

Schrödinger equation for a noninteracting Bose gas on a spatiotemporal lattice

V. V. Konotop* and A. Spire†

Centro de Física da Matéria Condensada, Universidade de Lisboa, Complexo Interdisciplinar, Avenida Prof. Gama Pinto 2, Lisboa 1649-003, Portugal

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We propose a spatiotemporal discretization of the Schrödinger equation for field operators of noninteracting bosons. The scheme, being based on the associated space of the creation and annihilation operators and on a discretization of the Schrödinger equation, preserves equal time commutation relations, possesses Hermitian action, unitary evolution operator, and all relevant integrals which are counterparts of the respective conservation quantities in the continuum limit. Although the scheme is implicit, it allows a reduction to a nonlocal but explicit scheme. In the limit of small time steps the scheme is reduced to a model studied earlier. Some particular examples of the discrete-time Schrödinger equation in the presence of external potentials are given.

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I. INTRODUCTION

There exist several reasons for interest in developing difference-difference schemes for quantum-mechanical operator equations. The traditional ones are lattice formulations of the quantum field [1] and statistical [2] theories, which represent a natural approximation to the path-integral approach displaying no ultraviolet divergences. One more reason is that the finite element approach (borrowed from the numerical techniques) to the continuum-time Heisenberg equation can be employed for numerical solution of operator field equations [3]. Since the evolution equations are now written for operators rather than for c numbers, one of the main requirements for that approach is the preserving equal time commutation relation (ETCR) under the discretization. The finite elements method, proposed in Ref. [3] does take into account the operator nature of the equations and does preserve ETCR, resulting, however, in an implicit scheme. This last property of the discretization due to [3] stimulated appearing of an alternative approach based on the “leapfrog” method of finite differencing [4], which preserves ETCR as well, but coincides with the exact solution only in the continuum limit. Finally, as it has been shown in Ref. [5] (see, also, Ref. [6] for review) a discrete time approach allows rather elegant and simple estimation of spectra of quantum-mechanical systems.

The present work is motivated by several factors. First of all, after famous experiments [7], where Bose-Einstein condensate has been obtained, one can observe an explosion of studies of low-temperature behavior of Bose gases. The original problem is formulated in terms of the field operators in the presence of an external trap potential. The study of the spectra, starting with the quantum problem (rather than with the mean-field approach known as the Gross-Pitaevskii equation) is of natural interest. An approach based on the discrete-time evolution of the field operators in the Heisenberg picture is an alternative way of solving the problem. The second factor is that, the studies of the discrete-time

evolution problem for operators, have been performed, so far, directly for the field operators. On the other hand, in the conventional quantum theory, where time is continuous, the field operators are constructed by means of the second-quantization procedure on the basis of the creation and annihilation operators and the associated Schrödinger picture. Understanding the discrete analog of that procedure seems to be of practical interest. To be more specific, in the present paper we will be interested in the discrete analog of the Schrödinger equation [8]

$$i\psi_t = \psi_{xx} + V(x)\psi \quad (1)$$

for field operator possessing the canonical ETCR:

$$[\psi(x,t), \psi(x',t)] = [\psi^\dagger(x,t), \psi^\dagger(x',t)] = 0 \quad (2)$$

$$[\psi(x,t), \psi^\dagger(x',t)] = \delta(x-x')$$

describing the one-dimensional Bose gas in an external potential $V(x)$. We will be looking for a discretization that resembles as much as possible the dynamics of the continuum model (1) and (2) and reduces to it when a step of discretization goes to zero. Finally, the third motivation for the present work is the intention to make an improvement of the existing results on the discretization of Eq. (1) at $V(x) = 0$, which has been considered in Ref. [9] where two discretizations of Eqs. (1) and (2) have been proposed. However, one of the schemes presented in Ref. [9] which displays main physical properties including conservation quantities and existence of a Hermitian action, does not preserve ETCR, while another scheme, preserving ETCR (for a uniquely defined step of discretization) does not possess a number of essential physical properties.

In the present work we report a discretization of Schrödinger field equation which (i) preserves ETCR, (ii) possesses a Hermitian action, (iii) does not show the spectrum doubling in a homogeneous case, (iv) holds the main physical properties of the field existing in the continuum case (i.e., possesses all necessary integrals of motion), and (v) is unitary (the unitary evolution operator is found explicitly). Naturally, the step of discretization of our scheme is arbitrary (unlike in Ref. [9]).

*Electronic address: konotop@cii.fc.ul.pt

†Electronic address: spire@cii.fc.ul.pt

The organization of the paper is as follows. In Sec. II, we provide a discretization of a Schrödinger equation for the case of free noninteracting bosons, which preserves ETCR and possesses the main conserved quantities: the number of particles, momentum, and the energy. In Sec. III we construct the Hermitian action and relate the proposed discretization to an explicit scheme. The theory is generalized in Sec. IV, where examples of three different potentials are presented. The results are summarized in the Conclusion.

II. UNITARY DISCRETIZATION OF THE SCHRÖDINGER EQUATION

Let us introduce discrete time $t = \tau n$ and space $x = hl$ variables, where n and l are integers and τ and h are temporal and spatial steps of the discretization, respectively. Consider the following difference-difference Schrödinger equation for the field operator $\psi_l^n = \psi(hl, \tau n)$:

$$\begin{aligned} \psi_l^{n+1} - \psi_l^n = & -i\gamma[\beta_1\psi_{l-1}^{n+1} + \beta_2\psi_{l+1}^{n+1} - \beta_3\psi_l^{n+1}] \\ & -i\gamma[\alpha_1\psi_{l+1}^n + \alpha_2\psi_{l-1}^n - \alpha_3\psi_l^n], \end{aligned} \quad (3)$$

where $\gamma = \tau/h^2$ and the complex parameters satisfy the conditions (i) $\alpha_j = \bar{\beta}_j$ (the overbar stands for the complex conjugation) and (ii) $\text{Re}(\alpha_1 + \alpha_2 - \alpha_3) = 0$. It is a straightforward algebra to ensure that when $\tau \rightarrow 0$ and $h \rightarrow 0$ Eq. (3) is reduced to Eq. (1) with $V(x) \equiv 0$. Equation (3) is nothing but a generalization of the implicit scheme proposed for the Schrödinger equation in Ref. [10] to the operator case.

Now we show that Eq. (3) preserves ETCR. To this end, considering the lattice to be infinite we employ the discrete Fourier transform and introduce operators $a^n(k)$ according to the formula

$$\psi_l^n = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ikl} a^n(k) dk. \quad (4)$$

Substituting this representation in Eq. (3) we obtain

$$a^{n+1}(k) = e^{i\mu(k)} a^n(k) = e^{i\mu(k)(n+1)} a(k), \quad (5)$$

where $a(k) \equiv a^0(k)$ and

$$\mu(k) = 2 \arg(1 + i\gamma\alpha_3 - i\gamma\alpha_1 e^{ik} - i\gamma\alpha_2 e^{-ik}). \quad (6)$$

Let us now impose the following commutation relation at the initial moment of time $n=0$,

$$[\psi_l^0, \psi_m^0] = [\psi_l^{\dagger 0}, \psi_m^{\dagger 0}] = 0, \quad [\psi_l^0, \psi_m^{\dagger 0}] = \frac{1}{h} \delta_{ml}, \quad (7)$$

which is the simplest discretization of Eq. (2). Then, using Eq. (4) one ensures that Eq. (7) means

$$[a(k), a^\dagger(k')] = \frac{1}{h} \delta(k - k'), \quad (8)$$

and the imposed ETCR hold after the first temporal step, i.e., at $n=1$. Then, using the induction we suppose that at some time n , the ETCR are verified, i.e.,

$$[\psi_l^n, \psi_m^n] = [\psi_l^{\dagger n}, \psi_m^{\dagger n}] = 0, \quad [\psi_l^n, \psi_m^{\dagger n}] = \frac{1}{h} \delta_{ml}, \quad (9)$$

and compute them for the next step of time $n+1$,

$$\begin{aligned} [\psi_l^{n+1}, \psi_m^{\dagger n+1}] &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dk' e^{i(\mu(k) - \mu(k'))} \\ &\quad \times e^{ikl - ik'm} [a^n(k), a^{\dagger n}(k')] \\ &= [\psi_l^n, \psi_m^{\dagger n}]. \end{aligned} \quad (10)$$

Thus we have proven that ETCR are preserved during the discrete time evolution. It is to be emphasized here, that the obtained results are essentially based on the particular form of discretization (3) subject to the conditions (i) and (ii) of the coefficients of the discretization.

As it is clear from the construction of the operators $a^\dagger(k)$ and $a(k)$ they can be interpreted as creation and annihilation operators of a quasiparticle in the quantum state k . Notice that the quantum-state space is restricted to the first Brillouin zone: $k \in [-\pi, \pi]$ which is a natural consequence of the discretization. Then one can verify that scheme (3) is unitary. Indeed, introducing the unitary operator

$$U = \exp\left(ih \int_{-\pi}^{\pi} \mu(k) a^\dagger(k) a(k) dk\right), \quad (11)$$

and using that $U^\dagger a(k) U = a(k) \exp[i\mu(k)]$ one arrives at the equation which determines the evolution of the field operator on the spatiotemporal lattice

$$\psi_l^{n+1} = U^\dagger \psi_l^n U. \quad (12)$$

The last formula implies conservation of ETCR as well as conservation of the total number of particles: $N^{n+1} = N^n = N$, where

$$N^n = \sum_l \rho_l^n = \sum_l \psi_l^{\dagger n} \psi_l^n \quad (13)$$

and $\rho_l^n = \psi_l^{\dagger n} \psi_l^n$ is an operator of the density of particles (i.e., the number of particles at a lattice site l at time n). This follows from the fact that N^n is a functional of $a^\dagger(k) a(k)$ and thus commutes with the unitary operator U . Alternatively, using relations (4) and (5) one can obtain

$$\begin{aligned} \sum_l \psi_l^n \psi_l^n &= \frac{1}{(2\pi)^2} \sum_l \int \int_{-\pi}^{\pi} e^{i(p-k)l + i(\mu(p) - \mu(k))n} \\ &\quad \times a^\dagger(k) a(p) dk dp \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} a^\dagger(k) a(k) dk, \end{aligned} \quad (14)$$

i.e., N^n indeed does not depend on discrete time n . It is to be mentioned here that the operator of number of particles N

given by Eq. (13) and having natural representation through the density operator differs from the definition of a charge Q^n ,

$$Q^n = \frac{1}{2} \sum_l (\psi_l^\dagger \psi_l^{n+1} + \psi_l^{\dagger n+1} \psi_l^n) \quad (15)$$

introduced in Ref. [9], although the both quantities coincide in the continuum limit. In this context it is interesting to mention that discretization (3) preserves also Q^n : $Q^{n+1} = Q^n = Q$ [this can be proven by a slight modification of relations (14)].

Other physically relevant conserved quantities are the energy

$$E^n = \frac{1}{2h^2} \sum_l [(\psi_{l+1}^\dagger - \psi_{l-1}^\dagger)(\psi_{l+1}^{n+1} - \psi_{l-1}^{n+1}) + (\psi_{l+1}^{\dagger n+1} - \psi_{l-1}^{\dagger n+1})(\psi_{l+1}^n - \psi_{l-1}^n)], \quad (16)$$

and the momentum

$$P^n = \frac{i}{2h} \sum_l [(\psi_{l+1}^{\dagger n+1} + \psi_{l-1}^{\dagger n})(\psi_{l+1}^{n+1} - \psi_{l-1}^n) + (\psi_{l+1}^\dagger - \psi_{l-1}^{\dagger n+1})(\psi_{l+1}^n + \psi_{l-1}^{n+1})]. \quad (17)$$

Demonstration of the conservation of these two quantities is slightly more complicated. We start from the observation that in terms of new operators

$$q_l^n = (-1)^n e^{-2i\xi n} \psi_l^n, \quad (18)$$

where $\xi = \arg[i - \gamma(\alpha_3 + \alpha_1)]$, Eq. (3), can be rewritten in the form

$$q_l^{n+1} + \bar{a}_2 q_{l+1}^{n+1} + \bar{a}_1 q_{l-1}^{n+1} = q_l^n + a_1 q_{l+1}^n + a_2 q_{l-1}^n, \quad (19)$$

where $|a_j| = \gamma|\alpha_j|/[i - \gamma(\alpha_3 + \alpha_1)]$. Let us choose $a_1 = a_2 = ig$, from Eq. (19) it follows that

$$\begin{aligned} I^n &= \sum_l (q_l^\dagger + ig q_{l+1}^\dagger + ig q_{l-1}^\dagger) \\ &\quad \times (q_l^{n+1} - ig q_{l+1}^{n+1} + -ig q_{l-1}^{n+1}) \\ &= \sum_l q_l^\dagger q_l^{n+1} - g^2 \sum_l (q_{l+1}^\dagger + q_{l-1}^\dagger)(q_{l+1}^{n+1} + q_{l-1}^{n+1}) \end{aligned} \quad (20)$$

is a conserved quantity: $I^n = I^{n+1}$. The first term of the last relation is conserved [by an analogy with Eq. (14)], then it follows that the second term is conserved, as well. Using Eq. (14) and the last conserved relation, we obtain that

$$J^n = \sum_l (q_{l+1}^{\dagger n+1} - q_{l-1}^{\dagger n+1})(q_{l+1}^n - q_{l-1}^n) \quad (21)$$

is a conserved quantity. Returning to the initial operator ψ_l^n it gives that

$$\tilde{J}^n = \sum_l (\psi_{l+1}^\dagger - \psi_{l-1}^\dagger)(\psi_{l+1}^{n+1} - \psi_{l-1}^{n+1}) \quad (22)$$

is conserved. As it follows from definition (16) and (17) the energy and the momentum are composed of \tilde{J}^n and $\tilde{J}^{\dagger n}$, and hence the conservation of \tilde{J}^n implies conservation laws: $E^{n+1} = E^n$ and $P^{n+1} = P^n$.

Then the scheme we have chosen appears to be stable in the sense that all physical properties given at initial time ($n=0$) are conserved for any time.

III. EQUATION OF MOTION: IMPLICIT AND EXPLICIT SCHEMES

Let us show now that the discretization (3) possesses other necessary conditions such as existence of a Hermitian action and absence of spectrum doubling. Moreover, we will show that the initially implicit scheme can be rewritten in a form of a nonlocal but explicit one. To simplify the consideration we reduce the scheme to a one-parametric one, by requiring the following conditions to be fulfilled:

- (i) $a_1 = a_2 = ig$,
- (ii) $2|\alpha_1| \cos(\phi_1) = -\sin(\phi_1)$,
- (iii) $4\gamma|a_1|^2 - |a_1| + \gamma = 0$

(the last requirement can be satisfied for $\gamma < 1/4$). Then discrete-time evolution equation (3) takes the form

$$\begin{aligned} &(\psi_{l+1}^{n+1} - \psi_{l+1}^n + \psi_{l-1}^{n+1} - \psi_{l-1}^n) + 2\beta^2(\psi_l^{n+1} - \psi_l^n) \\ &= i\beta(\psi_{l+1}^{n+1} + \psi_{l-1}^{n+1} - 2\psi_l^{n+1} + \psi_{l+1}^n + \psi_{l-1}^n - 2\psi_l^n), \end{aligned} \quad (23)$$

where $\beta = 1/(2|a_1|)$.

Now one can write down the action in a simple form

$$\begin{aligned} S &= i \sum_{l,n} [(\psi_{l+1}^\dagger + \psi_{l-1}^\dagger + 2\beta^2 \psi_l^\dagger)(\psi_l^{n+1} - \psi_l^n) \\ &\quad + \beta \psi_l^\dagger(\psi_{l+1}^{n+1} + \psi_{l-1}^{n+1} - 2\psi_l^{n+1} + \psi_{l+1}^n + \psi_{l-1}^n - 2\psi_l^n)]. \end{aligned} \quad (24)$$

Passing to the dispersion relation of Eq. (23) we look for a solution in a form $\psi_l^n = A_{h,\tau}(k) e^{i(klh - \omega\tau n)}$, where $A_{h,\tau}(k)$ is a space and time-independent operator and substitute it into the both sides of Eq. (23). This gives

$$\omega = \frac{2}{\tau} \arctan \left(\frac{2\beta \sin^2 \left(\frac{kh}{2} \right)}{\cos(kh) + \beta^2} \right). \quad (25)$$

The obtained formula shows the absence of the spectrum doubling.

In order to rewrite implicit scheme (3) in an explicit form we introduce the second-order shift operators (acting in the operator space)

$$B \psi_l = -\beta(\psi_{l+1} + \psi_{l-1} - 2\psi_l),$$

$$T \psi_l = \psi_{l+1} + \psi_{l-1} + 2\beta^2 \psi_l,$$

and the time-shift operator \mathcal{U} given by the formula $\psi_l^{n+1} = \mathcal{U}\psi_l^n$. Then we obtain that Eq. (23) can be rewritten as follows:

$$i(\mathcal{U}-I)T_l\psi_l^n = \beta(\mathcal{U}+I)B_l\psi_l^n, \quad (26)$$

where I is a unity operator. Thus formally

$$\mathcal{U}^n = [(iT+B)^{-1}(iT-B)]^n, \quad (27)$$

i.e., \mathcal{U} appears to be a unitary operator. Taking into account that $[T,B]=0$ we finally arrive at the conclusion that the field operators obey to the temporal dynamics $\psi_l^n = (\mathcal{U})^n \psi_l^0$ [c.f. Eq. (12)], which formally coincides with the equation for the evolution of the wave function in the quantum mechanics where a wave function should be used instead of the operator.

Consider now the limit when the temporal step goes to zero $\tau \rightarrow 0$ ($\beta \rightarrow \infty$). Then $\beta = h^2/2\tau + O(2\tau/h^2)$ and the evolution operator takes the form

$$\psi_l^{n+1} = \mathcal{U}\psi_l^n = \psi_l^n - \frac{2\tau}{ih^2}(\psi_{l+1}^n + \psi_{l-1}^n - 2\psi_l^n) + O\left(\frac{\tau^2}{h^4}\right).$$

Thus, in this limit we arrive at the straightforward discrete scheme for the ‘‘Schrödinger field’’ on a Galileo lattice, which was discussed in Ref. [9].

To conclude this section we compute the non-equal-time commutation relations $C(k,l) \equiv [\psi_l^{n+1}, \psi_k^{\dagger n}]$. It follows from Eq. (23) that they obey the lattice equation

$$C(k,l) = F(k,l) + igC(k,l+1) + igC(k,l-1), \quad (28)$$

where $F(k,l) = \delta_{k,l} + ig(\delta_{k,l+1} + \delta_{k,l-1})$. Using the discrete Fourier transform one obtains

$$C(k,l) \equiv \tilde{C}(k-l) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq e^{iq(l-k)} \frac{1+2ig \cos q}{1-2ig \cos q}. \quad (29)$$

In particular, $\tilde{C}(0) = 2(1+4g^2)^{-1/2} - 1$ and $\tilde{C}(\pm 1) = (i/g)[1 - (1+4g^2)^{-1/2}]$.

IV. GENERALIZATIONS: BOSONS IN AN EXTERNAL POTENTIAL

The approach developed above for the simplest case of free bosons, can be generalized to a number of cases, when external potential is present. This can be done using the associated Schrödinger picture and the analogy with the procedure of the second quantization. To this end we consider a discrete space-time version of the Schrödinger equation for the wave function φ_l^n in a form

$$\varphi_l^{n+1} - \varphi_l^n = i\gamma \sum_m (H_{m,l} \varphi_m^{n+1} + \bar{H}_{l,m} \varphi_m^n). \quad (30)$$

Then the analog of the stationary Schrödinger equation reads

$$\begin{aligned} \varphi_l(k) + i\gamma \sum_m \bar{H}_{l,m} \varphi_m(k) \\ = e^{i\mu(k)} \left(\varphi_l(k) - i\gamma \sum_m H_{m,l} \varphi_m(k) \right), \end{aligned} \quad (31)$$

where $\varphi_l(k)$ is the eigenstate corresponding to the ‘‘energy’’ $\mu(k)$ and k is a spectral parameter which plays the role of the quantum state number. It follows from Eq. (31) that the temporal dependence of the eigenstate $\varphi_l(k)$ is given by $e^{i\mu(k)n} \varphi_l(k)$ such that the wave function φ_l^n can be represented as

$$\varphi_l^n = \sum_k e^{i\mu(k)n} \varphi_l(k) \quad (32)$$

(for the sake of simplicity in the present section we consider a finite lattice subject to the periodic boundary conditions). A value k_0 giving the minimum of $|\mu(k)|$ corresponds to the ground state of the system.

Before providing the second quantization of Eq. (30), let us consider in more details spectral problem (31). First of all one can ensure that $\mu(k)$ is real. To this end, multiplying Eq. (31) by $\bar{\varphi}_l(k)$ and computing the sum over l we obtain

$$\mu(k) = 2 \arg \left(\sum_l |\varphi_l(k)|^2 + i\gamma \sum_{l,m} \bar{\varphi}_l(k) \bar{H}_{l,m} \varphi_m(k) \right). \quad (33)$$

Next multiplying Eq. (31) by $\bar{\varphi}_l(k')$ with $k' \neq k$ and summing over all l we obtain the orthogonality conditions

$$\sum_l \bar{\varphi}_l(k') \varphi_l(k) + i\gamma \sum_{l,m} \bar{\varphi}_l(k') \bar{H}_{l,m} \varphi_m(k) = 0 \quad (34)$$

and an additional condition

$$\sum_{l,m} (\bar{H}_{l,m} + H_{m,l}) \bar{\varphi}_l(k') \varphi_m(k) = 0, \quad k' \neq k. \quad (35)$$

It is worth pointing out here that in the continuum time limit [$\gamma \rightarrow 0$ and hence $\mu(k) \rightarrow 0$] eigenvalue problem (31) is reduced to

$$\varphi_l(k) \mu(k) = \gamma \sum_m (\bar{H}_{l,m} + H_{m,l}) \varphi_m(k) + O(\gamma^2) \quad (36)$$

and thus Eqs. (34) and (35) coincide in the leading order and take the form of the conventional orthogonality conditions.

For the sake of simplicity the consideration in the rest of this section will be restricted to the case $H_{m,l} = \bar{H}_{l,m}$ [which is the most interesting case from the physical point of view and corresponds to the supposition (i) from Sec. III]. Then for the coefficients

$$a_{l,m} = \sum_k \bar{\varphi}_l(k) \varphi_m(k) \quad (37)$$

one obtains the equation

$$\sum_m [a_{n,m} \text{Re}(H_{l,m}) - a_{m,l} \text{Re}(H_{n,m})] = 0, \quad (38)$$

which must be valid for all n and l and $a_{n,m} \rightarrow 0$ for $|n - m| \rightarrow \infty$. This is satisfied by $a_{n,m} = \delta_{nm}$, i.e.,

$$\sum_k \bar{\varphi}_l(k) \varphi_m(k) = \delta_{lm}, \quad (39)$$

which can be interpreted as the completeness condition.

Now we can construct the field operators

$$\psi_l = \sum_k \varphi_l(k) a(k), \quad \psi_l^\dagger = \sum_k \bar{\varphi}_l(k) a^\dagger(k). \quad (40)$$

Then requiring $[a(k), a^\dagger(k')] = (1/\hbar) \delta_{kk'}$, we obtain $[\psi_l, \psi_{l'}^\dagger] = (1/\hbar) \delta_{ll'}$.

Finally, we define temporal evolution for the field operators by the relation $\psi_l^{n+1} = U^\dagger \psi_l^n U$ with unitary operator U defined as in Eq. (11) with integral substituted by a sum and μ being an eigenvalue of problem (31). This immediately leads to the Schrödinger equation on a Galileo lattice:

$$\psi_l^{n+1} - \psi_l^n = i\gamma \sum_m (H_{m,l} \psi_m^{n+1} + \bar{H}_{l,m} \psi_m^n), \quad (41)$$

i.e., as it is expected it has formally the same form as the Schrödinger equation for the wave function φ_l^n (30). As it is clear the discretization (3) is of the type of Eq. (41) with

$$H_{m,l} = -\beta_1 \delta_{m+1,l} - \beta_2 \delta_{m-1,l} + \beta_3 \delta_{m,l}.$$

The discretization (41) preserves ETCR, which now follows directly from the definition of the temporal evolution.

As far as the link between Schrödinger, Eq. (30), and Heisenberg, Eq. (41), pictures on a lattice is established, one can take advantage of the absence of interactions, and use the fact that is solvable, even inhomogeneous, Eq. (30) means solvability [the solvability is understood here in the sense of possibility to represent the field operator ψ_l^n in an explicit form (40), where all $\varphi_l(k)$ are known] of the discretized Schrödinger equation (41). Let us consider three examples, allowing one to construct some exact solutions.

A. Reflectionless sech-like potential

First of all we observe, that the discretization of the Schrödinger equation corresponding to Eq. (3) is nothing but the linear part of the integrable discretization of the classical nonlinear Schrödinger equation [11]. We make use of the explicit form of the respective static (i.e., having an envelope independent on n) one-soliton solution

$$\varphi_l^{(s)n} = \frac{\sinh(2w)}{\cosh(2lw)} e^{i\mu_0 n}, \quad (42)$$

where

$$\mu_0 = \arctan\left(\frac{4a \cosh(2w)}{1 + 2a^2 + 4a^2 \cosh(4w)}\right), \quad (43)$$

where w is a real parameter characterizing the soliton amplitude and $a = |\gamma \alpha_1 / (i - \gamma(\alpha_3 - \alpha_1))|$. Considering Eq. (31) with

$$H_{m,l} = \delta_{m,l} [\beta_3 - \beta_1 (\varphi_{m-1}^{(s)} \bar{\varphi}_m^{(s)} + \varphi_{m+1}^{(s)} \bar{\varphi}_m^{(s)})] + \beta_1 [\delta_{m,l-1} + \delta_{m,l+1}], \quad (44)$$

we obtain the following discrete model

$$i \frac{\psi_l^{n+1} - \psi_l^n}{\gamma} = -\beta_3 \psi_l^{n+1} + \beta_1 (\psi_{l-1}^{n+1} + \psi_{l+1}^{n+1}) - \alpha_3 \psi_l^n + \alpha_1 (\psi_{l+1}^n + \psi_{l-1}^n) - \beta_1 (\varphi_{l-1}^{(s)} \bar{\varphi}_l^{(s)} + \varphi_{l+1}^{(s)} \bar{\varphi}_l^{(s)}) \psi_l^{n+1} - \alpha_1 (\varphi_{l-1}^{(s)} \bar{\varphi}_l^{(s)} + \varphi_{l+1}^{(s)} \bar{\varphi}_l^{(s)}) \psi_l^n. \quad (45)$$

Equation (45) represents the discretization of the equation

$$i \psi_t = \psi_{xx} + \frac{\mathcal{A}^2}{\cosh^2(\mathcal{A}x)} \psi. \quad (46)$$

The respective potential possesses one discrete level, and thus the condensate at the zero temperature is approximately described by the field operator $\psi_l^n = \varphi_l a_0 e^{i\mu_0 n}$. Thus μ_0 is nothing but the energy of the background state of the discrete model.

B. Bosons in a linear potential

Let us consider another consequence of the fact that Eq. (3) is a linearization of the integrable discrete-time nonlinear Schrödinger equation. Namely, we use that once a classical integrable model is found, and thus admits the Lax representation, one can construct a new integrable model by applying gauge transformation [12]. Such a transform may give a non-trivial, from the physical point of view, generalization of the model, which in particular happens with inclusion of a linear force into consideration [13]. Namely, we are interested on the discretization

$$i \frac{\psi_l^{n+1} - \psi_l^n}{\gamma} = -\beta_3 \psi_l^{n+1} + \beta_2 \psi_{l+1}^{n+1} e^{ihF(2l+1)} + \beta_1 \psi_{l-1}^{n+1} e^{-ihF(2l-1)} - \alpha_3 \psi_l^n + \alpha_1 \psi_{l+1}^n e^{-ihF(2l-1)} + \alpha_2 \psi_{l-1}^n e^{ihF(2l+1)}, \quad (47)$$

which come from Eq. (3) after the transform $\psi_l^n \rightarrow \psi_l^n e^{ihFl^2}$. The continuum limit corresponds to a noninteracting Bose gas subject to the linear force:

$$i \psi_t = \psi_{xx} + 2Fx \psi. \quad (48)$$

Equation (47) is obtained from Eq. (41) using the matrix

$$H_{m,l} = -\beta_3 \delta_{m,l} + \beta_2 \delta_{m,l+1} e^{ihF(2m-1)} + \beta_1 \delta_{m,l-1} e^{-ihF(2m+1)}. \quad (49)$$

C. Potential with nonlocal interactions

To construct the last example we take into account that the development in Secs. II and III has been based on the discrete Fourier transform. Thus inclusion potential energy

terms in a form of convolution with the field (i.e., the case $H_{l,m} = H_{l-m}$) does not change properties of the system with respect to the Fourier transform. This allows us to write the discrete model (30) using

$$H_{m,l} = \beta_3 \delta_{l,m} - \beta_1 \delta_{l-1,m} - \beta_2 \delta_{l+1,m} - \sum_{l_1} h V_{l,m} \delta_{l_1,m}.$$

Then, we obtain discrete equation for wave function of bosons with nonlocal interactions

$$i \frac{\varphi_l^{n+1} - \varphi_l^n}{\gamma} = -\beta_3 \varphi_l^{n+1} + \beta_1 \varphi_{l-1}^{n+1} + \beta_2 \varphi_{l+1}^{n+1} - \alpha_3 \varphi_l^n + \alpha_1 \varphi_{l+1}^n + \alpha_2 \varphi_{l-1}^n + \sum_{l_1} h V_{l-l_1} (\varphi_{l_1}^{n+1} + \varphi_{l_1}^n). \quad (50)$$

The continuum limit of this equation reads

$$i \varphi_t = \varphi_{xx} + \int dy V(x-y) \varphi(y). \quad (51)$$

And the explicit form of Eq. (33) is now

$$\mu(k) = 2 \arg[1 + i \gamma \alpha_3 - i \gamma \alpha_1 e^{ik} - i \gamma \alpha_2 e^{-ik} - i V(k)] \quad (52)$$

and thus the whole analysis for free bosons provided the Sec. II can be reproduced here for the case of the nonlocal potential.

V. CONCLUSION

To conclude, we have obtained a discretization of the Schrödinger field equation which on one hand preserves ETCR and on the other hand possesses in the linear case all

relevant properties of the underline continuum field. Although the scheme is implicit it is reducible to a nonlocal explicit one. Our discretization can be viewed as a generalization of the implicit scheme due to [10] the operator case. In the limit of relatively small time step our discretization coincides with the straightforward one discussed in details in Ref. [9].

The main approach was based on the link between filed operators and creation and annihilation operators, which were introduced through the associate discretization of the time-dependent Schrödinger equation. The stationary discrete Schrödinger equation defines a spectral problem, which is to be investigated in more details elsewhere.

Discretizations of three different inhomogeneous models have been presented. Meantime, in this communication we left open the problem of application of the procedure to more general physical models, i.e., including potentials of a more general form, for the sake of the definition of their spectra by numerical methods. We also believe that the proposed approach will be fruitful for description of weakly nonlinear nonintegrable models on a perturbative basis, when known exact methods [14] are not applicable, as well as for the generalization to two- and three-dimensional cases. Finally, we mention that the discretization based on the associated discrete Schrödinger picture is a natural way for introducing two- and three-dimensional discrete Schrödinger models.

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- [1] See, e.g., J.B. Kogut, *Rev. Mod. Phys.* **55**, 775 (1983).
 [2] See, e.g., L.P. Kadanoff, *Rev. Mod. Phys.* **49**, 267 (1977).
 [3] C.M. Bender and D.H. Sharp, *Phys. Rev. Lett.* **50**, 1535 (1983).
 [4] V. Moncrief, *Phys. Rev. D* **28**, 2485 (1983).
 [5] C.M. Bender, K.A. Milton, D.H. Sharp, L.M. Simmons, and R. Stong, *Phys. Rev. D* **32**, 1476 (1985); C.M. Bender and M.L. Green, *ibid.* **34**, 3255 (1986); L. Vázquez, *Phys. Lett. A* **144**, 15 (1990).
 [6] G. Dattoli, P.L. Ottaviani, A. Torre, and L. Vázquez, *Nuovo Cimento Soc. Ital. Fis., A* **20**, 21A (1997).
 [7] M.H. Andersen, J.R. Enscher, M.R. Matthewes, C.E. Wieman, and E.A. Cornell, *Science* **269**, 198 (1995); C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995); K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, and W. Ketterle, *ibid.* **75**, 3969 (1995).
 [8] Although Eq. (3) is written for the field operators following the terminology of Refs. [9,14], we call it Schrödinger equation, due to its apparant similarity to the conventional Schrödinger equation in the quantum mechanics.
 [9] L. Vázquez, *Phys. Rev. D* **34**, 3253 (1986).
 [10] M. Delfour, M. Fortin, and G. Payre, *J. Comput. Phys.* **44**, 277 (1981).
 [11] T.R. Taha and M.J. Ablowitz, *J. Comp. Physiol.* **55**, 192 (1984).
 [12] L.D. Faddeev and L.A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons* (Springer-Verlag, Berlin, Heidelberg, 1987).
 [13] V. Konotop, *Phys. Lett. A* **258**, 18 (1999).
 [14] V.E. Korepin, N.M. Bogoliubov, and A.G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge University Press, Cambridge, 1993).