R}^3 \) does not depend on the way how it has been parametrized, the embedding \( x(z) \) transforms as a scalar i.e. it has weight \( h = 0 \) under reparametrizations. Similarly, the curvature (5) and torsion (6) are scalars under reparametrizations. Infinitesimally,

\[
\delta \kappa(s) = -\epsilon(s) \frac{d\kappa}{ds} \equiv -\epsilon \kappa_s
\]

\[
\delta \tau(s) = -\epsilon(s) \frac{d\tau}{ds} \equiv -\epsilon \tau_s
\]

Generic functions can be composed by taking derivatives, multiplying and summing up functions that have definite weights.

If \( f(s) \) is a function on \( \gamma \) that has a definite weight, in general its derivative does not have a definite weight. For the derivative to acquire a definite weight, we need to extend it into a covariant derivative along \( \gamma \). Given the metric \( g_{zz} \) along \( \gamma \), we can deduce the covariant derivative by considering its action on a function \( f \) with weight \( h \). For this we demand that under the infinitesimal transformation \( \mathfrak{g} \)

\[
\left( \frac{d}{dz} + \Gamma(z) \right) \tilde{f}(z) - \left( \frac{d}{ds} + \Gamma(s) \right) f(s)
\]

\[= - \left( \epsilon \frac{d}{ds} + (h + 1) \epsilon_s \right) \left( \frac{d}{ds} + \Gamma(s) \right) f(s)
\]

Here \( \Gamma \) is the connection on \( \gamma \). Explicitely, we can choose

\[
\Gamma(z) = h \partial_z \ln \sqrt{g} \equiv h \partial_z \ln ||x_z(z)||
\]

(9)

where we have used (4). More generally, we may also choose

\[
\Gamma(z) \rightarrow \Gamma(z) + \mathcal{A}(z)
\]

(10)

Here \( \mathcal{A}(z) \) is a quantity with weight \( h = 1 \).

A general frame is related to the Frenet frame by a local \( \text{SO}(2) \) rotation, that sends

\[
\begin{pmatrix}
\mathbf{n} \\
\mathbf{b}
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\mathbf{e}_1 \\
\mathbf{e}_2
\end{pmatrix}
= \begin{pmatrix}
\cos \eta(z) & -\sin \eta(z) \\
\sin \eta(z) & \cos \eta(z)
\end{pmatrix}
\begin{pmatrix}
\mathbf{n} \\
\mathbf{b}
\end{pmatrix}
\]

(11)
The ensuing rotated version of the Frenet equation is

$$\frac{d}{dz} \begin{pmatrix} e_1 \\ e_2 \\ t \end{pmatrix} = \sqrt{g} \begin{pmatrix} 0 & \tau - \eta_z & -\kappa \cos \eta \\ -\tau + \eta_z & 0 & -\kappa \sin \eta \\ \kappa \cos \eta & \kappa \sin \eta & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ t \end{pmatrix}$$

(12)

We can write this as

$$\frac{d}{dz} \begin{pmatrix} e_1 \\ e_2 \\ t \end{pmatrix} = \sqrt{g} \begin{pmatrix} 0 & \tau_r - \kappa_g \\ -\tau_r & 0 & -\kappa_n \\ \kappa_g & \kappa_n & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ t \end{pmatrix}$$

(13)

Here $\kappa_g$ is the geodesic curvature, and $\kappa_n$ is the normal curvature, and $\tau_r$ is the relative torsion of the curve on a two dimensional surface $S \in \mathbb{R}^3$; we obtain the surface by deforming the osculating plane, around the point of contact with the curve, and different values of $\eta$ can also be interpreted in terms of different choices of the surface $S$. Notice that while $\kappa_g$ and $\kappa_n$ in (13) both depend on the surface, that is they are both frame dependent, the modulus

$$\rho = \bar{\psi} \psi = \bar{\kappa} \kappa = \kappa_g^2 + \kappa_n^2$$

(14)

is a frame independent characteristic of the curve $\gamma$. In particular, $\rho$ is a scalar under reparametrizations.

We introduce the combination

$$\psi(z) = \kappa(z) \exp \left( i \int_0^z \tau \sqrt{g} \, dz' \right)$$

(15)

Alternatively, we may introduce the more symmetric

$$\psi(z) = \kappa(z) \exp \left( i \frac{z}{2} \int_0^z \tau \sqrt{g} \, dz' + i \frac{z}{2} \int_0^L \tau \sqrt{g} \, dz' \right)$$

(16)

The decomposition (15) is essentially the Hasimoto variable of fluid dynamics [30], [31]. It has weight $h = 0$, and it is invariant under the frame rotation (12): When

$$\tau(s[z]) \rightarrow \tau(s[z]) - \frac{d\eta}{ds} \equiv \tau(z) - \frac{1}{\sqrt{g}} \frac{d\eta}{dz}$$

(17)

and

$$\kappa \rightarrow e^{i\eta} \kappa$$

(18)

we get

$$\psi(z) \rightarrow \kappa e^{i\eta(z)} \cdot \exp \left( i \int_0^z \sqrt{g} \tau - i\eta(z) \right) \equiv \tilde{\psi}(z)$$

(19)

We also note that there are the following two natural, frame independent realizations of the quantity $A$ with weight $h = 1$ in (10),

$$A \sim j_z(z) = \partial_z \ln \psi$$

(20)

and

$$A \sim \tilde{j}_z(z) = \partial_z \ln \tilde{\psi}$$

(21)

They both appear in our construction.
III. NLSE HIERARCHY OF CURVES

We are interested in frame independent energy functions of curves, that have definite
and identifiable transformation properties under curve reparametrizations. We first observe
that there are several frame independent energy functions, that have a natural geometric
interpretation. The length \( H_{-1} \equiv L \) in (1) is an example. Additional familiar examples are
the total torsion (total helicity)

\[
H_{-2} = \int_0^L \tau(s) ds
\]

and the total squared curvature

\[
H_1 = \frac{1}{2} \int_0^L \kappa^2(s) ds = \frac{1}{2} \int_0^L |t_s|^2 ds
\]

The latter determines the Worm Like Chain (Kratky-Porod) model that has been extensively
applied e.g. to study elastic properties of DNA [41]; for applications of (23) to random
surfaces, see [24]. The Bernoulli elastic curve is defined by the following linear combination
of (23) and (1),

\[
H_1 + H_{-1} = \frac{1}{2} \int_0^L \{ \kappa^2(s) + \lambda \} ds
\]

Here \( \lambda \) is a Lagrange multiplier that enforces the length constraint. Finally, we also mention
the following combination of curvature and torsion

\[
H_K = \frac{1}{2} \int_0^L \{ \alpha \kappa^2(s) + \beta \tau^2(s) \} ds
\]

This defines the Kirchhoff elastic energy of a filament, that has also been studied extensively
in the literature [5]-[7]. Here we have assumed the arc-length parametrization; recall that
both \( \tau \) and \( \kappa \) are scalars under reparametrizations.

In the context of three dimensional fluid dynamics, the length (1) is commonly employed
as the Hamiltonian of a vortex filament [5]-[11]. The dynamics of the filament is given by
the localized induction approximation

\[
\frac{d\mathbf{x}}{dt} = \mathbf{x}_s \times \mathbf{x}_{ss} = \kappa \mathbf{b}
\]

where the time evolution follows from the Rasetti-Regge bracket [23], with symplectic one-
form

\[
\int ds dt \, \mathbf{x} \cdot \mathbf{x}_s \times \mathbf{x}_t
\]

Similarly, the energy (23) has the form of standard Hamiltonian of Heisenberg spin chain,
with \( \mathbf{t}(s) \) the spin vector. The dynamics is given by

\[
\frac{d\mathbf{t}}{dt} = \mathbf{t} \times \mathbf{t}_{ss}
\]
and now the Poisson bracket is

$$\{t^{a}(s), t^{b}(s')\} = -\epsilon^{abc} t^{c}(s) \delta(s - s')$$

(27)

Hasimoto [30], [31] utilized the variable (15) to establish an equivalence between (25) and (26). For this he showed that both are equivalent to the equation of motion of the non-linear Schrödinger (NLSE) Hamiltonian

$$H_{3} = \int ds \{\bar{\psi}s \psi_{s} + \lambda(\bar{\psi}\psi)^{2}\}$$

(28)

when the Poisson bracket is

$$\{\psi(s), \bar{\psi}(s')\} = i\delta(s - s')$$

(29)

Here we have introduced a generic coupling parameters $\lambda$, it can be scaled to $\lambda = 1$ by suitable redefinitions.

In the following we adopt (29), its representations in terms of the Hasimoto decomposition, and its discrete version as the standard bracket that we denote with the subscript $s$.

The NLSE Hamiltonian system (28), (29) can be elegantly presented in a form which is manifestly covariant under reparametrizations of the curve: When we introduce an arbitrary parametrization $s \to z$, the NLSE Hamiltonian becomes

$$H_{3} = \int \sqrt{g} dz \{g^{zz}\bar{\psi}_{z}\psi_{z} + \lambda(\bar{\psi}\psi)^{2}\}$$

(30)

where we have used the definition (4) of the induced metric on $\gamma$. The Poisson bracket is similarly reparametrization covariant,

$$\{\psi(z), \bar{\psi}(z')\} = \frac{i}{\sqrt{g}} \delta(z - z')$$

(31)

The NLSE equation is known to be integrable on the finite segment $[0, L]$, when appropriate boundary conditions are imposed. In fact, the equations (25), (26) constitute a bi-hamiltonian pair that determines the NLSE hierarchy. Consequently there is an infinite set of conserved charges in involution with respect to the ensuing brackets,

$$\{H_{n}, H_{m}\} = 0 \quad n, m \in \mathbb{Z}^{+}$$

(32)

The charges are integrals of densities

$$H_{n} = \int_{0}^{L} \sqrt{g} dz \mathcal{H}_{n}(z)$$

that are functionals of $\psi$, $\bar{\psi}$ and their derivatives.

In general, we can expect that the densities in an integrable hierarchy are determined only up to an additive derivative contribution,

$$\mathcal{H}_{n} \simeq \mathcal{H}_{n} + d\Lambda$$

(33)
where \( \Lambda(z) \) is some functional of \( \psi \) and \( \bar{\psi} \) and their derivatives, and subject to an integrable boundary condition such as \( \Lambda(0) = \Lambda(L) \). Recall that in one dimension, any function can be represented as a derivative of its own integral. Consequently, we limit our attention in (33) to such functionals \( \Lambda(z) \) that are local in the fields \( \psi(z) \) and \( \bar{\psi}(z) \) and their derivatives. In that case, we call \( d\Lambda(z) \) a perfect derivative. In an integrable hierarchy the density \( H_n(z) \) of a conserved charge is in general an equivalence class, where two representatives are equivalent to each other when they share the same Poisson bracket relations and deviate from each other only by a perfect derivative. This equivalence relation defines a structure akin de Rham cohomology. A mutually consistent choice of the perfect derivative contributions in a hierarchy of conserved charges in involution, can be viewed as a "choice of gauge".

Our aim is to utilize the NLSE hierarchy to introduce frame independent energy functions, in a manner which is manifestly reparametrization covariant. Occasionally, we find it convenient to introduce \( j_z(z) \) in (20) and \( \rho(z) = \bar{\psi}(z)\psi(z) \) as the canonical variables, in lieu of the Hasimoto variables \( \psi(s) \) and \( \bar{\psi}(s) \). Note that alternatively the complex conjugate \( \bar{j}_z(z) \) in (21) could be used instead of \( j_z(z) \), and even a linear combination of the two could be utilized. In terms of the variables \( j_z \) and \( \rho \), the NLSE Hamiltonian has the following manifestly covariant representation

\[
H_3 = \int \sqrt{g} dz \left\{ g^{zz} j_z \rho - \rho g^{zz} j_z j_z + \lambda \rho^2 \right\}
\]

and the standard bracket (31) is the inverse symplectic two-form

\[
\Omega^{-1}_{33}(z, z') = \left( \begin{array}{cc} \{ j_z(z), j_z(z') \}_s & \{ j_z(z), \rho(z') \}_s \\ \{ \rho(z), j_z(z') \}_s & \{ \rho(z), \rho(z') \}_s \end{array} \right) = i \left( \begin{array}{cc} 0 & \frac{1}{\sqrt{g}} \frac{d}{dz} \\ \frac{1}{\sqrt{g}} \frac{d}{dz} & 0 \end{array} \right) \delta(z - z')
\]

We also record the ensuing NLSE equations of motion, in terms of the arc-length parameter:

\[
\frac{d}{dt} j = \{ H_3, j(s) \}_s = i \frac{d}{ds} \left[ \frac{d}{ds} j - j^2 - 2 \lambda \rho \right]
\]

and

\[
\frac{d}{dt} \rho = \{ H_3, \rho(s) \}_s = -i \frac{d}{ds} \left[ (\frac{d}{ds} - 2j) \rho \right]
\]

We remark that both (36) and (37) are perfect derivatives. Here and in the sequel we denote

\[
j \equiv j_s
\]

the variable \( j_z(z) \), in arc-length parametrization.

Instead of (25) and (26), it is often more convenient to base the bi-Hamiltonian structure on (34), (35), and with the conserved momentum

\[
P \equiv H_2 = \int ds \, j \rho = \int \sqrt{g} dz \, g^{zz} j_z \rho \quad \{ H_3, H_2 \}_s = 0
\]
as the second Hamiltonian, together with \( H_3 \). In the arc-length parametrization, the symplectic structure corresponding to \( H_2 \) is

\[
\Omega^{-1}_{2}(s, s') = \left( \{j(s), j(s')\}, \{\rho(s), j(s')\}, \{\rho(s), \rho(s')\} \right)
\]

\[
= i \left( \begin{array}{cc}
2\lambda \frac{d}{ds} & -\frac{d}{ds}(\frac{d}{ds}j) \\
(d_j - j) \frac{d}{ds} & -(\frac{d}{ds}\rho + \rho \frac{d}{ds}) \\
\end{array} \right) \delta(s - s')
\]

(39)

It is straightforward to confirm that with (38), (39) we obtain (36), (37) as the equations of motion. The infinite number of conserved densities \( H_n(s), n = 1, \ldots \) of the NLSE hierarchy can be iteratively constructed as follows,

\[
\left( \begin{array}{c}
\frac{\delta H_{n+1}}{\delta j(s)} \\
\frac{\delta H_{n+1}}{\delta \rho(s)} \\
\end{array} \right) = \Omega_3 \Omega^{-1}_{2} \left( \begin{array}{c}
\frac{\delta H_n}{\delta j(s)} \\
\frac{\delta H_n}{\delta \rho(s)} \\
\end{array} \right)
\]

(40)

and the construction is conventionally started from the conserved charge (23)

\[
H_1 = \int ds \mathcal{H}_1 = \frac{1}{2} \int ds \bar{\psi} \psi \equiv \frac{1}{2} \int ds \kappa^2
\]

(41)

We note that the length (1) and the total torsion (22) are also conserved charges in the NLSE hierarchy, even though they do not have a natural place in the standard hierarchy relations; the square of the torsion that appears in (24) is not the density of a conserved charge in the NLSE hierarchy. As a consequence, both (1) and (22) are commonly interpreted as additional conserved charges, with negative order \( H_{-1} \) and \( H_{-2} \) respectively (see e.g. [6], [8]), and included ad hoc. We may also choose

\[
H_0 = 0
\]

Finally, we point out the following relation between the NLSE hierarchy and the classical Virasoro (Witt) algebra of diffeomorphisms on the segment \([0, L] \in \mathbb{R}^1\). If we define

\[
\rho(s) = \frac{1}{L^2} \sum_{-\infty}^{\infty} \mathcal{L}_n e^{2\pi in \frac{s}{L}}
\]

(42)

and

\[
j(s) = \frac{1}{L^2} \sum_{-\infty}^{\infty} \mathcal{J}_n e^{2\pi in \frac{s}{L}}
\]

(43)

and substitute in (39) the coefficients obey the Poisson brackets

\[
\{\mathcal{L}_n, \mathcal{L}_m\}_s = 2\pi (n - m) \mathcal{L}_{n+m} + \frac{cL}{12} (n^3 - n) \delta_{n,-m}
\]

(44)

\[
\{\mathcal{L}_n, \mathcal{J}_m\}_s = -2\pi m \mathcal{J}_{n+m} - i 4\pi^2 n^2 \delta_{n,-m} L
\]

(45)

\[
\{\mathcal{J}_n, \mathcal{J}_m\}_s = -4\pi \lambda n \delta_{n,-m} L
\]

(46)

and

\[
\{L, \mathcal{L}_n\}_s = \{L, \mathcal{J}_n\}_s = 0
\]

(47)
where (44) is the classical Virasoro (Witt) algebra and \( J_n \) extends it with a current algebra; the central charge \( c \) is classically absent but in general it is non-vanishing, in the quantum theory. Note that we have here interpreted the length \( l \) as an additional element of the algebra; it is after all a conserved charge in the NLSE hierarchy. We have also renormalized the coupling \( \lambda \) in (28) as follows,

\[
\lambda \to \lambda(L) = L \lambda \equiv \hat{\lambda}
\]

Moreover,

\[
H_1 \simeq \int ds \bar{\psi} \psi \equiv \int d\rho \propto L_0
\]

where we use (42). Since \( \Omega_3 \) in (35) is field independent and \( \Omega_2 \) can be presented in terms of the current algebra generators (44)-(46) we conclude that all the classically conserved charges \( H_n \) are polynomials of the classical Virasoro-current algebra generators \( L_n \) and \( J_n \), and length \( L \).

### IV. REPARAMETRIZATION COVARIANCE OF RECURSION RELATIONS

Besides (40), the NLSE hierarchy of conserved densities \( H_n(s) \) with \( n \in \mathbb{Z}^+ \) can be constructed using the following recursive relation [33], [32]

\[
\omega_{n+1}(s) = -i \frac{d\omega_n}{ds} + \lambda \bar{\psi} \sum_{j=1}^{n-1} \omega_j \omega_{n-j}
\]  

(48)

We assume that the arc-length parametrization is used, in the case of curves in \( \mathbb{R}^3 \). We also note that alternatively, the recursion could be based on the complex conjugate of (48). When the construction in (48) is started with

\[
\omega_0(s) = 0 \\
\omega_1(s) = \frac{1}{4} \psi(s)
\]  

(49)

we reproduce the densities \( H_n(s) \) of all the higher order conserved charges as follows [32], [33],

\[
H_n(s) = \bar{\psi} \omega_n \quad n \in \mathbb{Z}^+
\]  

(50)

For a generic parametrization \( s \to z \) of the curve, we need to covariantize the recursive relation (48), with due care. For this we remind that the Hasomoto variable \( \psi(z) \) is a scalar \( i.e. \) has weight \( h = 0 \) under reparametrizations. Thus we obtain the reparametrization covariant expression of the charge \( H_1 \) in (23) by interpreting the ensuing density \( \omega_1 \) as a scalar. In a generic parametrization,

\[
\omega_1(z) = \frac{1}{4} \psi(z)
\]

\[
H_1 = \int \sqrt{g} dz H_1(z) = \int \sqrt{g} dz \bar{\psi} \omega_1
\]
Next, we aim to compute $\omega_2(z)$ from the proper reparametrization covariant version of (48). Since $\omega_1$ is a scalar, we conclude that we may set

$$\omega_2 = -i \frac{d}{dz} \omega_1$$

so that $\omega_2$ has weight $h = 1$. In (38) we have displayed the corresponding conserve charge $H_2$, in a covariant form.

We proceed to $H_3$. Since $\omega_1$ has weight $h = 1$, for a covariant charge we need to interpret the derivative term in (48) accordingly, as the weight $h = 1$ covariant derivative using the connection (9). The ensuing covariant version of (48) then reproduces (30):

$$\omega_3 \equiv \omega_{31} + \omega_{32} = -i(\frac{d}{dz} + \Gamma)g^{zz}\omega_2 + \lambda \bar{\psi}\omega_1^2$$

$$= -\frac{1}{\sqrt{g}} \partial_z (\sqrt{g}g^{zz}\partial_z \omega_1) + \lambda \bar{\psi}\omega_1^2$$

$$\Rightarrow H_3 = \int \sqrt{g} dz \bar{\psi} \omega_3 = \frac{1}{4} \int \sqrt{g} dz \{g^{zz}\bar{\psi}_z \psi_z + \lambda (\bar{\psi}\psi)^2\}$$

Note that in $\omega_3(z)$, the first term $\omega_{31}$ has weight $h = 2$ while the second term $\omega_{32}$ has weight $h = 0$. Consequently, when we proceed to $H_4$ and onwards, and compute the derivative of $\omega_3$ etc. in the recursive relation (48), the derivative operator must be replaced by the appropriate covariant derivative: In the case of $H_4$ we need to introduce a covariant derivative with weight $h = 2$ when the derivative is acting on the first term $\omega_{31}$, and a covariant derivative with $h = 0$ when acting on the second term in $\omega_{32}$,

$$-i \frac{d}{ds} \omega_3 \rightarrow -i (\partial_z + 2\Gamma)\omega_{31} - i\partial_z \omega_{32}$$

In this manner, by successively interpreting the derivative in (48) as the appropriate covariant derivative, we generate the manifestly reparametrization covariant versions of the densities $\omega_{n+1}(z)$, order by order. These densities are linear combinations of terms with different weights, and the highest weight term has weight $h = n$.

V. HIERARCHY WITH POSITIVE ORDER

We first remind that the densities $\mathcal{H}_n(s)$ are not necessarily uniquely determined. In particular, there may be the latitude (33) to add a perfect derivative to the density. In the case of an integrable model, this latitude can be restricted by imposition of proper (integrable) boundary conditions at the end points of the segment $[0, L]$. Here, our goal is to utilize the NLSE hierarchy to find frame independent and reparametrization covariant energy functions for curves. For this we note, that the end points of our curves can move freely in $\mathbb{R}^3$. As a consequence the boundary conditions that we need to impose at the end points $z = 0$ and $z = L$, are to be open. In particular, we may deform the energy density of the curve by an appropriate perfect derivative term, as long as this term does not interfere with frame independence and reparametrization covariance.

From the point of view of algebraic relations in integrable models the canonical pair of complex variables $(\psi, \bar{\psi})$ is adequate. But we are interested in describing curves. For
this, more work is necessary. We need, in addition of solving the integrable equations, to construct a solution to the Frenet equation (3), (13), followed by an integration of the curve reconstruction equation (2). For this reason we proceed to investigate the recursion relation (48) explicitly, in terms of the (Frenet frame) curvature and torsion. For clarity, in the sequel we use the arc-length parametrization, a reparametrization covariantization is straightforward following Section IV, and will be performed when conceptually desirable.

We first observe that the relation (50) between the density $H_n$ and the quantity $\omega_n$ admits the following internal symmetry: The density remains intact, when we send

$$\omega_n(s) \rightarrow e^{i\alpha(s)}\omega_n(s)$$

$$\bar{\psi}(s) \rightarrow \bar{\psi}(s)e^{-i\alpha(s)}$$

where $\alpha(s)$ is some function. Note that $\alpha(s)$ can also depend on the canonical variables. In particular, (51) does not need to be a canonical transformation. The transformation (51) converts the recursion relation (48) into

$$\omega_{n+1}(s) = -\left( i \frac{d}{ds} + \frac{d\alpha}{ds} \right) \omega_n + \lambda \bar{\psi} \sum_{j=1}^{n-1} \omega_j \omega_{n-j}$$

We recall the Hasimoto variable (15) in the arc-length parametrization

$$\psi(s) = \kappa(s) \exp \left( i \int_0^s \tau ds' \right)$$

with $(\kappa, \tau)$ the Frenet curvature and torsion, and choose

$$\alpha(s) = -\int_0^s \tau(s) ds'$$

This gives us

$$\omega_{n+1}(s) = -\left( i \frac{d}{ds} - \tau(s) \right) \omega_n + \lambda \bar{\psi} \sum_{j=1}^{n-1} \omega_j \omega_{n-j}$$

which is manifestly covariant under frame rotations.

We record the following five terms, for later reference; in computing these, we employ the Frenet frame a.k.a. unitary gauge relation (48), in which the curvature $\kappa(s)$ is a real valued quantity.

$$\omega_0 = 0$$

$$\omega_1 = \frac{1}{4} \kappa$$

$$\omega_2 = \frac{1}{4} \tau \kappa - \frac{i}{4} \kappa'$$

$$\omega_3 = -\frac{1}{4} \kappa'' + \frac{1}{4} \tau^2 \kappa + \frac{\lambda}{16} \kappa^3 - \frac{i}{4} (\tau' \kappa + 2 \tau \kappa')$$

$$\omega_4 = \frac{1}{16} \left( 4 \kappa \tau^3 - 4 \kappa \tau'' - 12 \tau \kappa'' - 12 \tau' \kappa' + 3 \lambda \kappa^3 \tau \right) + \frac{i}{16} \left( 4 \kappa''' - 12 \tau \tau' \kappa - 12 \kappa' \tau^2 - 5 \lambda \kappa^2 \kappa' \right)$$

13
We multiply these with \( \bar{\kappa} \) to obtain the ensuing versions of the integrable densities \( \mathcal{H}_n \); we remind in the Frenet frames the curvature is real so that \( \bar{\kappa} = \kappa \). We list the following four for later reference:

\[
\begin{align*}
\mathcal{H}_1 &= \frac{1}{4} \kappa^2 \\
\mathcal{H}_2 &= \frac{1}{4} \tau \kappa^2 - \frac{i}{8} \frac{d}{ds} (\kappa^2) \\
\mathcal{H}_3 &= \frac{1}{4} (\kappa')^2 + \frac{1}{4} \tau^2 \kappa^2 + \frac{\lambda}{16} \kappa^4 - \frac{i}{4} \frac{d}{ds} (\tau \kappa^2 - i \kappa \kappa') \\
\mathcal{H}_4 &= \frac{i}{2} \kappa \kappa''' \\
&\quad + \frac{1}{16} \left( 8 \kappa \kappa'' \tau + 4 \kappa^2 \tau^3 - 4 (\kappa')^2 \tau + 3 \lambda \kappa^4 \tau \right) \\
&\quad + \frac{i}{64} \frac{d}{ds} \left( -24 \kappa^2 \tau^2 + 5 \lambda \kappa^4 + 16 i \left[ \kappa^2 \tau' + \kappa \kappa' \tau \right] \right)
\end{align*}
\]

We identify in \( \mathcal{H}_1 \) the mass (number) density of NLSE. In \( \mathcal{H}_2 \) we identify the canonical momentum density, in addition of a perfect derivative term. In \( \mathcal{H}_3 \) we have the NLSE Hamiltonian density, in addition of a perfect derivative term. Finally, \( \mathcal{H}_4 \) is the complex modified KdV density together with a perfect derivative term. Note that the form of the perfect derivative terms is fully dictated by the recursion relation. Even though the presence of a perfect derivative does not contribute to the charge at the given order, it does influence the functional form of higher order conserved charges.

We can also present the recursion relation directly in terms of the integrable densities. The result is

\[
\begin{align*}
\mathcal{H}_0 &= 0 \\
\mathcal{H}_1 &= \frac{1}{4} \kappa^2 \\
\mathcal{H}_{n+1} &= -i \mathcal{D} \mathcal{H}_n + \lambda \sum_{j=1}^{n-1} \mathcal{H}_j \mathcal{H}_{n-j} \\
\mathcal{D} &= \frac{d}{ds} + (i \tau - [\ln \kappa]') = \frac{d}{ds} - \frac{d}{ds} \ln \bar{\psi} \equiv \frac{d}{ds} - \tilde{j}(s)
\end{align*}
\]

It is notable that the \( h = 1 \) quantity \( (21) \) appears.

**VI. HIERARCHY WITH NEGATIVE ORDER**

We observe that the derivative operator \( \mathcal{D} \) that appears in \( (56) \) and its conjugate

\[
\bar{\mathcal{D}} = \frac{d}{ds} + j(s)
\]

are related by the Weyl transformation,

\[
\mathcal{D} = e^{-\theta} \bar{\mathcal{D}} e^\theta
\]

when we choose

\[
e^\theta = |\psi|^2
\]
This symmetry between the two quantities (20) and (21) is most natural, and proposes us to introduce the following extension (Weyl dual) of (48), for all negative integers: We simply map

$$\omega_n \rightarrow \omega_{-n} = e^{-\theta} \omega_n$$

This gives

$$\omega_{-(n+1)} = -i \left( \frac{d\omega_{-n}}{ds} + \omega_{-n} \frac{d \ln |\psi|^2}{ds} \right) + \lambda \bar{\psi} |\psi|^2 \sum_{j=1}^{n-1} \omega_{-j} \omega_{-(n-j)}$$

with

$$\omega_{-1} = \frac{1}{\psi}$$

We define

$$\mathcal{H}_{-n} = \bar{\psi} \omega_{-n}$$

to arrive at the following recursion relations of densities

$$\mathcal{H}_0 = 0$$

$$\mathcal{H}_{-1} = 1$$

$$\mathcal{H}_{-(n+1)} = -i \bar{D} \mathcal{H}_{-n} + \lambda |\psi|^2 \sum_{j=1}^{n-1} \mathcal{H}_{-j} \mathcal{H}_{-(n-j)}$$

$$\bar{D} = \frac{d}{ds} + j(s) \equiv \frac{d}{ds} + \frac{d}{ds} \ln \psi$$

where

$$\mathcal{H}_{-n} = e^{-\theta} \mathcal{H}_n$$

We present the following three negative order densities, for reference and scrutiny, using the Frenet frame:

$$\mathcal{H}_{-2}(s) = -i \frac{d}{ds} \ln \psi = \tau - i \frac{d}{ds} \ln \kappa$$

$$\mathcal{H}_{-3}(s) = -\frac{d^2}{ds^2} \ln \psi - \left( \frac{d}{ds} \ln \psi \right)^2 + \lambda |\psi|^2$$

$$= \left[ \tau - i (\ln \kappa) \right]^2 + 1 + \lambda \kappa^2 - i \left[ \tau + i (\ln \kappa) \right]'$$

$$\mathcal{H}_{-4}(s) = \frac{i}{\psi} \frac{d^2}{ds^2} \psi - i \lambda \left( \psi \frac{d}{ds} \bar{\psi} + 4 \bar{\psi} \frac{d}{ds} \psi \right)$$

Remarkably, the two conserved charges (1) and (22) of the NLSE hierarchy now appear naturally, as quantities in the negative order recursive relation. We remind that in a conventional approach to NLSE, these two charges do not arise from the recursion relations (48). Instead, they are introduced in an ad hoc manner [6], [8] as additional charges. Furthermore, the density \( \mathcal{H}_{-3} \) can be given a familiar interpretation in terms of quantities that relate to gauge theories. This density is like the gauge invariant Proca mass for \( \tau \), when we interpreted \( \tau \) as a gauge field and \( \ln \kappa \) as the ensuing Stueckelberg field; the combination is gauge invariant under the analog U(1) gauge transformation (17), (18). See also next Section.

Unlike (1) and (22), the integral of \( \mathcal{H}_{-3} \) is not a conserved quantity in the NLSE hierarchy. For example, we find, using the standard bracket (29)

$$\{ H_3, H_{-3} \}_s = 2i \int ds \left[ \left( \frac{\ln \psi}{\psi} \right)^{\prime\prime} - 2 \lambda |\psi|^2 (\ln \psi)^{\prime\prime} \right] \neq 0$$
However, the iterative relation (59) is suggestive that the negative order densities \( \mathcal{H}_{-n} \) determine an independent hierarchy of conserved charges that are in involution amongst themselves, and possibly including \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \), in terms of the Poisson bracket (29).

\[
\{H_{-n}, H_{-m}\}_s = 0 \quad \text{for } n, m \geq 0
\]  

(62)

We have confirmed this to the densities given in (61), for example we find

\[
\{H_{-3}, H_{-4}\}_s = 3A^2 \int ds \frac{d}{ds}(\bar{\psi}\psi) \simeq 0
\]

At the moment we lack a simple proof that all the negative order charges are in involution, the integrability (62) is a conjecture; the fact that the first four charges are in involution strongly suggests that the conjecture could be correct.

In Figure 1 we summarize schematically the positive and negative order hierarchies, and the correspondence for the quantities that have a familiar interpretation, together with their Weyl duality relations.

FIG. 1: Schematic relations between those conserved densities that have a natural interpretation in terms of gauge field theory, in the positive order (55) and negative order (59), (61) hierarchies. AHM/NLSE is for Abelian Higgs Model a.k.a. nonlinear Schrödinger equation, Weyl denotes relation by the Weyl duality between the hierarchies, and Z-S stands for Zakharov-Shabat recursive relation. Both hierarchies amalgamate at \( H_0 = 0 \).

VII. FRAME INDEPENDENCE AND GAUGE STRUCTURE

We employ the recursion relations (56), (59) to specify Hamiltonian energy functions, that describe curves and their dynamics in \( \mathbb{R}^3 \). The explicit recursion relations that we
have presented utilize a fixed variable $s \in [0, L]$ that we have chosen to identify with the arc-length parameter of the curve. However, we have also explained how reparametrization covariant generalizations can be introduced, order by order in the recursion.

Notwithstanding, in order to describe a curve in $\mathbb{R}^3$ we need in addition to solve the Frenet equation \[3\], \[13\]. The Frenet equation involves the curvature and torsion, and as such it is frame dependent. We proceed to complement reparametrization covariance with manifest frame independence.

According to \[17\], \[18\] the curvature and torsion ($\kappa, \tau$) transform exactly like an Abelian Higgs multiplet ($\phi, A$) under frame rotations, provided we identify the Frenet frame curvature $\kappa$ as the modulus of a complex (Higgs) scalar field $\phi$, and the torsion $\tau$ as the one dimensional $U(1)$ gauge field $A$. In the arc-length parametrization, the action of frame rotation can thus be summarized as follows:

$$\phi(s) \sim \kappa(s) \rightarrow e^{i\eta(s)}\kappa(s)$$

$$A(s) \sim \tau(s) \rightarrow \tau(s) - \eta(s)$$

Consequently frame independent Hamiltonians for curves can be constructed in parallel with $U(1)$ gauge invariant Hamiltonians of the Higgs multiplet ($\phi, A$). An example of the latter is the standard Abelian Higgs model Hamiltonian

$$H_3 = \int ds \left\{ |(\frac{d}{ds} + i A)\phi|^2 + \lambda|\phi|^4 \right\}$$

(63)

If we identify the Hasimoto variable as follows,

$$\psi(s) = \phi(s) \exp\left\{i \int A \right\}$$

(64)

we recover the NLSE Hamiltonian \[28\]. On the other hand, if in \[63\] we introduce the change of variables

$$\kappa \simeq \phi \rightarrow \sigma e^{i\theta}$$

$$\tau \simeq A \rightarrow J = A - i \frac{d}{ds} \ln \phi + i \frac{d}{ds} \ln \phi^*$$

(65)

the NLSE Hamiltonian becomes

$$H_3 = \int ds \left\{ \left( \frac{d\sigma}{ds} \right)^2 + e^2 \sigma^2 J^2 + \lambda \sigma^4 \right\}$$

(66)

Like $\psi$ in \[64\], both $J$ and $\sigma$ are manifestly frame (gauge) independent variables; $J$ is commonly called the supercurrent variable, in the context of Abelian Higgs model; $\sigma$ is the Higgs condensate.

The entire NLSE hierarchy can be similarly presented in terms of the frame independent variables \[65\]. For example, for $H_2$ we get from \[38\] (note: $\sigma = \sqrt{\rho}$)

$$H_2 = \int ds \sigma^2 J$$

(67)
In the Abelian Higgs model, this is the canonical momentum; for $H_1$ we have in (56)

$$H_1 = \int ds \sigma^2$$

(68)

which is the Higgs mass term, in the Abelian Higgs model.

For the negative order density $H_{-2}$ we get from (61)

$$H_{-2} = \tau - i \frac{d}{ds} \ln \kappa \simeq \tau + \frac{d}{ds} \arg \kappa - i \frac{d}{ds} \ln \sigma$$

The charge is

$$H_{-2} = \int ds J$$

(69)

We identify (69) as a one dimensional version of helicity, or Abelian Chern-Simons term, for the gauge invariant variable $J$. For the density of $H_{-3}$ we get similarly

$$H_{-3} = \left( i \tau - \frac{d \ln \kappa}{ds} \right)^2 + i \frac{d}{ds} \left[ \tau - i \frac{d \ln \kappa}{ds} \right] + 1$$

$$\simeq -J^2 + i \frac{d}{ds} J + 1$$

(70)

The conserved charge is

$$H_{-3} = \int ds J^2 + L$$

(71)

where $L$ is the length of the curve. In the Abelian Higgs model, we identify the first term in (70), (71) as the one dimensional version of the gauge invariant i.e. frame independent Proca mass, for the variable $J$.

VIII. DISCRETE CHAINS

In the discrete case of a piecewise linear space polygon i.e. chain, the reparametrization i.e. diffeomorphism covariance is not of concern. However, the requirement of invariance under frame rotations persists. Consequently, we start by revisiting the construction of frames for a piecewise linear polygonal chain in $\mathbb{R}^3$ [39]. We take $r_i$ ( $i = 1, ..., N$) to be the coordinate sites of the vertices, and at each vertex site $i$ we introduce the unit tangent vector

$$t_i = \frac{r_{i+1} - r_i}{|r_{i+1} - r_i|}$$

(72)

We frame the chain by introducing at each vertex $i$ the unit binormal vector

$$b_i = \frac{t_{i-1} \times t_i}{|t_{i-1} \times t_i|}$$

(73)

and the unit normal vector

$$n_i = b_i \times t_i$$

(74)
The orthogonal triplet \((\mathbf{n}_i, \mathbf{b}_i, \mathbf{t}_i)\) defines the discrete Frenet frame at the vertex \(\mathbf{r}_i\) of the chain. The bond angles along the chain are

\[
\kappa_i \equiv \kappa_{i+1,i} = \arccos (\mathbf{t}_{i+1} \cdot \mathbf{t}_i)
\]

and the torsion angles are

\[
\tau_i \equiv \tau_{i+1,i} = \text{sign}\{\mathbf{b}_{i-1} \times \mathbf{b}_i \cdot \mathbf{t}_i\} \cdot \arccos (\mathbf{b}_{i+1} \cdot \mathbf{b}_i)
\]

If these angles are known, we can use the discrete Frenet equation

\[
\begin{pmatrix}
\mathbf{n}_{i+1} \\
\mathbf{b}_{i+1} \\
\mathbf{t}_{i+1}
\end{pmatrix} =
\begin{pmatrix}
\cos \kappa \cos \tau & \cos \kappa \sin \tau & -\sin \kappa \\
-\sin \tau & \cos \tau & 0 \\
\sin \kappa \cos \tau & \sin \kappa \sin \tau & \cos \kappa
\end{pmatrix}_{i+1,i}
\begin{pmatrix}
\mathbf{n}_i \\
\mathbf{b}_i \\
\mathbf{t}_i
\end{pmatrix}
\]

(77)

to construct the frame at vertex \(i + i\) from the frame at vertex \(i\). Once we have the frames we get the entire chain, up to global rotations and translations, using

\[
\mathbf{r}_k = \sum_{i=0}^{k-1} |\mathbf{r}_{i+1} - \mathbf{r}_i| \cdot \mathbf{t}_i
\]

(78)

This amounts to an integration of (2), in the discrete case. For simplicity, in the sequel we assume that the bond lengths \(i.e.\) distances between the neighboring vertices are constant

\[
|\mathbf{r}_{i+1} - \mathbf{r}_i| = a
\]

(79)

With no loss of generality we can set \(\mathbf{r}_0 = 0\), and choose \(\mathbf{t}_0\) so that it points along the positive \(z\)-axis, so

\[
\mathbf{r}_1 = a \hat{z}
\]

In parallel with the continuum curves, (77) proposes us to construct energy functions for discrete chains in terms of the bond and torsion angles.

We note that (78) does not involve the vectors \(\mathbf{n}_i\) and \(\mathbf{b}_i\). Thus, as in the case of continuous curves, we may introduce an arbitrary SO(2) rotation between them, without affecting the chain. At each vertex site \(i\) this frame rotation acts as follows,

\[
\begin{pmatrix}
\mathbf{n} \\
\mathbf{b} \\
\mathbf{t}
\end{pmatrix}_i \rightarrow
\begin{pmatrix}
\cos \Delta_i & \sin \Delta_i & 0 \\
-\sin \Delta_i & \cos \Delta_i & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\mathbf{n} \\
\mathbf{b} \\
\mathbf{t}
\end{pmatrix}_i
\]

(80)

Here the \(\Delta_i\) are the arbitrarily chosen local rotation angles. On the bond angles, the effect of frame rotations can be presented as follows,

\[
\kappa_i T^2 \rightarrow \kappa_i (\cos \Delta_{i+1} T^2 + \sin \Delta_{i+1} T^1)
\]

(81)

This is the real SO(2) version of the complex U(1) rotation (18). Thus we may consider \(\kappa_i\) as a complex variable so that its real part coincides with the \(T^2\) component of (81), and the imaginary part is the \(T^1\) component of (81). The frame transformation property is

\[
\kappa_i \rightarrow e^{i\Delta_{i+1}} \kappa_i
\]

(82)
The bond angle (73) is the modulus of this variable. On the torsion angles, the frame rotation has the following effect

\[ \tau_i \rightarrow \tau_i - \Delta_{i+1} + \Delta_i \]  

(83)

A priori, the fundamental range of the bond angle \( \kappa_i \) is \([0, \pi]\). For the torsion angle the range is \( \tau_i \in [-\pi, \pi) \). Consequently we may identify \((\kappa_i, \tau_i)\) with the canonical latitude and longitude angles of a two-sphere \( S^2 \). However, in the sequel we find it useful to extend the range of \( \kappa_i \) into \([-\pi, \pi] \ mod(2\pi)\), but with no change in the range of \( \tau_i \). We compensate for this two-fold covering of \( S^2 \) by introducing the following \( \mathbb{Z}_2 \) symmetry

\[ \kappa_j \rightarrow -\kappa_j \quad \text{for all } j \geq i \]

\[ \tau_i \rightarrow \tau_i - \pi \]  

(84)

This is a special case of (80), with

\[ \Delta_l = \pi \quad \text{for } l \geq i + 1 \]

\[ \Delta_l = 0 \quad \text{for } l < i + 1 \]

IX. THE DISCRETIZED NONLINEAR SCHRÖDINGER EQUATION

Two a priori different integrable discrete versions of the continuum NLSE have been presented, the one in [35] and the one in [36]. We review these models, before we proceed to derive a discretization of [53], [56], using the frame independence of a discrete chain as our guiding principle. Following [32], we denote the two discrete models by LNS\(_1\) and LNS\(_2\), respectively. It can be shown, that LNS\(_1\) is equivalent to the lattice Heisenberg spin chain model (LHM) [32]. In [40] it has also been shown, that LNS\(_1\) and LNS\(_2\) are gauge equivalent the sense, that their Lax pair representations can be gauge transformed to each other. But a proof based on gauge equivalence of the Lax pair does not give an explicit relation between the variables. In particular, it does enable us to reveal, how to describe discrete curves, transferably in terms of the two versions of discretized non-linear Schrödinger equation. For this reason, we show how to establish the equivalence of LHM and LNS\(_2\) in terms of an explicit change of variables.

We start by describing the lattice Heisenberg spin chain model i.e. LHM. With \( s_i \) a three component unit vector at site \( i = 1, ..., N \), the Hamiltonian is (for notational simplicity we set bond length \( a = 2 \) in (79) and take the classical spin parameter \( s \) in [32] to have value \( s = 1 \))

\[ H_{LHM} = - \sum_{i=1}^{N-1} \ln(1 + s_i \cdot s_{i+1}) \]  

(85)

and the Poisson bracket is the discrete version of (27),

\[ \{ s^a_i, s^b_j \} = -\epsilon^{abc} s^c_j \delta_{ij} \]  

(86)

The equation of motion for \( s_i \) is the Landau-Lifschitz equation

\[ \frac{ds_i}{dt} = \{ H_{LHM}, s_i \} = -s_i \times \frac{\partial H_{LHM}}{\partial s_i} \]  

(87)
It reproduces (26) in the continuum limit $a \to 0$.

We may use (85) to introduce an energy function for discrete polygonal chains. For this we simply identify the spin variable $s_i$ with the tangent vector $t_i$, defined in (72). Note that since only $s_i \sim t_i$ appears in (85), (86) the energy function (85) determines chain dynamics which is manifestly invariant under the local frame rotations (80). In terms of the discrete Frenet frame, the equation of motion (87) becomes

$$\frac{dt_i}{dt} = 1/2 \left( \tan \frac{\kappa_{i+1}}{2} b_{i+1} - \tan \frac{\kappa_i}{2} b_i \right)$$

so that for our polygonal chain we obtain, from (72), the discrete version of the localized induction approximation (25),

$$\frac{dr_i}{dt} = \tan \frac{\kappa_i}{2} b_i$$

Since the Landau-Lifschitz equation is integrable there are conserved quantities, equal in number with the canonical coordinates (or momenta). In particular, we note that the equation of motion (88) preserves the closure condition of the chain

$$\frac{d}{dt} \left\{ \sum_{i=1}^{N} t_i \right\} = 0$$

This is the discrete version of the continuum statement that $H_{-1}$ in (1), (59) is a conserved quantity.

In terms of the Frenet frame bond (75) and torsion (76) angles, with $(\kappa_{i+1,i}, \tau_{i+1,i}) \equiv (\kappa_i, \tau_i)$ the Poisson bracket (86) is

$$\{ \kappa_i, \kappa_{i+1} \} = \sin \tau_{i+1}$$

$$\{ \kappa_{i-2}, \tau_i \} = -\cos \tau_{i-1} \csc \kappa_{i-1}$$

$$\{ \kappa_{i-1}, \tau_i \} = \cot \frac{\kappa_{i-1}}{2} + \cos \tau_i \cot \kappa_i$$

$$\{ \kappa_i, \tau_i \} = -\cot \frac{\kappa_i}{2} - \cos \tau_i \cot \kappa_{i-1}$$

$$\{ \kappa_{i+1}, \tau_i \} = \cos \tau_{i+1} \csc \kappa_i$$

$$\{ \tau_{i-1}, \tau_i \} = \csc \kappa_{i-1} \left( \sin \tau_i \cot \kappa_i + \sin \tau_{i-1} \cot \kappa_{i-2} \right)$$

$$\{ \tau_{i-1}, \tau_{i+1} \} = \sin \tau_i \csc \kappa_{i-1} \csc \kappa_i$$

The Hamiltonian is

$$H = -\sum_i \ln (1 + t_i \cdot t_{i+1}) = -2 \sum_i \ln \cos \frac{\kappa_i}{2}$$

and the equation of motion (88) is

$$\frac{d\kappa_i}{dt} = \tan \frac{\kappa_{i-1}}{2} \sin \tau_i - \tan \frac{\kappa_{i+1}}{2} \sin \tau_{i+1}$$

(92)
\[
\frac{d\tau_i}{dt} = \cos \tau_i \left( \cot \kappa_i \tan \frac{\kappa_{i-1}}{2} - \cot \kappa_{i-1} \tan \frac{\kappa_i}{2} \right) \\
\quad + \tan \frac{\kappa_{i+1}}{2} \csc \kappa_i \cos \tau_{i+1} - \tan \frac{\kappa_{i-2}}{2} \csc \kappa_{i-1} \cos \tau_{i-1}
\]

(93)

From (93) we immediately compute

\[
\frac{d}{dt} \sum_i \tau_i = 0
\]

This is the discrete version of the conservation of total torsion \(H_{-2}\) in (22). We also note that in the continuum limit, (91) becomes (23).

We now show that the equations of motion (92), (93) coincide with those of the LNS\(_2\) model. For this we introduce the following discrete variable,

\[
\psi_i = \tan \frac{\kappa_i}{2} e^{i\vartheta_i}
\]

(94)

where we have the (anti)symmetrized combination

\[
\vartheta_i = \frac{1}{2} \left( \sum_{k=1}^i \tau_k - \sum_{k=i+1}^N \tau_k \right)
\]

Note that (94) does not remain invariant under (82), (83). It should not be interpreted as the proper discretized version of the frame independent Hasimoto variable (16). Consequently we proceed by explicitly assuming the Frenet framing.

A direct computation, using (90), gives

\[
\frac{d\psi_i}{dt} = \frac{1}{2} \sec^2 \frac{\kappa_i}{2} e^{i\vartheta_i} \frac{d\kappa_i}{dt} + i \tan \frac{\kappa_i}{2} e^{i\vartheta_i} \frac{d\vartheta_i}{dt}
\]

On the other hand,

\[
(1 + |\psi|^2)(\psi_{i+1} + \psi_{i-1}) = \sec^2 \frac{\kappa_i}{2} \left( \tan \frac{\kappa_{i+1}}{2} e^{i\tau_{i+1}} + \tan \frac{\kappa_{i-1}}{2} e^{-i\tau_{i}} \right) e^{i\vartheta_i}
\]

By absorbing a factor of 2 in the definition of \(t\) and redefining

\[
\psi_i \rightarrow \psi_i e^{it}
\]

we obtain the LNS\(_2\) equation [35]

\[
\frac{i}{dt} \frac{d\psi_i}{dt} = -(\psi_{i+1} - 2\psi_i + \psi_{i-1}) - |\psi|^2 (\psi_{i+1} + \psi_{i-1})
\]

This is a Hamiltonian equation of motion, with

\[
H = -\sum_i \left( \psi_i^* \psi_{i+1} + \psi_i^* \psi_{i+1} \right) = -2 \sum_i \tan \frac{\kappa_i}{2} \tan \frac{\kappa_{i+1}}{2} \cos \tau_{i+1}
\]

and Poisson brackets

\[
\{ \psi_i, \psi_j^* \} = i \left( 1 + |\psi|^2 \right) \delta_{ij}
\]

\[
\{ \psi_i, \psi_j \} = \{ \psi_i^*, \psi_j^* \} = 0
\]

These relations define the LNS\(_2\) model. Thus we have established the equivalence between the LHM and LNS\(_2\) models, by a direct computation in terms of the discrete Frenet frames.
X. DISCRETIZED RECURSION RELATIONS OF THE POSITIVE ORDER

As an energy function for a discrete chain, the LHM (85), (86) engages only the tangent vector \( \mathbf{t}_i \approx \mathbf{s}_i \) and consequently it is, as such, manifestly frame independent. But the combined variable (94) that relates LHM and LNS does not transform covariantly under frame rotations. Consequently it can not be interpreted as a discrete frame invariant version of the Hasimoto variable. Our goal, in the following, is to derive a proper \( i.e. \) manifestly frame independent discretized version of the continuum NLSE hierarchy (53) of conserved charges. These can be utilized as energy functions, in the case of piecewise linear polygonal chains.

As the guiding principle we shall utilize \( solely \) the concept of invariance under frame rotations, in terms of the formal identification as gauge transformations: We demand that the discretized versions of the conserved charges should be manifestly invariant under the local frame rotations (80) \( i.e. \) they should derive from a gauge principle. They should go over to their continuum NLSE hierarchy counterparts, including the perfect derivative contributions, and smoothly in the limit where the bond length \( a \) between the neighboring vertices (79) vanishes.

We note that the primary emphasis here is on ensuring frame independence rather than on preserving integrability. The former is a necessary requirement for constructing meaningful energy functions for discrete chains, while the latter is a bonus. We presume that if the discretized recursion relations are carefully constructed so that frame invariance is preserved, these relations will also lead to integrability, if indeed the latter can be consolidated with the former. For this, we shall confirm that in a carefully executed continuum limit we indeed obtain the conserved charges of the NLSE hierarchy, including the perfect derivative contributions. In combination with frame independence, this is a strong indication that the discrete hierarchies we present are integrable.

We introduce the following discrete version of the Hasimoto variable (15),

\[
\psi_i = \kappa_i \exp\{ia \sum_{k=1}^{i} \tau_{k+1,k}\}
\]  

(95)

Note that (95) is different from (94). The latter is not manifestly frame independent, while (95) is constructed to be so. We continue to identify the \( \kappa_i \equiv \kappa_{i+1,i} \) as the bond angles (75). But from the conceptual point of view, there is now an advantage to consider the bond angles \( \kappa_i \) as variables that have support at the corresponding \( i^{th} \) vertex.

Similarly, the variables \( \tau_{k+1,k} \) are related to the chain geometry, as torsion angles according to (76). Unlike the bond angles that reside at the vertices, the \( \tau_{k+1,k} \) are now interpreted as variables that have support on the link that connects the vertices \( k \) and \( k + 1 \).

As geometric bond and torsion angles, \( (\kappa_i; \tau_{i+1,i}) \) relate to the discrete Frenet framing of the chain. Again, in the general frames, we extend \( \kappa_i \) into a complex variable. The site dependent frame rotation that sends

\[
\kappa_{i+1,i} \equiv \kappa_i \rightarrow \kappa_i \exp\{i\Delta_{i+1}\}
\]

\[
\tau_{i+1,i} \rightarrow \tau_{i+1,i} - \frac{1}{a}(\Delta_{i+1} - \Delta_i)
\]

(96)

leaves the Hasimoto variable (95) intact (with \( \Delta_1 = 0 \)). Note that in relation to (83), we have re-defined the torsion angles by scaling them with the bond length \( a \).
We shall now introduce the discrete analogs of the densities $\omega_n(s)$ in (48). We denote them $w_n[i]$. We propose to evaluate the $w_n[i]$ from the following discretization of the (general frame) recursion relation (53),

$$w_{n+1}[i] = \frac{i}{a} \left\{ w_n[i] - e^{-i\alpha_{i+1,i}} w_n[i-1] \right\} + \lambda \bar{\kappa}_i \sum_{l<n} w_l[i] w_{n-l}[i], \quad (97)$$

The recursion starts with

$$w_0[i] = 0$$

$$w_1[i] = \frac{1}{4} \kappa_i \simeq \frac{1}{4} \kappa_{i+1,i} \quad (98)$$

We have here carefully constructed (97) using the standard lattice gauge theory [42] discretization of covariant derivative. We note that there are variants of this discretization [42]. In particular we may introduce

$$w_{n+1}[i] = \frac{i}{a} \left\{ w_n[i + 1] e^{i\alpha_{i+1,i+1}} - w_n[i] \right\} + \lambda \bar{\kappa}_i \sum_{l<n} w_l[i] w_{n-l}[i],$$

But for the present purposes it is sufficient to consider the version (97). We note that with the initialization (98), the quantities $w_n[i]$ transform according to

$$w_n[i] \rightarrow e^{i\Delta_{i+1} \cdot w_n[i]}$$

under discrete frame rotations. In particular, (97) is covariant under frame rotations.

In analogy with (50), we introduce the following frame invariant quantities,

$$N_n[i] = \bar{\kappa}_i w_n[i] \quad (99)$$

and in the following we proceed by using the Frenet framing where $\bar{\kappa}_i \equiv \kappa_i$. We verify that in the continuum limit $a \rightarrow 0$ the ensuing quantities (99) reproduce the densities (56), including the perfect derivative contributions. In combination with discrete frame rotation covariance, this will support the conjecture, that (99) are the proper discrete versions of the continuum conserved NLSE charges. We confirm this explicitly, for the four densities in (55).

In the case of $w_1[i]$, it is clear that in the continuum limit the quantity $N_1[i]$ is reduced to

$$\lim_{a \rightarrow 0} N_1[i] = \frac{\kappa^2}{4}, \quad (100)$$

which coincides with the density $H_1$ in (55).

For $w_2[i]$, we get

$$w_2[i] = \frac{i}{a} \left[ w_1[i] - e^{-i\alpha_{i+1,i}} w_1[i-1] \right]$$

$$= \frac{i}{a} \left[ \kappa_i - e^{-i\alpha_{i+1,i}} \frac{\kappa_{i-1}}{4} \right] \quad (101)$$

In the continuum limit, this gives

$$\lim_{a \rightarrow 0} N_2[i] = \frac{\tau \kappa^2}{4} - \frac{i}{8} \frac{d}{ds} \left( \kappa^2 \right) \quad (102)$$

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which is the conserved density $H_2(s)$ of NLSE hierarchy, including the perfect derivative contribution.

The $w_3[i]$ reads

$$w_3[i] = \frac{i}{a} \left\{ w_2[i] - e^{-ia\tau_{i+1,i}} w_2[i - 1] \right\} + \lambda \kappa_i w_1[i] w_1[i]$$

$$= \frac{i}{a} \left\{ \frac{i}{a} \left[ \frac{\kappa_i}{4} - e^{-ia\tau_{i+1,i}} \frac{\kappa_{i-1}}{4} \right] - e^{-ia\tau_{i+1,i}} \left( \frac{i}{a} \left[ \frac{\kappa_{i-1}}{4} - e^{-ia\tau_{i,i-1}} \frac{\kappa_{i-2}}{4} \right] \right) \right\} + \lambda \kappa_i \frac{\kappa_i \kappa_i}{4} \frac{\kappa_i}{4}$$

In the continuum limit,

$$\lim_{a \to 0} N_3[i] = -\frac{1}{4} \kappa^2 \kappa'' - \frac{i}{2} \tau \kappa' \kappa - \frac{i}{4} \tau' \kappa^2 + \frac{1}{4} \tau^2 \kappa^2 + \frac{\lambda}{16} \kappa^4$$

$$= \left( \frac{\kappa' \kappa'}{4} - \frac{i}{4} \kappa'' \kappa \right) + \left( \frac{\kappa' \kappa'}{4} + \frac{\tau^2 \kappa^2}{4} + \frac{\lambda}{16} \kappa^4 \right)$$

This coincides with the density of the nonlinear Schrödinger Hamiltonian, together with the perfect derivative term in (55).

For the fourth quantity,

$$w_4[i] = \frac{i}{a} \left\{ w_3[i] - e^{-ia\tau_{i+1,i}} w_3[i - 1] \right\} + 2 \kappa_i w_2[i] w_1[i]$$

In the continuum limit, we have verified that the ensuing charge $N_4[i]$ reproduces $H_4(s)$ in (55), inclusive the perfect derivative term.

**XI. DISCRETIZED RECURSION RELATIONS OF THE NEGATIVE ORDER**

We proceed to the discrete version of the negative order hierarchy (59). We propose the following manifestly frame rotation invariant discretization,

$$w_{-(n+1)}[i] = -\frac{i}{a \kappa_i} \left\{ \kappa_i^2 w_{-n}[i] - \kappa_{i-1}^2 e^{-ia\tau_{i+1,i}} w_{-n}[i - 1] \right\} + \lambda \kappa_i^2 \sum_{l<n} w_{-l}[i] w_{-(n-l)}[i]$$

As before,

$$w_0[i] = 0$$

and we initialize the recursion by setting

$$w_{-1}[i] = \frac{1}{\kappa_i}$$

This ensures that $w_{-(n+1)}[i]$ transforms covariantly under discrete frame rotations,

$$w_{-n}[i] \to e^{-i\Delta_{i+1}} w_{-n}[i]$$

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The higher order negative order quantities \( N_{-n}[i] \) are defined as

\[
N_{-n}[i] = \kappa_i w_{-n}[i]
\]  

(107)

In the following we proceed using the Frenet frames; by construction, the final results are frame independent.

We have explicitly confirmed, that in the continuum limit this produces the correct Frenet frame densities in (61), including the perfect derivative contributions. For example, we immediately confirm that

\[
N_{-1} = 1,
\]

Similarly, for \( w_{-2}[i] \) we have

\[
w_{-2}[i] = -\frac{i}{a\kappa_i^2} \left\{ \kappa_i^2 w_{-1}[i] - \kappa_{i-1}^2 e^{-i\alpha_{i+1}^j} w_{-1}[i-1] \right\}
\]

(108)

In the continuum limit, (107) gives immediately

\[
\lim_{a \to 0} N_{-2}[i] = \tau - i(\ln \kappa)'
\]

(109)

which coincides with the density \( H_{-2} \) in (61), including the perfect derivative. Similarly, we find that \( N_{-3}[i] \) produces the Proca mass term \( H_{-3}(s) \) in (61) including the perfect derivative term: We have

\[
\omega_{-3}[i] = -\frac{i}{2\kappa_i^2} \left( \kappa_i^2 w_{-2}[i] - \kappa_{i-1}^2 e^{-i\alpha_{i+1}} w_{-2}[i-1] \right) + \lambda \kappa_i^3 w_{-1}[i] w_{-1}[i]
\]

We have also confirmed by explicit computation, that \( N_{-4}[i] \) produces \( H_{-4}(s) \) in (61), including the perfect derivative. Consequently, we conjecture that this is the case to all negative order terms.

Finally, we note that if we introduce the discrete version of the Weyl transformation

\[
N_{-n}[i] \to e^{\theta[i]} N_{-n}[i] \equiv N_{-n}^\theta[i]
\]

with

\[
\theta[i] = \ln |\kappa_i|^2
\]

we find that in the continuum limit we recover the densities with positive order,

\[
N_{-n}[i] \to N_{-n}^\theta[i] \simeq N_n[i] \xrightarrow{a \to 0} H_n(s)
\]

We have confirmed this explicitly, to order \( n = 4 \).

XII. ENERGY FUNCTIONS FOR DISCRETE CHAINS

In [25]-[29], the following energy function has been introduced and applied to model folded proteins as space filling piecewise linear polygonal chains,

\[
E = \sum_{i=1}^{N} \left\{ -2\sigma_{i+1}\sigma_i + b \sigma_i^2 J_i^2 + c(\sigma_i^2 - m^2)^2 \right\} + \sum_{i=1}^{N} \left\{ d J_i + q \sigma_i^2 J_i + e J_i^2 \right\} \quad (\sigma_{N+1} = 0)
\]

(110)
The functional form of this energy function is justified by a naive discretization of the following linear combination of charges $H_a \ (a = -3, -2, 1, 2, 3)$, that appear in the continuum NLSE hierarchy and its Weyl dual hierarchy; see equations (66)-(71)

$$E = \int ds \left\{ \left( \frac{d\sigma}{ds} \right)^2 + e^2 \sigma^2 J^2 + \lambda \sigma^4 + \mu^2 \sigma^2 \right\} + \int ds \left\{ dJ + q\sigma^2 J + e J^2 \right\} \tag{111}$$

Here the frame independent i.e. gauge invariant supercurrent variables are utilized. The energy function (111) has a natural gauge theory interpretation: The first line is the Abelian Higgs model in the supercurrent variables, with spontaneously broken potential term when $\mu^2 < 0$. The second line displays the Chern-Simons term, the canonical momentum and the Proca mass term, respectively. When a naive discretization of the derivative contribution is implemented, 

$$\left( \frac{d\sigma}{ds} \right)^2 \to (\sigma_{i+i} - \sigma_i)^2 \sim 2\sigma_i^2 - 2\sigma_{i+i} \sigma_i$$

we clearly arrive at (110). This discretization of the energy function (111) appears to correctly describe various properties of folded proteins [26]-[29].

Unfortunately, (110) also leads to a conceptual predicament. As the bond angle, the variable $\sigma_i$ in (110) is by construction a non-negative quantity, and in particular the first term in (110) does not remain invariant under a local transformation that send $\sigma_k \to -\sigma_k$ at one given site. On the other hand, (111) is even in $\sigma$ and consequently in this continuum energy function, $\sigma(s)$ can be extended into a real valued variable. In the discrete case, we have previously used the $\mathbb{Z}_2$ symmetry transformation (84) to extend the bond angle variable $\sigma_i \sim \kappa_i$ from positive values into both positive and negative values. This symmetry transformation leaves the vectors $t_i$ intact, and as a consequence the discrete chain constructed from (78) is also intact. Consequently, from the point of view of discrete chains, it might be desirable to have a discrete energy function that remains invariant under this symmetry transformation. Unfortunately, (110) does not have this property.

We note that the continuum version of the $\mathbb{Z}_2$ transformation corresponds to a discontinuous frame flipping by $\pi$ at an inflection point of the curve; the continuum version of (84) engages both the unit step and the Dirac $\delta$-function [39].

Our goal is to minimally improve (110) into a discrete energy function which is constructed from the densities in the discrete NLSE hierarchy, so that the ensuing energy has the local $\mathbb{Z}_2$ symmetry (84). In parallel with (111), we are instructed to try and proceed by using the discretized versions of the charges $H_a \ (a = -3, -2, 1, 2, 3)$. These charges have been derived in the previous two Sections, these are the quantities $N_a[i]; \ a \in \mathbb{Z}$. These quantities are by construction fully frame independent and consequently invariant under the local symmetry transformation (84). Consequently we start by introducing the $\mathbb{Z}_2$ invariant discrete combination

$$\alpha_3 N_3[i] + \alpha_2 N_2[i] + \alpha_1 N_1[i] + \alpha_{-2} N_{-2}[i] + \alpha_{-3} N_{-3}[i] \tag{112}$$

By construction, this overlays the putative energy function. In general the charges $N_a[i]$ have both a real part and an imaginary part,

$$N_a[i] = Re\ N_a[i] + iIm\ N_a[i]$$

and these are both independently invariant under the $\mathbb{Z}_2$ transformation; we have observed [55], [61] that in the continuum limit, the imaginary parts are perfect derivatives, except
for a term in $\mathcal{H}_{-3}$. As a consequence, whenever $N_a[i]$ is complex, we can interpret both the real part and the imaginary part, separately, as contributions to the energy. Accordingly, we account for them independently by substituting

$$N_a[i] \rightarrow \beta_1 \text{Re} N_a[i] + \beta_2 \text{Im} N_a[i] \quad \beta_{1,2} \in \mathbb{R}$$

in the expansion (112). The ensuing real-valued quantity can be used as an energy function:

According to the results in the previous Sections, its continuum limit contains the density in (111), in addition of terms that are perfect derivatives. In this way we can construct a discrete energy function that extends (110) in a manner which ensures invariance under the $\mathbb{Z}_2$ transformation (84).

Unfortunately, (112) is quite elaborate in comparison with (110). But we have found that a discrete energy density which extends (110) in a manner which is invariant under (84) and yields the density in (111) in the continuum, can also be obtained by considering only the three quantities $N_a[i]$ with $a = -2, 1, 2$.

We start with $N_1[i]$. It gives the following mass term contribution, we now work in the general frame where the $\kappa_i$ are complex

$$E_1[i] = m^2 \bar{\kappa}_i \kappa_i$$

with $m$ a parameter.

We proceed to $N_2[i]$ in (101). We obtain the contribution

$$N_2[i] \sim \bar{\kappa}_i \kappa_i - \bar{\kappa}_i e^{-ia\tau_{i+1,i}^{+1}} \kappa_i^{-1}$$

The first term can be combined with (114), it amounts to a redefinition of the a priori free parameter $m$.

Following Section VII, we conceptually identify the second term as the standard U(1) gauge invariant kinetic term that is commonly introduced in lattice Abelian Higgs model [42]. For this, we simply interpret

$$\kappa_i \sim \phi_{i+1}$$

as the complex lattice Higgs field, and

$$\tau_{i+1,i} \sim A_{i+1,i}$$

the ensuing gauge field so that the second term is the familiar [42]

$$\bar{\phi}_{i+1} e^{ia A_{i+1,i} \phi_i}$$

We write the second term in (115) as follows,

$$\bar{\kappa}_i e^{-ia\tau_{i+1,i}^{+1} \kappa_i^{-1}} = |\kappa_i|^2 \exp\left\{-i a \tau_{i+1,i} + \ln \frac{\kappa_i^{-1}}{\kappa_i}\right\}$$

$$= \sigma_i \sigma_i^{-1} \exp\{-ia J_{i+1,i}\}$$

(116)

where, in analogy with (65), we have introduced the gauge i.e. frame independent variables

$$\sigma_i = |\kappa_i|$$

$$J_{i+1,i} = \tau_{i+1,i} - \frac{1}{a} \{\arg(\kappa_i) - \arg(\kappa_{i-1})\}$$

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The quantity \[ (116) \] has both a real part and an imaginary part, that are independently frame rotation invariant. Consequently, in line with \((113)\), we obtain two independent quantities that we utilize to introduce the following contribution to discrete energy density

\[
E_2[i] = \sum_i \left\{ -2\sigma_i \sigma_{i-1} \cos(aJ_{i+1,i}) + \frac{q}{a} \sigma_i \sigma_{i-1} \sin(aJ_{i+1,i}) \right\}
\]

(117)

where the parameters are chosen for easy comparison with \((110)\).

Following Section VIII we proceed and extend the variables \(\sigma_i\) from their \textit{a priori} positive to arbitrary real values. For this we introduce the local \(\mathbb{Z}_2\) symmetry \((84)\), that acts on the present variables at a given site \(k\) as follows:

\[
\sigma_j \rightarrow -\sigma_j \quad \text{for all} \quad j \geq k
\]

(118)

Unlike \((110)\), the energy \((117)\) remains intact under this symmetry, thus we can utilize it to extend \(\sigma_i\) in \((117)\) from positive values to arbitrary real values.

When we expand \((117)\) in the bond length parameter \(a\), we get

\[
\approx -2\sigma_i \sigma_{i-1} + q \sigma_i \sigma_{i-1} J_{i+1,i} + a^2 \sigma_i \sigma_{i-1} J_{i+1,i}^2 + \mathcal{O}(a^3)
\]

which is reminiscent of the first, fifth and second terms in \((110)\), respectively. The difference is a higher order correction in the bond length parameter \(a\).

We now proceed to the negative order term \(N_{-2}[i]\). From \((108)\) we extract the following discrete energy density contribution. As in \((113)\) we account for the real and imaginary part separately, and write

\[
E_{-2}[i] = -\frac{2e}{a^2} \frac{\sigma_i}{\sigma_{i-1}} \cos(aJ_{i+1,i}) + \frac{d}{a} \frac{\sigma_i}{\sigma_{i-1}} \sin(aJ_{i+1,i})
\]

(119)

\[
= \frac{d}{a} \sin(aJ_{i+1,i}) - \frac{2e}{a^2} \cos(aJ_{i+1,i})
\]

\[
+ \frac{1}{\sigma_{i-1}} \left( \frac{\sigma_i - \sigma_{i-1}}{a} \right) \left\{ d \sin(aJ_{i+1,i}) - \frac{2e}{a} \cos(aJ_{i+1,i}) \right\}
\]

(120)

Again, this remains intact under the \(\mathbb{Z}_2\) transformation \((118)\) so that we are able to take \(\sigma_i\) to be a real valued quantity. When we expand in the bond length parameter \(a\), the first line gives modulo a constant

\[
\approx d J_{i+1,i} + e J_{i+1,i}^2 + \mathcal{O}(a^2)
\]

which is reminiscent of the fourth and sixth terms in \((110)\) with corrections that are of higher order in \(a\). The second line in \((120)\) gives

\[
\approx -\frac{2e}{a} \frac{1}{\sigma_{i-1}} \left( \frac{\sigma_i - \sigma_{i-1}}{a} \right) + \left( \frac{\sigma_i - \sigma_{i-1}}{\sigma_{i-1}} \right) \left( d J_{i+1,i} + e J_{i+1,i}^2 \right) + \mathcal{O}(a^2)
\]

where, in the continuum limit, the first term becomes a perfect derivative,

\[
\frac{1}{\sigma_{i-1}} \frac{\sigma_i - \sigma_{i-1}}{a} \rightarrow \frac{d \ln \sigma}{ds}
\]
and the second term vanishes in this limit, as $\mathcal{O}(a)$.

Finally, the quartic self-interaction of $\sigma_i$ arises naturally from (112), see (103), (104). Here, we propose to add it essentially ad hoc, as the square of the density (114); any even polynomial of $\kappa_i$ is invariant under the discrete transformation (118) and as such admissible in energy. Most likely this is in violation of integrability. But in applications to proteins, it is desirable to have soliton solutions for which (discrete) translation invariance becomes broken, by a Peiers-Nabarro barrier [43].

We combine (114), (117) and (119) to arrive at the following improved and $\mathbb{Z}_2$ invariant version of the energy density (110),

$$E = \sum_{i=1}^{N} \left\{-2\sigma_i\sigma_{i-1}\cos(aJ_{i+1,i}) + \frac{q}{a}\sigma_i\sigma_{i-1}\sin(aJ_{i+1,i})\right\} + \sum_{i=1}^{N} c(\sigma_i^2 - m^2)^2$$

$$+ \sum_{i=1}^{N} \left\{\frac{d}{a}\frac{\sigma_i}{\sigma_{i-1}}\sin(aJ_{i+1,i}) - \frac{2c}{a^2}\frac{\sigma_i}{\sigma_{i-1}}\cos(aJ_{i+1,i})\right\}$$

(121)

It would be interesting to see, how (121) models folded proteins.

XIII. SUMMARY

In summary, we have addressed the problem how to utilize extrinsic geometry, to derive Hamiltonian energy functions for continuous and discrete strings that move in three dimensional space. The approach we have chosen, is based on a simple geometric principle: We insist, that the energy density must remain invariant under local frame rotations and, in the case of continuous strings, transform covariantly under reparametrizations. In this manner we arrive naturally to energy densities, that relate to the integrable hierarchy of the nonlinear Schrödinger equation. Furthermore, we have found that there is a Weyl dual to this hierarchy, that also relates to the energy densities that are relevant for strings in three space dimensions. We have argued that this additional hierarchy is also integrable, and we have confirmed the integrability explicitly in the case of the first few nontrivial quantities. In addition, we have established, by explicit computation, the equivalence of the two known integrable discrete nonlinear Schrödinger hierarchies. We have also shown, how a discretized generalization of the nonlinear Schrödinger equation that has been previously shown to describe folded proteins, can be obtained as a particular limit of the quantities that appear in the discretized Zakharov-Shabat recursion relations that we have proposed.

We hope that our approach can provide a systematic basis for the general description of both continuous and discrete string-like configurations in three space dimensions, in particular space filling ones.

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