Higher-order quantum bright solitons in Bose-Einstein condensates show truly quantum emergent behavior

Christoph Weiss\textsuperscript{1,} and Lincoln D. Carr\textsuperscript{2,}†
\textsuperscript{1}Joint Quantum Centre (JQC) Durham–Newcastle, Department of Physics, Durham University, Durham DH1 3LE, United Kingdom
\textsuperscript{2}Department of Physics, Colorado School of Mines, Golden, Colorado 80401, USA

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When an interaction quench by a factor of four is applied to an attractive Bose-Einstein condensate, a higher-order quantum bright soliton exhibiting robust oscillations is predicted in the semiclassical limit by the Gross-Pitaevskii equation. Combining matrix-product state simulations of the Bose-Hubbard Hamiltonian with analytical treatment via the Lieb-Liniger model and the eigenstate thermalization hypothesis, we show these oscillations are absent. Instead, one obtains a large stationary soliton core with a small thermal cloud, a smoking-gun signal for non-semiclassical behavior on macroscopic scales and therefore a fully quantum emergent phenomenon.

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The quantum-classical correspondence is well-established for single-particle quantum mechanics but is known to be problematic for some many-body quantum problems such as strongly correlated systems and even materials as simple as the antiferromagnet. A key macroscopic prediction of Bose-Einstein condensates (BECs) is the bright soliton, appearing as a localized rigid ground state “lump” for attractive BECs. Based on the ubiquity of semiclassical limits for non-interacting and weakly interacting bosons, such as lasers and BECs, one might expect a well-defined emergent macroscopic classical behavior generically from such systems. To date, most aspects of matter-wave bright soliton experiments \cite{1–11} seem to be explained on the semiclassical mean-field level via the Gross-Pitaevskii equation (GPE): thus they display quantum behavior on a single-particle level matching classical wave experiments such as nonlinear photonic crystals \cite{12} and spin-waves in ferromagnetic films \cite{13, 14}. This statement is supported by the fact that quantum-quantum bright solitons \cite{15–22} — matter-wave bright solitons that display quantum behavior beyond the single-particle mean-field level — for many practical purposes show mean-field behavior predicted by the GPE emerging already for particle numbers as low as $N \gtrsim 3$ \cite{23}. So far, beyond-mean field effects only seem to play a role if two or more distinct bright solitons are involved: two matter-wave quantum bright solitons can behave quite differently from matter-wave mean-field bright solitons. Only the latter necessarily have a well-defined relative phase \cite{24}. Both the limit of well-defined phase \cite{7} and the limit involving a superposition of many phases \cite{25, 26} are experimentally relevant for matter-wave bright solitons \cite{7, 26}. In this Letter we show that truly quantum many-body effects are responsible for the dynamics of a single quantum-quantum bright soliton, a smoking-gun signal for quantum emergence in BEC experiments.

For far-from equilibrium dynamics of beyond-ground state quantum bright solitons, we are only at the beginning of a journey similar to the case of quantum dark solitons. That scientific voyage required multiple lines of investigations \cite{27–31} to arrive at the state-of-the art explanation that atom losses are necessary to obtain mean-field properties from many-body quantum solutions \cite{32}. Dark solitons were also realized experimentally in BECs \cite{33} and have been further explored in detail over the years in comparison to such predictions, e.g. \cite{34}. In contrast, bright solitons to-date lack for instance a phase coherence measurement, let alone the kind of far-from-equilibrium dynamics we are predicting here. Thus we focus on a quantum bright soliton experiment easily accessible in current platforms. Specifically, one first prepares a single ground-state bright soliton and then rapidly changes the interaction, an “interaction quench” via a Feshbach resonance, a well-established experimental technique. For one-dimensional Bose gases recent work related to quenches includes positive-to-negative quenches \cite{21, 35}, and zero-to-positive quenches \cite{36}. Quenches involving dark-bright solitons \cite{37, 38}, quenched dynamics of two-dimensional solitary waves \cite{39}, and breathers in discrete nonlinear Schrödinger equations \cite{40–42} were also investigated, as well as the breathing motion after a quench of the strength of a harmonic trap \cite{43}.

For attractive BECs, there are very specific mean-field predictions \cite{44}: in particular, for an interaction quench by a factor of four there are exact analytical mean-field results available that predict robust perfectly oscillatory behavior for all times \cite{45}. However, how quantum bright solitons would behave in such a situation is an open question which we address in the current Letter. One GPE interpretation of a higher-order soliton is $N_s$ bound bright solitons, here $N_s = 2$, a kind of diatomic solitonic molecule in a nonlinear vibrational mode. One might therefore expect quantum fluctuations to cause the two solitons to unbind via e.g quantum tunneling out of a many-body potential, resulting in two equal-sized solitons moving away from each other \cite{46}. This is not at all what we...
find, and is inconsistent with exact results for the center-of-
mass wave function [47]. Moreover, our beyond-mean-field
results are distinct from the GPE failing for strongly correlated
systems like Mott insulators [48–50]; as well as from many-
body systems on short timescales with differences disappear-
ing for typical experimental parameters and large BECs [51].
We will show that an interaction quench leaves a large soliton
core with small emissions of single particles. Experimentally
these dynamics will appear as a “fizzled” higher order bright
soliton, a stationary soliton core with a small thermal cloud.
Thus we establish a new kind of quantum macroscopicity in
weakly interacting bosonic systems.

The mean-field approach via the GPE is a powerful ap-
proximation which provides physical insight into weakly in-
teracting ultracold atoms. In a quasi-one-dimensional wave
guide [1–11, 52] the GPE reads
\[ i\hbar \partial_t \psi(x,t) = -(\hbar^2/2m)\partial_{xx} \psi(x,t) + (N-1)g_{1D}\psi(x,t)^2 \psi(x,t), \]
where \( \psi(x,t) \) is a complex wave function normalized to unity
and \( N \) is the number of atoms of mass \( m \). The attractive interac-
tion
\[ g_{1D} = 2\hbar \omega_{\perp} a < 0 \]
is proportional to the \( s \)-wave scattering length \( a \) and the per-
pendicular angular trapping-frequency, \( \omega_{\perp} \) [53]. Some GPE
predictions for repulsive BECs even become exact [54, 55] in
the mean-field limit
\[ g_{1D} \to 0, \quad N \to \infty, \quad (N-1)g_{1D} = \text{const.} \quad (1) \]

While quantum bright solitons in their internal ground
state in addition have a center-of-mass wave function (see
Refs. [56, 57] and references therein), for measurements both
many-body quantum physics [17, 58] and the GPE [59]
predict bright solitons localized at \( x_0 \) with a single-particle den-
sity profile of form
\[ \rho(x) \equiv |\psi(x)|^2 = (2\xi_N \cos[(x-x_0)/(2\xi_N)]^2)^{-1}, \]
where the soliton length \( \xi_N \) and the related soliton time \( \tau_N \)
\[ \xi_N \equiv h^2/[m(N-1)|g_{1D}|]^{-1}; \quad \tau_N \equiv mg_{1D}^2/h. \quad (2) \]
remain constant when approaching the mean-field limit (1).

In this Letter we use an interaction quench
\[ g_{1D}(t) = \begin{cases} g_0 : & t \leq 0 \\ \eta g_0 : & t > 0 \end{cases}; \quad \eta \geq 1, \quad g_0 < 0. \]

After an interaction quench by a factor of \( \eta = 4 \), the GPE
yields the analytical result [45, p 300]
\[ \rho(x,t) = \frac{\cosh[3x/(2\xi_N)] + 3e^{-i/\tau_N} \cosh[x/(2\xi_N)]}{3 \cos(t/\tau_N) + 4 \cosh(x/\xi_N) + \cosh(2x/\xi_N)} \]
\[ \times \left( \frac{\cosh[3x/(2\xi_N)] + 3e^{-i/\tau_N} \cosh[x/(2\xi_N)]}{3 \cos(t/\tau_N) + 4 \cosh(x/\xi_N) + \cosh(2x/\xi_N)} \right)^2, \quad (3) \]
which is depicted in Fig. 1. For \( 3/2 < \eta/2 < 5/2 \) mean-field
predictions also are very specific: after losing a few atoms the

![FIG. 1: Semiclassical emergent dynamics. After an interaction quench by a factor of four, the GPE mean-field theory predicts perfect oscillatory behavior, Eq. (3) [45]. Is it realistic to expect BEC experiments to reproduce these oscillations? (a) GPE density, normalized to its maximum for the first two oscillation periods as a function of space and time in soliton units. (b) 2D projection of (a).](image)
this can be included by adding a diverging system size to the mean-field limit (1) to get \[ g_{1D} \rightarrow 0, N \rightarrow \infty, L \rightarrow \infty, \xi_N = \text{const.}, N/L = \text{const.} \]

Reaching such a limit is a difficult numerical problem [64]. However, by replacing the Hamiltonian (6) by the Bose-Hubbard model (BHM) used to model quantum bright solitons by e.g. [56, 57, 65, 66], we introduce thermalization mechanisms present in real experiments such as a weak imperfectly harmonic trap, or a one-dimensional waveguide embedded in a 3D geometry; for the BHM thermalization is due specifically to a lattice, in our case in the limit of very weak discretization. The BHM takes the form

\[
\hat{H}_{\text{BHM}} = -J \sum_j (\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j) + \frac{1}{2} U \sum_j \hat{n}_j (\hat{n}_j - 1)
\]

where \( \hat{b}_j^\dagger \) (\( \hat{b}_j \)) creates (annihilates) a particle on lattice site \( j \), \( U < 0 \) quantifies the interaction energy of a pair of atoms and \( \hat{n}_j \) counts the number of atoms on lattice site \( j \). In order to use this in a way we can directly use the physical insight gained from the LLM (6), we choose for the hopping matrix element (cf. [56, Eq. (17)])

\[
J = \hbar^2 / (2m \delta_\perp^2)
\]

such that both models have the same single-particle dispersion in the long wavelength limit \( k \delta_\perp \ll \pi \), with \( \delta_\perp \) the lattice constant. The interaction

\[
U = g_{1D} (32 J \hbar^2 m + m^2 g_{1D}^2) / (4\hbar^2)
\]

is chosen such that the two-particle ground state has the same ground-state energy as Eq. (6) compared to the free gas [56].

While both the weak lattice introduced by Eq. (8) and a weak harmonic trap [67, 68] break the integrability of the LLM, we can still approximately describe eigenstates by Eq. (7). Furthermore, from a modeling point of view, by choosing the lattice we avoid the divergence of the energy fluctuations of the initial state immediately after the interaction quench, caused by delta functions squared, in \( \langle \Delta \hat{H}_{\text{new}} \rangle_0 = (\eta - 1)^2 \left[ \langle \hat{H}_{\text{int old}} \rangle_0 \right]^2 \). While in physics distributions with well-defined mean and diverging variance are well-known [69], a more severe reason for avoiding the LLM limit is that this limit seems to be mathematically ill-defined – an initial wave function with the wrong boundary conditions at \( x_j = x_t \) (\( j \neq \ell \)) has to be expressed in terms of eigenfunctions with the correct boundary conditions [17]. Summarizing, we note that these energy fluctuations are consistent with the LLM predicting the presence of quantum superpositions involving many solitonlets in the initial state, but inconsistent with simple pictures predicting two large solitonlets that either oscillate [45] around each other or separate from each other [46] as the latter cannot happen rapidly [47].

We use time-evolving block decimation (TEBD) [70] — a numerical method based on matrix product states [71, 72] — to solve the BHM (8). In order to exclude both boundary effects and effects introduced by additional traps, we start with a very weak harmonic trap, such that opening it hardly introduces atom losses [73] and thus the analytical result (3) remains valid. In our simulations, we switch this trap off at the same time as we introduce the interaction quench.

If for \( N \gtrsim 3 \) quantum bright solitons indeed already show mean-field behavior [23], we should be able to see the mean-field oscillations depicted in Fig. 1 already for \( N = 3 \). Figures 2 and 3 show that the mean-field oscillations are absent from the many-body TEBD data for \( N = 3 \) and \( N \) up to 16, respectively. For the BHM (8), we note that the relative particle measurement of Eq. (5) can be rewritten in second quantized form appropriate to TEBD by replacing \( \langle (x_1 - x_2)^2 \rangle \) with \( \sum_j (j - \ell)^2 \langle \hat{b}_j^\dagger \hat{b}_j \rangle \).

Within the LLM, for relative distances large compared to the soliton length \( \xi_N \), the leading-order contributions to excited states consists of \( N_S \) solitonlets of terms corresponding to \( N_S \) individual solitonlets moving apart \([17]\) In order to obtain a physical understanding on the time scales on which these solitonlets can move apart if they initially sit on top of each other, we recall the text book result for the variance of an initially Gaussian single-particle wave function [74],

\[
\Delta \chi^2 = \Delta \chi_0^2 (1 + \hbar t / (2M \Delta \chi_0^2)^2).
\]

For the relative motion the mass \( M = Nm \) has to be replaced by the relative mass \( m_{\text{rel}} \equiv m N_1 N_2 / (N_1 + N_2) \). If initially localized to \( \Delta \chi_0 \gg \xi_N \) (much stronger localization leads to too high kinetic energies while much weaker localization leads to a too wide initial wave function) and for a relative mass independent of \( N \), the relative wave function will expand to a size...
FIG. 3: Relative width measures for up to 16 particles. While the GPE predicts perfect oscillations, the predominant behavior in the matrix-product state numerics is that the relative distance of particles grows. (a) Relative width $\Delta_{1.2}$ as a function of time: mean-field oscillations (lowest black dotted curve); TEBD results ($N = 3, 4, 8, 16$ blue, fucia, brown, red curves from top to bottom); overall behavior is quadratic (fits shown as light blue curves). Here $J = 0.5$ and $U > -0.5, -0.33, -0.14, -0.07$. (b) Residual oscillations in panel (a) after subtracting the quadratic fit. (c) Relative error comparing TEBD data with distinct convergence parameters. From top to bottom: $N = 16; \chi_{\text{max}} = 60$ versus $\chi_{\text{max}} = 80, N = 8; \chi_{\text{max}} = 60$ vs. $\chi_{\text{max}} = 80, N = 4; \chi_{\text{max}} = 30$ vs. $\chi_{\text{max}} = 40, N = 3$ (too small to be visible): $\chi_{\text{max}} = 30$ vs. $\chi_{\text{max}} = 40$.

larger than the initial wave function on time scales [cf. Eq. (2)]

$$t \propto m \xi_N^2 \overline{\hbar} = [(N_1 N_2)/(N_1 + N_2)] \pi N. \quad (9)$$

The Hartree product states (4) are also ideal to calculate mean energies which in the mean-field limit (1) become identical to the exact many-body quantum results [17]. The kinetic energy prior to the interaction quench is $\langle E_{\text{int}}\rangle_{\text{old}} = N^3 m g_{1N}^2/(2 \hbar^2) = -E_0^{\text{old}},$ and the interaction energy $E_{\text{int}}^{\text{old}} = 2E_0^{\text{old}}$. Immediately after the interaction quench, the kinetic energy remains unchanged and the interaction energy is increased to $\langle E_{\text{int}}\rangle_{\text{new}} = \eta \langle E_{\text{int}}\rangle_{\text{old}} = 2\eta E_0^{\text{old}}$. In units of the new ground state energy $E_0^{\text{new}} = \eta^2 E_0^{\text{old}}$ we have a total average energy after the interaction quench of

$$\langle E \rangle = [(2\eta - 1)/\eta^2]E_0^{\text{new}} \quad (10)$$

where $0 < (2\eta - 1)/\eta^2 < 1$ for $\eta > 0.5$ and $\eta \neq 1$.

If ultracold attractive atoms are initially prepared in their ground state, by using the eigenstate thermalisation hypothesis [75, 76] we conjecture that an interaction quench by a factor of $\eta$ will on short time scales lead to a final state consisting of a single bright soliton containing $N_1$ atoms, as given by thermodynamic predictions, and $N - N_1$ free atoms. In the mean-field limit (1), for bright solitons thermodynamic predictions read [77]

$$N_1 = \left(2\eta - 1\right)^{1/3} N, \quad \xi_{N_1} = \frac{1}{[\eta(2\eta - 1)]^{1/3}} \xi_N, \quad \eta > \frac{1}{2}, \quad (11)$$
i.e., one large soliton with reduced particle number $N_1$ and reduced size $\xi_{N_1};$ and $N - N_1$ single atoms which are not bound in molecules.

FIG. 4: Extrapolation to large particle number. By applying the eigenstate thermalisation hypothesis [75, 76] we conjecture that after an interaction quench to more negative interactions by a factor of $\eta$, the attractive BEC approaches the equilibrium predictions for a thermally isolated gas of Ref. [77]. (a) New soliton length, in units of the original soliton length $\xi_{N,\text{old}}$ for a soliton containing all atoms (lower curve) versus $N_1$ emitted free atoms (upper curve) as a function of the quench $\eta$. (b) Fraction of atoms in the soliton (upper curve) and in the free gas (lower curve) [see also Eq. (11)].

To suggest that this might indeed be what happens seems counterintuitive at best, since following “thermalization” according to the eigenstate thermalisation hypothesis, all energetically accessible eigenfunctions will be involved [75, 76]; violating both the Landau hypothesis [78, very end], which at first glance seems to prevent co-existence of a large soliton and a free gas; argued against also by mean-field predictions [44, 45] as well as thermodynamic predictions for ultracold atoms in contact with a heat bath [62, 63]. However, the Landau hypothesis is based on assumptions that are not fulfilled for bright solitons [77] and thermally isolated ultracold atoms, arguably realised in state-of-the-art experiments with bright solitons [1–11], behave quite differently from those in contact with a heat bath [77]. Furthermore, contrary to rumours stating otherwise, one-dimensional Bose gases do thermalise, for example in the presence of a weak harmonic trap [67, 68].

As depicted in Fig. 4, we conjecture that after an interaction quench to more negative interactions, the system will relax towards the situation predicted in thermal equilibrium: the co-existence between one large soliton and a free gas [77]. The application of the eigenstate thermalisation hypothesis [75, 76] is supported by the fact that single atoms will move the initial cloud much faster than larger solitonlets [Eq. (9)] that can continue to thermalize. Two macroscopic solitons sitting on top of each other would have to remain at the same position [47]; a freely expending gas passes the convergence test of Ref. [47] but energy conservation and Eq. (10) would require at least one soliton(let) to be present.

To conclude, we have combined evidence from three distinct models (GPE, LLM and BHM) to show that truly quantum emergent behaviour for attractive Bosons happens after an interaction quench to more attractive interactions. Combining the numerical evidence with general considerations based on the eigenstate thermalization hypothesis for larger particle numbers, we conjecture that the final many-body quantum state consists of one smaller bright soliton and lots of sin-
gle atoms, thus yielding an ultimate example of a mean-field breakdown on time scales that remain experimentally relevant even in the mean-field limit (1). Our predictions are accessible to state-of-the-art experiments with thousands of atoms [1–11]. Furthermore, the above conjecture offers an explanation as to why experiments that quasi-instantaneously switch from repulsive to attractive interactions (see for example Ref. [5]) while avoiding the “Bose-nova” collapse or modulational instability can nevertheless lead to one large matter-wave bright soliton (and a thermal cloud) being formed.

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Data will be available online soon [79].

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1 Electronic address: christoph.weiss@durham.ac.uk
1 Electronic address: lcarr@mines.edu

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