Enigma of probability amplitudes in Hamiltonian formulation of integrable semidiscrete nonlinear Schrödinger systems

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An attempt to find a probability-amplitude-based Hamiltonian representation of the symmetrical version of integrable semidiscrete multicomponent nonlinear Schrödinger systems is made. Thus the on-cell locality of the general point transformation in combination with the model multicomponentness is shown to contradict the concept of canonical Hamiltonian representation in terms of probability amplitudes. Nevertheless, the above concept can be realized in a slightly adjusted semidiscrete multicomponent nonlinear Schrödinger system that preserves some physically valuable solutions of the original (either symmetric or asymmetric) integrable model. The advantages of the adjusted Hamiltonian model for the analysis of real physical systems are formulated. Examples of longitudinal and lateral soliton dynamics on multichain tubular lattices subjected to uniform electric and magnetic fields are given.

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I. INTRODUCTION

The driving force of the present research appears to have been ignited by academician Alexander S. Davydov in a discussion concerning some basic results [1] on the perturbation theory for the Ablowitz-Ladik version of a semidiscretized nonlinear Schrödinger system and mainly on its application to the Peierls-Nabarro problem in essentially nonlinear molecular chains presumably of biological origin. The principal question asked by Davydov was whether it is possible to rewrite the theory in more clear physical terms inasmuch as the direct sense of the Ablowitz-Ladik field amplitudes happens to be rather ambiguous. The positive answer would give the green light for the results [1] to be popularized in a new edition of the monograph *Solitons in Molecular Systems* [2].

Although the answer was not done during the time, the idea to make the theory more appropriate for physicists was reborn somewhat later [3,4] when we managed to reformulate the Ablowitz-Ladik model [5–7] in terms of probability amplitudes similar to their prototypes in a continuous Zakharov-Shabat system [8] and as a result to propose a physically motivated variational treatment of the Peierls-Nabarro problem in realistic physical systems modeled by one or another version of nonintegrable semidiscretized nonlinear Schrödinger equations.

For example, the original Ablowitz-Ladik equations, with the attractive nonlinearity [5–7]

$$+i\dot{q}(n)=[1+q(n)r(n)]\partial H/\partial r(n), \tag{1}$$

$$-i\dot{r}(n)=[1+r(n)q(n)]\partial H/\partial q(n), \tag{2}$$

turned out to be convertible into the standard Hamiltonian form [3,4]

$$+i\dot{Q}(n)=\partial H/\partial R(n), \tag{3}$$

$$-i\dot{R}(n)=\partial H/\partial Q(n), \tag{4}$$

by the following on-site point transformation:

$$q(n)=\sqrt{\{\exp[Q(n)R(n)]-1\}Q(n)/R(n)}, \tag{5}$$

$$r(n)=\sqrt{\{\exp[R(n)Q(n)]-1\}R(n)/Q(n)}. \tag{6}$$

Here the overdot stands for differentiation with respect to dimensionless time τ and the quantities $q(n)$ and $r(n)$ are complex-conjugate field amplitudes without clear physical meaning (referring to as nearly probability amplitudes), whereas $Q(n)$ and $R(n)$ are true complex-conjugate probability amplitudes to find the nth site of the discrete chain to be excited. The Hamiltonian function in original system (1) and (2) is given by

$$H=-\sum_{m=-\infty}^{\infty}[q(m)r(m+1)+q(m+1)r(m)], \tag{7}$$

while the Hamiltonian function in its transformed counterpart (3) and (4) is understood to be that obtained by inserting the relationships between the old $q(n)$ and $r(n)$ and new $Q(n)$ and $R(n)$ field variables (5) and (6) into the original Hamiltonian (7).

The interpretation of new amplitudes $Q(n)$ and $R(n)$ as the probability amplitudes is based upon the property

$$\frac{d}{d\tau}\sum_{m=-\infty}^{\infty}Q(m)R(m)=0, \tag{8}$$

readily recognizable as the conservation law for the total number of excitations within a chain. Namely, for this reason the transformed system (3) and (4) was called as the physically corrected [3] or physically acceptable [4] one.

Analogously with the Hamiltonian (7) the total momentum

$$P=\frac{i}{2}\sum_{m=-\infty}^{\infty}[q(m)r(m+1)-q(m+1)r(m)] \tag{9}$$

is also transformable to the corrected variables $Q(n)$ and $R(n)$ [4].

The question arises whether or not the similar probability amplitude Hamiltonian representation is possible for the multicomponent integrable semidiscrete nonlinear Schrödinger systems [9–16] which could be used as good candidates for modeling real quasi-one-dimensional structures of different physical origins.

For some of them the problem was solved positively [15]; however, for the systems of Manakov type [9–14] only an approximate approach is known [17,18]. The problem becomes even more intriguing inasmuch as it is precisely the quasi-one-dimensional (i.e., multichain) molecular aggregates but not purely one-chain ones that are able to demonstrate the structural robustness in a thermodynamical sense [19].

II. LAGRANGE-BRACKETS APPROACH TO THE TRANSFORMATION OF THE TSUCHIDA-UJINO-WADATI SYSTEM

Among the known integrable semidiscrete nonlinear Schrödinger systems of Manakov type the most reliable for seeking its Hamiltonian representation is the Tsuchida-Ujino-Wadati model [10]

$$+ i\dot{q}_\alpha(n) + \sum_{\beta=1}^{M} t_{\alpha\beta} q_\beta(n) + [1+\nu(n)][q_\alpha(n+1) + q_\alpha(n-1)] = 0, \tag{10}$$

$$- i\dot{r}_\alpha(n) + \sum_{\beta=1}^{M} r_\beta(n) t_{\beta\alpha} + [1+\nu(n)][r_\alpha(n+1) + r_\alpha(n-1)] = 0, \tag{11}$$

$$\nu(n) \equiv \sum_{\beta=1}^{M} q_\beta(n) r_\beta(n), \tag{12}$$

where $q_\alpha(n)$ and $r_\alpha(n)$ can be treated as field amplitudes on the αth chain within the nth unit cell, while $t_{\alpha\beta}$ as the parameters responsible for the linear resonant coupling between the chains; M is the number of chains. The parameter of intercell linear coupling is seen to be normalized to unity.

For the sake of brevity here and later in this paper we understand the term "Hamiltonian representation" as the Hamiltonian representation pretending to be written by means of probability amplitudes in contrast to the Hamiltonian structure in terms of scattering data developed by Gerdjikov and Ivanov [9]. For the same reason of brevity only the model with the attractive nonlinearity—i.e., the model (10)–(12) with field amplitudes $q_\alpha(n)$ and $r_\alpha(n)$ being complex conjugate and consequently with interchain resonant matrix $t_{\alpha\beta}$ being Hermitian $t_{\alpha\beta}=t^*_{\beta\alpha}$—will be inspected. It is worth while mentioning that the Tsuchida-Ujino-Wadati system (10)–(12) appears to be the only known integrable semidiscrete system of Manakov type where either the reduction $r_\alpha(n)=+q^*_\alpha(n)$ or the reduction $r_\alpha(n)=-q^*_\alpha(n)$ is naturally permitted. As the matter of fact it has been rather sophisticatedly designed precisely for such a purpose [10].

In order to distinguish the Manakov-type models admitting the reductions $r_\alpha(n)=\pm q^*_\alpha(n)$ from those where the reductions $r_\alpha(n)=\pm q^*_\alpha(n)$ are forbidden the adjectives "symmetric" and "asymmetric," respectively, appear to be useful [11].

Although the interchain coupling parameters $t_{\alpha\beta}$ in the Tsuchida-Ujino-Wadati (i.e., symmetric) system are usually assumed to be time independent [10], they similarly to another (i.e., asymmetric) model [14] might be arbitrary functions of time τ, thus allowing the system (10)–(12) to be parametrically driven [20–22]. We discard the latter opportunity as an unnecessary complication and adopt the traditional point of view. Then the terms with $t_{\alpha\beta}$ and $t_{\beta\alpha}$ can be eliminated by the gauge transformation [23] corresponding formally to the original model (10)–(12) with zero-valued $t_{\alpha\beta}$ and $t_{\beta\alpha}$. As a result the system (10)–(12) is converted into the following shorthand:

$$+ i\dot{q}_\alpha(n) = [1+\nu(n)]\partial H/\partial r_\alpha(n), \tag{13}$$

$$- i\dot{r}_\alpha(n) = [1+\nu(n)]\partial H/\partial q_\alpha(n), \tag{14}$$

where the function

$$H = -\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty} [q_\beta(m) r_\beta(m+1) + q_\beta(m+1) r_\beta(m)] \tag{15}$$

is taken as the linear combination of appropriate conserved quantities.

The trial assumption about expressions

$$\{q_\alpha(n), r_\beta(m)\} = i[1+\nu(n)]\delta_{\alpha\beta}\delta_{nm}, \tag{16}$$

$$\{q_\alpha(n), q_\beta(m)\} = 0 = \{r_\alpha(n), r_\beta(m)\}, \tag{17}$$

as some Poisson structure analogous to that for the Ablowitz-Ladik model [24–32] contradicts the Jacobi identities [despite formally producing the Hamiltonian-mimicry representation

$$\dot{q}_\alpha(n) = \{H, q_\alpha(n)\}, \tag{18}$$

$$\dot{r}_\alpha(n) = \{H, r_\alpha(n)\}, \tag{19}$$

for the inspecting equations (13)–(15)] and thus should be discarded as the wrong one. To put it differently, any other steps based on the pseudo-Hamiltonian formulation (16)–(19) are unable to achieve any true Hamiltonian formulation including that in terms of probability amplitudes.

In what follows we will rely upon another way of reasoning, assuming one-to-one functional correspondence between the old $q_\alpha(n)$ and $r_\alpha(n)$ and the new (abstract for the time being) $Q_\alpha(n)$, $R_\alpha(n)$ sets of dynamical variables, where n runs through the integers from minus to plus infinity, while α spans the integers from 1 to M. Then after some straightforward manipulations Eqs. (13) and (14) on the set of variables $q_\alpha(n)$ and $r_\alpha(n)$ are converted into the equations

$$-\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}[R_\alpha(n),Q_\beta(m)]\dot{Q}_\beta(m) - \sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}[R_\alpha(n),R_\beta(m)]\dot{R}_\beta(m) = \partial H/\partial R_\alpha(n), \tag{20}$$

$$-\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}[Q_\alpha(n),R_\beta(m)]\dot{R}_\beta(m) - \sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}[Q_\alpha(n),Q_\beta(m)]\dot{Q}_\beta(m) = \partial H/\partial Q_\alpha(n), \tag{21}$$

on the set of variables $Q_\alpha(n)$ and $R_\alpha(n)$. Here the quantities $[R_\alpha(n),Q_\beta(m)]$, $[R_\alpha(n),R_\beta(m)]$ and $[Q_\alpha(n),R_\beta(m)]$, $[Q_\alpha(n),Q_\beta(m)]$ are given by the definition

$$[F,G] = i\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}\frac{\frac{\partial q_\beta(m)}{\partial F}\frac{\partial r_\beta(m)}{\partial G} - \frac{\partial r_\beta(m)}{\partial F}\frac{\partial q_\beta(m)}{\partial G}}{1+\nu(m)}, \tag{22}$$

resembling the definition of Lagrange brackets [33]. Providing a proper enumeration of the variables the above quantities supplemented by the conditions of self-sufficiency become responsible for the symplectic representation of model under consideration [34,35].

III. DEPENDENCE OF OLD DYNAMICAL VARIABLES ON NEW ONES: STEP-BY-STEP SPECIFICATIONS

Analyzing the just obtained equations (20) and (21) we see that they acquire the canonical Hamiltonian form

$$+i\dot{Q}_\alpha(n) = \partial H/\partial R_\alpha(n), \tag{23}$$

$$-i\dot{R}_\alpha(n) = \partial H/\partial Q_\alpha(n), \tag{24}$$

under the conditions

$$[Q_\alpha(n),R_\beta(m)] = +i\delta_{\alpha\beta}\delta_{nm}, \tag{25}$$

$$[Q_\alpha(n),Q_\beta(m)] = 0, \tag{26}$$

$$[R_\alpha(n),Q_\beta(m)] = -i\delta_{\alpha\beta}\delta_{nm}, \tag{27}$$

$$[R_\alpha(n),R_\beta(m)] = 0, \tag{28}$$

serving as the first step in the specification of the previously abstract functional dependence of old variables on the new ones.

Likewise the original amplitudes $q_\alpha(n)$ and $r_\alpha(n)$ the transformed amplitudes $Q_\alpha(n)$ and $R_\alpha(n)$ are seen to be treated as complex-conjugated ones. As a consequence we can adopt the parametrizations

$$q_\alpha(n) = \sqrt{\nu_\alpha(n)}\exp[+i\varphi_\alpha(n)], \tag{29}$$

$$r_\alpha(n) = \sqrt{\nu_\alpha(n)}\exp[-i\varphi_\alpha(n)] \tag{30}$$

and

$$Q_\alpha(n) = \sqrt{\rho_\alpha(n)}\exp[+i\psi_\alpha(n)], \tag{31}$$

$$R_\alpha(n) = \sqrt{\rho_\alpha(n)}\exp[-i\psi_\alpha(n)], \tag{32}$$

where the moduli $\nu_\alpha(n)$ and $\rho_\alpha(n)$ and phases $\varphi_\alpha(n)$ and $\psi_\alpha(n)$ are assumed to be real-valued quantities. These substitutions draw the specification conditions (25)–(28) to be essentially modified and yield

$$[\rho_\alpha(n);\rho_\beta(m)] = 0, \tag{33}$$

$$[\psi_\alpha(n);\psi_\beta(m)] = 0, \tag{34}$$

$$[\rho_\alpha(n);\psi_\beta(m)] = +\delta_{\alpha\beta}\delta_{nm}, \tag{35}$$

$$[\psi_\alpha(n);\rho_\beta(m)] = -\delta_{\alpha\beta}\delta_{nm}, \tag{36}$$

where the bracket entries $[\rho_\alpha(n);\rho_\beta(m)]$, $[\psi_\alpha(n);\psi_\beta(m)]$ and $[\rho_\alpha(n);\psi_\beta(m)]$, $[\psi_\alpha(n);\rho_\beta(m)]$ are determined via the definition

$$[f;g] = \sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty}\frac{\frac{\partial \nu_\beta(m)}{\partial f}\frac{\varphi_\beta(m)}{\partial g} - \frac{\partial \varphi_\beta(m)}{\partial f}\frac{\partial \nu_\beta(m)}{\partial g}}{1+\nu(m)}. \tag{37}$$

Considering the physically corrected version (3) and (4) of basic Ablowitz-Ladik system (1), (2), and (7) it is easy to observe that on-site relationships (5) and (6) between original $q(n)$ and $r(n)$ and corrected $Q(n)$ and $R(n)$ variables are actually applicable to the whole Ablowitz-Ladik hierarchy defined as an infinite set of systems (1) and (2) with Hamiltonian functions running through real-valued superpositions of conserved quantities taken from the infinite set [22]. Generalizing the above point of view into the basic Tsuchida-Ujino-Wadati system (10)–(12) and its hierarchy it is plausible to suppose the functional relationships between the original $q_\alpha(n)$ and $r_\alpha(n)$ and corrected $Q_\alpha(n)$ and $R_\alpha(n)$ dynamical variables to be on-cell ones—i.e., to adopt that

$$\frac{\partial q_\alpha(n)}{\partial Q_\beta(m)} = \delta_{nm}\frac{\partial q_\alpha(m)}{\partial Q_\beta(m)}, \tag{38}$$

$$\frac{\partial q_\alpha(n)}{\partial R_\beta(m)} = \delta_{nm}\frac{\partial q_\alpha(m)}{\partial R_\beta(m)}, \tag{39}$$

$$\frac{\partial r_\alpha(n)}{\partial R_\beta(m)} = \delta_{nm}\frac{\partial r_\alpha(m)}{\partial R_\beta(m)}, \tag{40}$$

$$\frac{\partial r_\alpha(n)}{\partial Q_\beta(m)} = \delta_{nm}\frac{\partial r_\alpha(m)}{\partial Q_\beta(m)}. \tag{41}$$

This is the second step of our argument.

The third step consists in the identification of the quantity $\ln[1+\nu(n)]$ with the number of excitations within the nth unit cell,

$$\rho(n) = \sum_{\beta=1}^{M} \rho_\beta(n), \tag{42}$$

begetting the explicit functional dependence

$$\nu(n) = \exp[\rho(n)] - 1. \tag{43}$$

This step is naturally dictated by the lowest conservation law

$$\frac{d}{d\tau} \sum_{m=-\infty}^{\infty} \ln[1 + \nu(m)] = 0 \tag{44}$$

of the Tsuchida-Ujino-Wadati system.

Despite of all steps directed to concretization of mapping the set of $q_\alpha(n)$ and $r_\alpha(n)$ onto the set of $Q_\alpha(n)$ and $R_\alpha(n)$ the resulting specification formulas, in general, remain extremely complicated for the analysis and practical calculations. Thus, several attempts dealing with a number of plausible mapping *Ansätze* have failed to give a positive result stumbling on this or that contradiction.

For this reason we decided making the next move without any particular *Ansatz* but restricting ourselves to the simplest nontrivial case of a two-chain model when $M=2$. In so doing the parametrizations

$$\nu_1(n) = \frac{1}{2}[1 - \tanh y(n)]\nu(n), \tag{45}$$

$$\nu_2(n) = \frac{1}{2}[1 + \tanh y(n)]\nu(n), \tag{46}$$

$$\varphi_1(n) = \varphi(n) + \theta(n), \tag{47}$$

$$\varphi_2(n) = \varphi(n) - \theta(n) \tag{48}$$

and

$$\rho_1(n) = \frac{1}{2}[1 - \tanh x(n)]\rho(n), \tag{49}$$

$$\rho_2(n) = \frac{1}{2}[1 + \tanh x(n)]\rho(n), \tag{50}$$

$$\psi_1(n) = \psi(n) + \lambda(n), \tag{51}$$

$$\psi_2(n) = \psi(n) - \lambda(n), \tag{52}$$

when having been applied to the basic specification conditions (33)–(36) in combination with the second-step and third-step assumptions (38)–(41) and (42),(43), are proven to be very helpful. After straightforward but somewhat lengthy calculations we have

$$\frac{\partial y(n)}{\partial x(n)}\frac{\partial \theta(n)}{\partial \lambda(n)} - \frac{\partial y(n)}{\partial \lambda(n)}\frac{\partial \theta(n)}{\partial x(n)} = \frac{\cosh^2 y(n)}{\cosh^2 x(n)}\frac{\rho(n)}{1 - \exp[-\rho(n)]}, \tag{53}$$

$$\frac{\partial y(n)}{\partial x(n)}\frac{\partial \theta(n)}{\partial \psi(n)} - \frac{\partial y(n)}{\partial \psi(n)}\frac{\partial \theta(n)}{\partial x(n)} = 0, \tag{54}$$

$$\frac{\partial y(n)}{\partial \psi(n)}\frac{\partial \theta(n)}{\partial \lambda(n)} - \frac{\partial y(n)}{\partial \lambda(n)}\frac{\partial \theta(n)}{\partial \psi(n)} = 0, \tag{55}$$

$$\frac{\partial \varphi(n)}{\partial x(n)} = \frac{\partial \theta(n)}{\partial x(n)} \tanh y(n) + \left[\frac{\partial y(n)}{\partial \rho(n)}\frac{\partial \theta(n)}{\partial x(n)} - \frac{\partial y(n)}{\partial x(n)}\frac{\partial \theta(n)}{\partial \rho(n)}\right]\frac{1 - \exp[-\rho(n)]}{\cosh^2 y(n)}, \tag{56}$$

$$\frac{\partial \varphi(n)}{\partial \lambda(n)} = \frac{\partial \theta(n)}{\partial \lambda(n)} \tanh y(n) - \tanh x(n) + \left[\frac{\partial y(n)}{\partial \rho(n)}\frac{\partial \theta(n)}{\partial \lambda(n)} - \frac{\partial y(n)}{\partial \lambda(n)}\frac{\partial \theta(n)}{\partial \rho(n)}\right]\frac{1 - \exp[-\rho(n)]}{\cosh^2 y(n)}, \tag{57}$$

$$\frac{\partial \varphi(n)}{\partial \psi(n)} = \frac{\partial \theta(n)}{\partial \psi(n)} \tanh y(n) + 1 + \left[\frac{\partial y(n)}{\partial \rho(n)}\frac{\partial \theta(n)}{\partial \psi(n)} - \frac{\partial y(n)}{\partial \psi(n)}\frac{\partial \theta(n)}{\partial \rho(n)}\right]\frac{1 - \exp[-\rho(n)]}{\cosh^2 y(n)}. \tag{58}$$

This set of equations, despite its rather unwieldy essentially nonlinear structure, permits a simple test of compatibility. Indeed the demand of cross differentiation

$$\frac{\partial^2 \varphi(n)}{\partial \lambda(n) \partial x(n)} = \frac{\partial^2 \varphi(n)}{\partial x(n) \partial \lambda(n)} \tag{59}$$

checked on two equations (56) and (57) for $\partial\varphi(n)/\partial x(n)$ and $\partial\varphi(n)/\partial\lambda(n)$ with using the first equation (53) of the set is reduced to the condition

$$\rho(n) = \exp[-\rho(n)], \tag{60}$$

which at an arbitrary $\rho(n)$ can never be satisfied.

Thus, we came to the contradiction indicating that the Hamiltonian representation in terms of probability amplitudes for the Tsuchida-Ujino-Wadati model (13)–(15) is impossible at least under the adopted though very plausible assumptions.

IV. APPROXIMATE HAMILTONIAN REPRESENTATION PRESERVING EXACT FACTORIZED SOLUTIONS

It would not be right to conclude the paper with the sole proclamation of a negative result as concerns a particular very promising integrable model (10)–(12).

Of course, integrable models play a significant role in physical investigations serving as the foundation for the development of some approximate procedure to solve or analyze the physically motivated equations. However, as a matter of fact the wide nominal potentialities of any integrable

model are usually restricted to the exploration of its simplest (supposedly one-soliton) solutions. In this respect there is no principal difference between an exact integrable model and its slightly adjusted though presumably nonintegrable counterpart preserving some valuable class of solutions. More important is the ability of the adjusted model to be properly used for the purposes of approximate integration of the original physical system.

Fortunately, the basic symmetric Manakov-type system (10)–(12) as well as the asymmetric ones [9,11–14] can be readily adjusted to meet the above demands of weakened integrability to say nothing of a Hamiltonian formulation of the adjusted system or more strictly of its transformed version rewritten in terms of probability amplitudes.

The main step of an approximate approach is common for all systems of Manakov type, either symmetrical or asymmetrical. It assumes the trivial substitution of point on-cell transformations

$$q_\alpha(n) = Q_\alpha(n)E(n), \tag{61}$$

$$r_\alpha(n) = R_\alpha(n)E(n), \tag{62}$$

with

$$E(n) = \sqrt{\frac{\exp \rho(n) - 1}{\rho(n)}} \tag{63}$$

and $\rho(n)$ given by formula (42) directly into the system under consideration. As a result dealing, for instance, with the Tsuchida-Ujino-Wadati symmetrical system (10)–(12) the exact equations for the probability amplitudes $Q_\alpha(n)$ and $R_\alpha(n)$ are found to be

$$\begin{aligned} +i\dot{Q}_\alpha(n) = {} & \frac{\partial H_a}{\partial R_\alpha(n)} + 2E(n+1)\frac{dE(n)}{d\rho(n)} \\ & \times \sum_{\beta=1}^{M} [Q_\alpha(n)Q_\beta(n+1) - Q_\alpha(n+1)Q_\beta(n)]R_\beta(n) \\ & + 2E(n-1)\frac{dE(n)}{d\rho(n)} \\ & \times \sum_{\beta=1}^{M} [Q_\alpha(n)Q_\beta(n-1) - Q_\alpha(n-1)Q_\beta(n)]R_\beta(n), \end{aligned} \tag{64}$$

$$\begin{aligned} -i\dot{R}_\alpha(n) = {} & \frac{\partial H_a}{\partial Q_\alpha(n)} + 2E(n+1)\frac{dE(n)}{d\rho(n)} \\ & \times \sum_{\beta=1}^{M} [R_\alpha(n)R_\beta(n+1) - R_\alpha(n+1)R_\beta(n)]Q_\beta(n) \\ & + 2E(n-1)\frac{dE(n)}{d\rho(n)} \\ & \times \sum_{\beta=1}^{M} [R_\alpha(n)R_\beta(n-1) - R_\alpha(n-1)R_\beta(n)]Q_\beta(n), \end{aligned} \tag{65}$$

where

$$H_a = H_\perp + H_\parallel, \tag{66}$$

while

$$H_\perp = -\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty} R_\alpha(m)t_{\alpha\beta}Q_\beta(m), \tag{67}$$

$$\begin{aligned} H_\parallel = {} & -\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty} E(m+1)E(m) \\ & \times [Q_\beta(m+1)R_\beta(m) + R_\beta(m+1)Q_\beta(m)]. \end{aligned} \tag{68}$$

These equations conserve the quantities $H_\parallel$ and

$$N = \sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty} Q_\beta(m)R_\beta(m), \tag{69}$$

$$\begin{aligned} P = {} & \frac{i}{2}\sum_{\beta=1}^{M}\sum_{m=-\infty}^{\infty} E(m+1)E(m) \\ & \times [Q_\beta(m)R_\beta(m+1) - Q_\beta(m+1)R_\beta(m)], \end{aligned} \tag{70}$$

being the straightforward replicas of those yielded by the basic multicomponent system (10)–(12), but do not conserve the gauge-dependent quantity $H_\perp$ Eq. (67), even at time-independent interchain coupling parameters $t_{\alpha\beta}$ as is observed for genuine (continuous) Manakov-type systems [12] (N.B. Manakov himself had considered only the simplest version $M=2$ with $H_\perp \equiv 0$ [36]). The latter problem is caused by the second and third right-hand-side terms in each of transformed equations (64) and (65). The same right-hand-side terms destroy also the desirable canonical Hamiltonian structure

$$+i\dot{Q}_\alpha(n) = \partial H_a/\partial R_\alpha(n), \tag{71}$$

$$-i\dot{R}_\alpha(n) = \partial H_a/\partial Q_\alpha(n), \tag{72}$$

being further referred to as the adjusted semidiscrete multicomponent system.

The discrepancy between the integrable semidiscrete and integrable continuous Manakov-type systems with respect to a description of the transverse dynamics strengthens the positions of adjusted semidiscrete multicomponent models (66)–(68), (71), and (72) inasmuch as it removes the obstacles in providing the quantities $H_\perp$, Eq. (67), and $H_\parallel$ Eq. (68), with clear physical interpretation as the lateral and longitudinal parts of total Hamiltonian H_a, Eq. (66), respectively. The adjusted model preserves the total number of excitations, N, Eq. (69), and the longitudinal Hamiltonian $H_\parallel$, Eq. (68), to be conserved adding to them the conservation of transverse Hamiltonian $H_\perp$, Eq. (67), at $dt_{\alpha\beta}/d\tau \equiv 0$.

In this context it would be interesting to test the adjusted model (66)–(68), (71), and (72) on its complete integrability.

This important and maybe difficult question could be a matter for separate research. For example, the quantity P given by formula (70) fails to be conserved by the adjusted model and the correct expression claiming to describe the total momentum still has to be found.

Here we would like only to underline that the adjusted multicomponent system (66)–(68), (70), and (72) preserves a wide class of solutions typical of the basic multicomponent system taken in its transformed form (64)–(68)—namely, solutions of factorized type $Q_\alpha(n)=b_\alpha Q(n)$ and $R_\alpha(n)=b_\alpha^* Q^*(n)$ $(\Sigma_{\beta=1}^M b_\beta b_\beta^*=1)$ that naturally include the one-soliton solution [17,18]. Indeed inserting the above factorized *Ansatz* into the transformed basic equations (64)–(68) we see that the terms spoiling the Hamiltonian representation become zeros identically, thus making the basic and adjusted models indistinguishable. As a consequence the quantity P, Eq. (70), calculated on the factorized *Ansatz* is proven to be conserved by either model.

V. MAIN FEATURES OF THE ONE-SOLITON DYNAMICS ON TUBULAR LATTICES

Considering the multicomponent semidiscretized nonlinear Schrödinger system (66)–(68), (71), and (72) characterized by the adjusted Hamiltonian $H_a=H_\perp+H_\parallel$ we can underline its two valuable aspects: first, the presence of the transverse part $H_\parallel$ in the Hamiltonian H_a and, second, the mere Hamiltonian formulation of the system as a whole.

Indeed, the permitted variability in the transversal coupling parameters $t_{\alpha\beta}$ provides wide possibilities in modeling a practically arbitrary geometrical lattice structure in cross section when dealing with bunches of coupled one-dimensional chains typical of natural [37,38,2] or synthesized [39–41] essentially anisotropic macromolecules with α and n playing the role of lateral and longitudinal lattice coordinates of constituent molecules, respectively. For example, adopting $t_{\alpha\beta}$ as

$$t_{\alpha\beta}=t\exp(-i\Phi/M)\Delta(\alpha-\beta+1)+t\exp(+i\Phi/M)\Delta(\alpha-\beta-1), \tag{73}$$

we come to the tubular quasidimensional lattice structures resembling the well-known carbon nanotubes [39–41]. Here the notation

$$\Delta(\gamma)\equiv\frac{1}{M}\sum_{\varkappa=1}^{M}\exp\left(\frac{2\pi i}{M}\varkappa\gamma\right) \tag{74}$$

serves for the generalized delta Kronecker symbol being equal to unity for $\gamma=0,\ \pm M,\ \pm 2M,\ldots$ and zero otherwise, and the quantity Φ/M is reserved for the Peierls phase factor [42,13,14,16] responsible for the external magnetic field, while the parameter t determines the strength of coupling between the neighboring chains. For another example dealing this time with the arrangements of optical fibers we can choose the parameters $t_{\alpha\beta}$ as

$$t_{\alpha\beta}=t\Delta(\alpha-\beta+1)[1-\Delta(\beta-1)\Delta(\alpha-M)]+t\Delta(\alpha-\beta-1)[1-\Delta(\alpha-1)\Delta(\beta-M)] \tag{75}$$

and prescribe the variables α and n to mark fibers in plane orthogonal to the fiber axes with τ being the coordinate along the fibers. Thus essentially two-dimensional arrangements of fibers can be modeled in a generalization of models treating experiments on a purely one-dimensional array of coupled optical waveguides [43].

As for the aspect concerning the Hamiltonian formulation we bear in mind the good opportunity for a standard Legendre transformation from a Hamiltonian to Lagrangian representation with forthcoming application of a trial Lagrangian technique [44,3,45,17,18]. We demonstrate this approach for the analysis of the soliton dynamics on tubular lattice structure subjected to external magnetic and electric fields both directed along the tube axis assuming the probability amplitudes $Q_\alpha(n)$ and $R_\alpha(n)$ to be associated with charged carriers. The respective Lagrangian function is given by the expression

$$\begin{aligned}L=&\frac{i}{2}\sum_{\alpha=1}^{M}\sum_{n=-\infty}^{\infty}[R_\alpha(n)\dot{Q}_\alpha(n)-\dot{R}_\alpha(n)Q_\alpha(n)]\\&+\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\sum_{n=-\infty}^{\infty}R_\alpha(n)t_{\alpha\beta}Q_\beta(n)+\sum_{\alpha=1}^{M}\sum_{n=-\infty}^{\infty}E(n+1)E(n)\\&\times[Q_\alpha(n+1)R_\alpha(n)+R_\alpha(n+1)Q_\alpha(n)]\\&+\sum_{\alpha=1}^{M}\sum_{n=-\infty}^{\infty}n\mathcal{E}R_\alpha(n)Q_\alpha(n),\end{aligned} \tag{76}$$

where the term $\mathcal{E}$ describes the uniform electric field while the uniform magnetic field $\mathbf{B}$ is masked into the interchain resonant matrix $t_{\alpha\beta}$, Eq. (73), via dimensionless magnetic flux

$$\Phi=\frac{e}{c\hbar}|\mathbf{B}|S \tag{77}$$

through the cross section of tubular lattice structure. Here S is the area of an M-angular polygonal element with vertices located on the molecules of the same unit cell. The magnetic field $\mathbf{B}$ is supposed to be directed along the positive direction of the discrete longitudinal coordinate n.

The trial Lagrangian function $\mathcal{L}$ is set to be the Lagrangian function on the collective variables b_α, b_α^*, x, k, μ, and η obtained by the substitution of a one-soliton *Ansatz*

$$Q_\alpha(n)=b_\alpha\sqrt{\ln[1+\sinh^2\mu\,\mathrm{sech}^2\,\mu(n-z)]}\times\exp(ikn+i\eta) \tag{78}$$

into the main Lagrangian function L, Eq. (76), and calculation of all necessary sums over longitudinal n and transverse α coordinates under the normalizing condition

$$\sum_{\alpha=1}^{M}b_\alpha^*b_\alpha=1. \tag{79}$$

Fortunately, all sums including the last perturbative one are calculated exactly and the use of standard Lagrangian formalism can be readily performed. As a result the variables μ and η evolve according to the equations

$$\dot{\mu}=0, \tag{80}$$

$$\dot{\eta} = 2\cosh\mu\cos k, \tag{81}$$

while the other solitonic parameters form the $M+1$ pairs b_α, b_α^* and z, k of canonically conjugated variables that evolve according to the Hamiltonian equations

$$+i\dot{b}_\alpha = \partial\mathcal{H}/\partial b_\alpha^* \equiv -\sum_{\beta=1}^{M} t_{\alpha\beta}b_\beta, \tag{82}$$

$$-i\dot{b}_\alpha^* = \partial\mathcal{H}/\partial b_\alpha \equiv -\sum_{\beta=1}^{M} b_\beta^* t_{\beta\alpha}, \tag{83}$$

$$\dot{z} = \partial\mathcal{H}/\partial k \equiv 2\frac{\sinh\mu}{\mu}\sin k, \tag{84}$$

$$\dot{k} = -\partial\mathcal{H}/\partial z \equiv \mathcal{E}, \tag{85}$$

with the effective Hamiltonian $\mathcal{H}$ given by

$$\mathcal{H} = -\frac{2}{\mu}\sinh\mu\cos k - z\mathcal{E} - \sum_{\alpha=1}^{M}\sum_{\beta=1}^{M} b_\alpha^* t_{\alpha\beta}b_\beta. \tag{86}$$

The collective variables b_α, b_α^* and z, k are responsible, respectively, for the lateral and longitudinal dynamics of the soliton as a whole. These two sorts of dynamics are seen to be completely separated.

The parameter z is proven to coincide with the mean longitudinal coordinate of the nonlinear wave packet $[\Sigma_{n=-\infty}^{\infty} n\rho(n)/(\Sigma_{n=-\infty}^{\infty}\rho(n)]$ calculated on the one-solitonic *Ansatz* (78) and (79) and at a time-independent external electric field it is bound to be confined within the finite interval of length $z_{\max}-z_{\min}=(4/\mu\mathcal{E})\sinh\mu$. This effect known as Bloch dynamical localization [46,29,20] emanates from the interplay between the finiteness of the longitudinal kinetic energy band (the consequence of structure discreteness) and the monotonic dependence of longitudinal potential energy due to the conservation of total effective longitudinal energy [two first terms on right-hand side of formula (86)]. The direct integration of dynamical equations (84) and (85) confirms this statement, and we readily come to the Bloch oscillations with the amplitude $A_\parallel=(2/\mu\mathcal{E})\sinh\mu$ and the cyclic frequency $\omega_\parallel=\mathcal{E}$.

The most clear evidence of Bloch oscillations in their classical form has apparently been demonstrated in semiconductor superlattices [47] while the optical effects conceptually analogous to the Bloch oscillations are observable in the arrays of optical waveguides [48].

The lower the external electric field the longer is the interval of Bloch localization $z_{\max}-z_{\min}$. In the limit of zero field ($\mathcal{E}=0$) the longitudinal soliton dynamics becomes completely delocalized and degenerates into the trivial uniform motion $\ddot{z}=0$ as is seen from the respective dynamical equations (84) and (85).

Now let us look onto the lateral soliton dynamics. The respective dynamical equations (82) and (83) are linear ones and at time-independent external magnetic field can be easily integrated. Thus, using the explicit expression (73) for the transverse resonant matrix $t_{\alpha\beta}$ corresponding to the tubular lattice structure we obtain

$$b_\alpha(\tau) = \frac{1}{M}\sum_{\beta=1}^{M}\sum_{\varkappa=1}^{M} b_\beta(0) \times\exp\left[\frac{2\pi i\varkappa(\beta-\alpha)}{M} + 2it\tau\cos\left(\frac{2\pi\varkappa+\Phi}{M}\right)\right]. \tag{87}$$

This formula shows that in general there are M distinct modes of lateral oscillations with frequencies being essentially controlled by the magnitude of magnetic flux Φ. Nevertheless, at particular magnitudes of flux some of the frequencies may coincide or even can be softened to zero.

The most predictable and promising type of soliton dynamics is permissible on the lattices with two, three, four, or six cyclically coupled chains when all lateral eigenfrequencies

$$\omega(\varkappa) = 2t\cos\left(\frac{2\pi\varkappa+\Phi}{M}\right), \quad \varkappa = 1,2,\ldots,M, \tag{88}$$

taken under the absence of magnetic flux ($\Phi=0$), become commensurate. In such a case there is a principal possibility for the soliton density to be located completely on one of the lattice chains at some equidistant moments of time provided the initial conditions of soliton distribution have been properly chosen. This property seems to be very sound for transporting charge or energy (or both) to the particular site of a lattice so valuable, e.g., for biological macromolecules [2,38]. To make the task successful the lateral and longitudinal parts of the soliton dynamics must be properly synchronized whereas the typical longitudinal size of solitons should be as narrow as possible. On the other hand, the same property of momentary one-chain location allows the soliton to bypass the impure molecules under another proper synchronization of its lateral and longitudinal dynamics.

A detailed analysis of bypassing phenomena (soliton slalom in particular) on two-leg ladder lattices ($M=2$) is given in our previous articles [17,18], while the correct definition for the soliton longitudinal size in terms of parameter μ with account of the effect of breathing can be found in another of our papers [22].

We end this section by establishing the notion of mean lateral coordinates of soliton which alongside with the already mentioned definition of mean longitudinal coordinate of soliton (quoted as the mean longitudinal coordinate of nonlinear wave packet) could be useful in the visualization of the average soliton dynamics as well as in a qualitative understanding of soliton behavior under perturbations. Due to the two-dimensional character of lateral soliton dynamics, it is sufficient to introduce two lateral coordinates x and y according to the formula

$$x+iy=\frac{\sum_{\alpha=1}^{M}\exp\left(\frac{2\pi i\alpha}{M}\right)\sum_{n=-\infty}^{\infty}R_\alpha(n)Q_\alpha(n)}{\sum_{\alpha=1}^{M}\sum_{n=-\infty}^{\infty}R_\alpha(n)Q_\alpha(n)}. \tag{89}$$

Here and later x and y have nothing to do with $x(n)$ and $y(n)$ used for parametrizations (49), (50), (45), and (46) in Sec. III. Restricting ourselves to the one-solitonic *Ansatz* (78) accompanied by its normalizing condition (79) the definition (89) is readily reduced to the more simpler one

$$x+iy=\sum_{\alpha=1}^{M}\exp\left(\frac{2\pi i\alpha}{M}\right)b_\alpha^* b_\alpha. \tag{90}$$

In the particular case of solitons initially located on the γth chain of six-chain tubular lattices [i.e., the case specified by $b_\alpha(0)=\Delta(\alpha-\gamma)\exp(+i\delta_\alpha)$ with α running from unity to 6] this formula yields

$$\begin{aligned}x(\tau)+iy(\tau)=&\frac{1}{3}\exp\left(\frac{\pi i\gamma}{3}\right)\\&\times\left\{\cos\left[t\tau\left(\cos\frac{\Phi}{6}+\sqrt{3}\sin\frac{\Phi}{6}\right)\right]\right.\\&+\cos\left(2t\tau\cos\frac{\Phi}{6}\right)\\&\left.+\cos\left[t\tau\left(\cos\frac{\Phi}{6}-\sqrt{3}\sin\frac{\Phi}{6}\right)\right]\right\}.\end{aligned} \tag{91}$$

At the threading flux with Φ being equal to zero we see that all three frequencies of oscillations restore their commensurateness and the initial values $x(0)$ and $y(0)$ of lateral coordinates $x(\tau)$ and $y(\tau)$ resurrect repeatedly with the period $\tau_r=2\pi/t$. But it is precisely the challenging point which concerns the most effective use of solitonic transport (i) in achieving the prescribed site (e.g., the site with acceptor) or (ii) in bypassing the site with undesirable impurity.

VI. CONCLUSION

In conclusion, we have inspected the concept of probability amplitudes as a conjectural paradigm for the canonical Hamiltonian formulation of Manakov-type integrable semidiscrete nonlinear systems. It was shown that under rather general assumptions the above concept turned out to be contradictory.

Instead we proposed the direct on-cell substitution introducing the probability amplitudes though without converting an exact system into canonical Hamiltonian form. Alternatively the transformed exact system can be approximately adjusted to the canonical Hamiltonian form that preserves a wide class of physically interesting solutions and can serve as an appropriate basis for the analysis of realistic physical models on multileg ladder lattices. Indeed any real Hamiltonian system as a rule is characterized by the standard Poisson brackets. The study of its properties by means of a trial-adjusted system with the standard Poisson structure seems to be reliable since the meaning of field amplitudes during calculations remains unchanged, thus forbidding an incorrect treatment pathological to false (unphysical) effects.

In addition, we would like to stress that the proposed adjusted multicomponent nonlinear system opens the door for the notion of a lateral Hamiltonian, so natural and valuable for the description of slalom soliton dynamics on a ladder lattice with zigzag-distributed on-site impurities [17,18] as well as for understanding the origin of an attractive-repulsive alternative in an effective soliton interaction with modified transverse bond [18]. Both of the just mentioned effects are closely linked with the linear interchain coupling exactly reproducible by the adjusted model.

In this respect the dropping of terms with transverse coupling parameters $t_{\alpha\beta}$ under the good-looking pretext of their elimination by the proper gauge transformation (as sometimes takes place when seeking solutions of exact integrable models [10]) appears to be a completely incorrect procedure when dealing with perturbed multicomponent physical systems where mere effects are dictated by the interplay between the interchain coupling and the physical perturbation.

We presented two explicit expressions for the transverse coupling matrix associated with the tubular lattices (either natural or synthesized) and with the two-dimensional array of optical fibers.

Finally, we applied the trial Lagrangian approach to the description of the longitudinal and lateral soliton dynamics on tubular lattices subjected to uniform electric and magnetic fields, paying attention to the effect of Bloch oscillations (when the external electric field is turned on) and to the selective transportation of energy and charge due to the periodic shrinking of soliton density in the lateral direction accompanied by the proper synchronization with longitudinal solitonic motion (mainly when the external electric field is turned off). Here it is worth noticing that the uniform electric and magnetic fields happen to be treated by the effective dynamical equations (80)–(85) on an absolutely exact basis. In contrast, other types of external influence (e.g., the perturbations caused by impurities) may be caught by the trial Lagrangian formalism only approximately.

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