Nonlinear phenomenology from quantum mechanics: Soliton in a lattice

Juha Javanainen and Uttam Shrestha

Department of Physics, University of Connecticut, Storrs, CT 06269-3046

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We study a soliton in an optical lattice holding bosonic atoms quantum mechanically using both an exact numerical solution and Quantum Monte Carlo (QMC) simulations. The computation of the state is combined with an explicit account of the measurements of the numbers of the atoms at the lattice sites. In particular, importance sampling in the QMC method arguably produces faithful simulations of the outcomes of individual experiments. Even though the quantum state is invariant under lattice translations, an experiment may show a noisy version of the localized classical soliton.

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Quantum mechanics is widely accepted as the fundamental framework for physics. Nonetheless, a variety of nonlinear theories have met with unquestionable success in the modeling of macroscopic (many-body) systems. This state of the affairs begs for the question of how linear quantum mechanics mimics nonlinear behavior. Consider as an example a soliton of light propagating in a nonlinear optical fiber. Full quantum theory has solutions that in many respects resemble classical solitons [1], but finding such a quantum soliton does not solve the problem of linear versus nonlinear dynamics. For instance, in a translationally invariant optical fiber the quantum ground state may be chosen to be translationally invariant. Why is it, then, that localized solitons are so strongly favored by Nature that they form seemingly spontaneously?

It has been suggested that measurements play a part in the answer [2], but our tenet goes much further: Operationally, nonlinear phenomenology is created by the process of measurement. In this Letter we demonstrate our views by discussing bosonic atoms in an optical lattice, a problem that commands much current interest in its own right [3, 4] and also presents a discrete-space version of the soliton in nonlinear optics. We solve the quantum mechanical ground state either by exact diagonalization or by Quantum Monte Carlo (QMC) simulations [5, 6], but with a measurement theoretical twist. Namely, while a run of a QMC simulation produces the numbers of the atoms at each lattice site to be used in calculations of various ground-state expectation values, we argue that these occupation numbers are also a faithful simulation of what one would find in a single experiment that measures the occupation numbers. When classically one expects a soliton, each run of the QMC simulation, and hence each individual experiment, also shows a distribution of the atoms over the lattice sites like a classical soliton.

Quantum mechanically, we have the Bose-Hubbard model with the Hamiltonian

\[ H = \hbar \sum_k \left[ -\frac{\delta}{2}(\hat{b}_k^{\dagger} \hat{b}_{k+1} + \hat{b}_{k-1}^{\dagger} \hat{b}_k) + \kappa \frac{\delta}{2} \hat{b}_k^{\dagger} \hat{b}_k \hat{b}_{k+1} \hat{b}_{k-1} \right]. \]

Here \( \hat{b}_k \) annihilates an atom at the site \( k = 0, \ldots, L - 1 \), \( \delta \) is the amplitude for site-to-nearest-site tunneling, and \( \kappa \) characterizes on-site atom-atom interactions. Our \( L \)-site lattice is periodic so that \( k = L \) and \( k = 0 \) are the same site. This boundary condition, which would physically correspond to a ring lattice, is specifically chosen to make the Hamiltonian invariant under lattice translations. The total number of atoms \( \hat{N} = \sum_k \hat{b}_k^{\dagger} \hat{b}_k \) is a constant of the motion, and its value is denoted by \( N \).

The corresponding classical Hamiltonian is

\[ H = \hbar \sum_k \left[ -\frac{\delta}{2}(b_{k+1}^{*} b_k + b_{k-1}^{*} b_k) + \frac{\kappa}{2} |b_k|^2 \right]. \]

Here \( b_k \) are complex numbers such that \( |b_k|^2 \) stands for the number of atoms at the site \( k \). The quantities \( b_k \) and \( b_k^{*} \) are regarded as classical canonical conjugates with the Poisson brackets \( \{ b_k, b_k^{*} \} = -(i/\hbar) \delta_{k,k'} \). Hamilton’s equation of motion for \( b_k \),

\[ ib_k = -\frac{\delta}{2}(b_{k+1} + b_{k-1}) + \kappa |b_k|^2 b_k, \]

the lattice analog of the Gross-Pitaevskii equation, is commonly called Discrete Nonlinear Schrödinger equation (DNLSE). The total atom number \( N = \sum_k |b_k|^2 \) is again a constant of the motion.

The ground state of the classical Hamiltonian [2] is found, e.g., by integrating the DNLSE [3] in imaginary time. For repulsive interactions between the atoms, \( \kappa \geq 0 \), the lowest-energy state is spatially uniform, \( b_k = \sqrt{N} e^{i\varphi} \), where \( \varphi \) is a global phase. On the other hand, for a sufficiently strong attractive interaction \( \kappa < 0 \), the lowest-energy state is a soliton localized around some lattice site [2]. A soliton is a stationary state of the DNLSE; the amplitudes evolve in time according to \( b_{k}(t) = e^{-i\mu t/\hbar} b_k(0) \), where \( \mu \) is the chemical potential. Physically, the soliton reflects a balance between the tendencies of the atoms to collect together drawn by the attractive interactions, and to disperse as a result of the site-to-site hopping. A lattice-translated solitonic ground state is also a ground state, but a nontrivial superposition of ground-state solitons is not. Nonlinearity
makes localization an inescapable feature of the solitonic ground state.

In search of the quantum counterpart of a soliton we study the Hamiltonian \( \hat{H} \). Introduce the thermal density operator at the inverse temperature \( \beta \), \( \hat{\rho}(\beta) = e^{-\beta \hat{H}}/\text{Tr}[e^{-\beta \hat{H}}] \), the number operators of the sites \( k \), \( \hat{n}_k = \hat{b}_k^\dagger \hat{b}_k \), the collection of these operators \( \hat{n} = \{\hat{n}_0, \ldots, \hat{n}_{L-1}\} \), and the simultaneous eigenstates \( |\alpha\rangle \) of the number operators \( \hat{n} \) characterized by a collection of \( L \) integers \( \{n_0, \ldots, n_{L-1}\} \). We call such a set \( \alpha \) of the occupations numbers \( n_k \) a number state of the lattice. As the operators \( \hat{n}_k \) commute, according to standard quantum mechanics their values can be measured simultaneously. We say that the operator \( \hat{n} \) is measured. Any function \( f(\hat{n}) \) of the number state defined in a natural way the operator function \( f(\hat{n}) \), and the thermal expectation value of \( f(\hat{n}) \) equals

\[
\langle f(\hat{n}) \rangle = \sum_\alpha P(\alpha)f(\alpha) ; \quad P(\alpha) = \frac{\langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle}{\sum_\beta \langle \beta | e^{-\beta \hat{H}} | \beta \rangle} . \tag{4}
\]

On the other hand, suppose that by some means, call it importance sampling, it is possible to produce number states \( \alpha_m, m = 1, 2, \ldots \) at random, but with frequencies proportional to the corresponding \( P(\alpha_m) \) as in Eq. \( 4 \). The expectation value in Eq. \( 4 \) may then also be written

\[
\langle f(\hat{n}) \rangle = \langle f(\alpha) \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{m=1}^{M} f(\alpha_m) . \tag{5}
\]

Considering any quantity that can be expressed in terms of expectation values of functions of the form \( f(\alpha) \), the values from quantum measurements and from importance sampling agree. This applies to average atom number at a site, correlations of atom numbers between the sites, and so on: The measured values of the number operators \( \hat{n}_k \) agree in every possible statistical characterization with the occupation numbers \( n_k \) in the importance-sampled number states \( \alpha_m \). One experiment and one instance of sampling each produce a random set of occupation numbers, but in repeated runs the statistics of these random numbers could be verified to be the same for the experiments and for importance sampling. We therefore formulate our key interpretative hypothesis: Each number state \( \alpha_m \) coming from importance sampling is a representative outcome of an experiment measuring the operator \( \hat{n} \).

For brevity we focus on the low-temperature limit, \( \beta \to \infty \). If the ground state of the Hamiltonian \( \hat{H} \) is nondegenerate, the density operator is simply the projection onto the ground state. On the other hand, if the ground state is degenerate, the zero-temperature state is an equal mixture of the degenerate ground states. As a lattice translation is a symmetry operation of the Hamiltonian, it is possible to select all energy eigenstates so that they are invariant under lattice translations. Hence, the unique zero-temperature density operator must be invariant under lattice translations. Unlike the classical soliton, the quantum mechanical ground state (or, for that matter, any thermal-equilibrium state) will not single out any particular lattice site.

We first take up the two-site lattice, \( L = 2 \). Simple as the problem is, for parameters such as \( N\kappa/\delta = -2.309 \) we already have the conundrum that the classical ground state is a soliton with \( \frac{3}{4} \) of the atoms in one site and \( \frac{1}{4} \) in the other, whereas the quantum ground state is translation-invariant. So, what would the experiments see?

Here the quantum mechanical state space is spanned by the \( N+1 \) vectors \( |n, N-n\rangle \), where \( n \) is the number of the atoms in the site \( k=0 \) (\( k=1 \)). The two-site problem is trivial to solve numerically. For a fixed value of the parameter \( N\kappa/\delta \) that classically gives a soliton, and in the limit \( N \to \infty \), the ground state is doubly degenerate. Therefore we write the low-temperature ground state as a 50/50 statistical mixture of the two lowest-energy quantum states. As far as observed atom numbers are concerned, the complete statistics is determined by the probabilities \( P_\alpha \) that \( n \) of the atoms are found in the \( k = 0 \) site.

In Fig. \( 1 \) we plot the quantity \( \sqrt{N} P_n \) as a function of the fraction of the atoms in the \( k = 0 \) site, \( n/N \). Here \( N\kappa/\delta = -2.309 \) is fixed, and the atom number \( N \) is varied as indicated in the legend. Importance sampling would produce number states \( \alpha = \{n, N-n\} \) at frequencies proportional to \( P_\alpha \). As Fig. \( 1 \) shows, with an increasing atom number \( N \) the sampling, and the experiments, would give an increasingly accurate split of the atoms so that \( \frac{3}{4} \) of the them is in one site and \( \frac{1}{4} \) in the other, just like in the classical soliton. The reason for the \( \sqrt{N} \) multiplier for the probabilities is that one may then easily see from Fig. \( 1 \) that the fluctuations in the 3 : 1 split scales with the atom number \( N \) like \( 1/\sqrt{N} \).

While the Hamiltonian is invariant under a lattice
translation, an individual measurement result of the
atoms numbers with the approximate 3 : 1 split between
the sites is not. However, either one of the two sites
is the one with the higher occupation number with the
same probability, so that averaging over the experiments
restores the symmetry.

The resemblance of this situation to spontaneously
broken translation symmetry has been brought up in nu-
merous papers on the continuous soliton problem and
the attendant connection to measurement theory has also
been noted [2], but here we take a very direct approach.

Consider interference between two Bose-Einstein con-
densates, an analogous problem from the past [8, 10]
that continues to evoke new angles [11]. The traditional
view is that gauge symmetry of the condensate is broken,
which endows the BEC with a phase. The difference in
the phases is observable when two condensates are made
to overlap, which indeed produces an interference pat-
tern [12]. In contrast, we have predicted an interference pattern for two number-state condensates without ever
assuming any broken symmetry or phase [8]. The key
was to simulate the measurements of the positions of
the atoms. There are correlations between atomic po-
sitions in the state vector of the two overlapping conden-
sates. Every time the position of one atom is observed,
the state gets reduced so that it is compatible with the
newly gained measurement result. This reduction brings
out the correlations by modifying the position distribu-
tion for the next atom to be observed. Continuing in this
way, the measured positions of the atoms produce an in-
terference pattern. It comes about as a combination of
two elements: correlations between atomic positions in
the state, and measurements that convert the correla-
tions into the observations.

Easy as the corresponding measurement simulation
would be in the case of a two-site lattice [10,13], we have
not carried it out because the analog is clear enough as
it is. Even if the ground state is translationally invari-
ant, the potential for a soliton is there in the correlations
between the positions of the atoms: The attractive inter-
actions favor atoms collecting in the same site. However,
it is the observations that ultimately make the soliton.

With increasing numbers of atoms and lattice sites an
exact numerical solution [14] of the lattice system be-
comes impractical. Besides, the solution does not tell
what an experiment would see; one has to add a measure-
ment simulation along the lines of Refs. [8, 10, 13]. QMC
simulations may provide a sweeping answer to the ques-
tions of both finding the state and measuring it. This
is because importance sampling is a core idea in QMC
methods, and in Monte-Carlo simulations in general [15].

Our QMC simulations take place on a $L \times N_\beta$ grid [16],
where the first dimension represents the lattice sites and
the second dimension corresponds to $N_\beta$ steps in inverse
temperature with the size $\beta/N_\beta$. We use an elementary
world line algorithm combined with the checkerboard de-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Atom numbers $n_k$ at lattice sites $k$ for the classical soliton (solid circles) and for five solitons sampled from quantum mechanics; the symbols for the six solitons are all resolved at the site $k = 9$. The parameters are $L = 16$, $N = 256$, and $\kappa/\delta = -0.004$. The temperature is $\delta/100$ in units of frequency. Given the occupation numbers for the solitons $n_k^C$ and for the QMC results $n_k^Q$, the $\delta^2$ distances between the soliton and the five simulations, $d = \sqrt{\sum_k (n_k^Q - n_k^C)^2}$, equal 12.8, 20.9, 18.8, 17.8, and 15.8.}
\end{figure}
\( \kappa/\delta = -0.004 \), for which there is a classical soliton that spans several sites but is well contained inside the lattice length \( L \). In Fig. 2 we plot both the classical soliton (solid circles) and five importance-sampled solitons from the QMC method (various symbols, best resolved at the lattice site \( k = 9 \)). QMC results have been translated along the lattice so that the root-mean square difference from the classical soliton is minimized. The fluctuations in the simulations are rather large, but an eye would recognize every result of sampling as a soliton.

We have discussed explicitly two examples summarized in Figs. 1 and 2 but in our experience the results are generic: If for some fixed values of \( L \) and \( N \kappa/\delta \) there is a classical soliton, in the limit of large \( N \) a measurement on the quantum system will produce a soliton as well.

Our main technical point that each outcome from importance sampling faithfully represents an outcome of a single experiment may seem self-evident, but in practice it appears to be difficult to grasp this type of an argument. We therefore expand on the underlying philosophy.

Ultimately, the claim is that the statistics of a random variable, here \( \mathbf{n} \), determines how the realizations look like. We have resorted to the same idea before \[17, 18\], for instance when we predicted “quantum jumps” in the intensity of the light scattered off a three-level system with a long-lived “shelving state” ab initio from quantum mechanics \[17\]. The intensity correlation functions for the scattered light are continuous functions of their time arguments, but they are the correlation functions of a Markov jump process. Hence, the light intensity should look like a Markov jump process, i.e., execute abrupt jumps. These quantum jumps, originally envisaged by Dehmelt \[19\], were subsequently observed \[20\] and are now a standard laboratory technique for detecting weak transitions. In the present case we have no prior experience with the underlying random variable, but importance sampling shows that the realizations look like solitons. Hence, experiments should produce solitons.

To further illustrate the paradigm shift in our reasoning we compare with traditional QMC simulations. Ordinarily one would produce a number of samples and use them to calculate average quantities such as occupation numbers of the sites, standard deviations of the occupation numbers, correlations in atom numbers between adjacent sites, and so on; and maybe compare such averages with averages extracted from experiments. However, such a process may miss the forest from the trees: Even though the results from importance sampling display solitons, solitons may be difficult to uncover from the averaged quantities.

Recognizing the soliton as the basic outcome from measurements should inspire novel theoretical work. Consider analyzing fluctuations of a soliton using linearization of quantum mechanics around the classical soliton \[21\], which in the context of Bose-Einstein condensates is commonly called Bogoliubov theory. For a fixed number of sites the DNLSE can be rewritten so that the only dimensionless parameter containing the atom number is \( N \kappa/\delta \), the same applies to the linearization of the DNLSE that gives the Bogoliubov theory, and therefore also to atom number fluctuations around the classical soliton \[22, 23\]. We have here the interesting situation that the atom number fluctuations in the Bogoliubov theory can only depend on atom number through the parameter \( N \kappa/\delta \), which directly contradicts our Fig. 1.

There are many layers in our discussion. At the lowest level we introduce the measurement-theoretical idea that importance sampling in our simple QMC method literally simulates the experiments. New ways of comparing theory and experiment then open up. We apply this line of thought to predict localized solitons for atoms in an optical lattice from quantum mechanics in spite of the fact that the quantum state is translationally invariant and does not favor any particular lattice site. At the top level we promote the notion that classical nonlinear phenomena in a macroscopic system are implicit in the correlations within the quantum state, but measurements are the agent that ultimately brings them forth.

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