Temperatures are not useful to characterise bright-soliton experiments for ultra-cold atoms

Christoph Weiss* and Simon A. Gardiner†

Joint Quantum Centre (JQC) Durham–Newcastle, Department of Physics,
Durham University, Durham DH1 3LE, United Kingdom

Bettina Gertjerenken‡

Department of Mathematics and Statistics, University of Massachusetts, Amherst, MA 01003-4515, USA

(Dated: 28 October 2016)

PACS numbers: 03.75.Lm, 05.45.Yv, 67.85.Bc

Contrary to many other translationally invariant one-dimensional models, the low-temperature phase for an attractively interacting one-dimensional Bose-gas (a quantum bright soliton) is stable against thermal fluctuations. However, treating the thermal properties of quantum bright solitons within the canonical ensemble leads to anomalous fluctuations of the total energy that indicate that canonical and micro-canonical ensembles are not equivalent. State-of-the-art experiments are best described by the micro-canonical ensemble, within which we predict a co-existence between single atoms and solitons even in the thermodynamic limit — contrary to strong predictions based on both the Landau hypothesis and the canonical ensemble. This questions the use of temperatures to describe state-of-the-art bright soliton experiments that currently load Bose-Einstein condensates into quasi-one-dimensional wave guides without adding contact to a heat bath.

The experimental realization [1, 2] of a box potential opens new doors in investigating translationally invariant systems of ultra-cold atoms. For ideal gases in one-dimension there is no Bose-Einstein condensate (BEC), whereas the presence of a harmonic trap leads to a quasi-condensate [3]. For attractively interacting Bose gases, the ground state is a weakly bound molecule, a matter-wave bright soliton. Some of its properties are remarkably different from those of BECs: as we will see below, there is no off-diagonal long-range order. Thus, mathematical theorems about the non-existence [4, 5] of off-diagonal long-range order do not lead to additional physical insight for this model system.

Matter-wave bright solitons have been experimentally generated for ultracold atomic gases in quasi-one-dimensional wave guides for attractive interactions [6–15] and, in the presence of an optical lattice, also for repulsive interactions [16]. For dark solitons [17], developing a complete understanding by modeling them on the many-particle quantum level [18–23] is crucial. The same is true for bright solitons. We note that quasi-one-dimensional wave guides provide thermalisation mechanisms [24].

When modeling the statistical physics, experiments with ultracold atoms are best described by the micro-canonical ensemble (MCE), with fixed total energy \(E\) and fixed particle number \(N\) [25]. As long as the different ensembles are equivalent one can choose a simpler ensemble, such as the canonical ensemble (CE), which allows the energy to fluctuate; while the particle number \(N\) still is fixed, we now have the temperature \(T\) as a thermodynamic variable [23]). For attractive bosons in a quasi-one-dimensional wave guide the canonical ensemble even predicts that the thermal weakly-bound molecule–non-molecule crossover becomes a phase transition in the thermodynamic limit [26, 27]. However, as we will see, the energy fluctuations are anomalously large, making it necessary to re-investigate the transition on the level of the micro-canonical ensemble. Furthermore, this implies that while the canonical ensemble is a powerful tool to describe both the high- and low-temperature phases [26, 27], it fails to capture the physics of the crossover itself correctly for thermally isolated systems with ultracold atoms.

For \(N\) attractively interacting atoms \((g_{1D} < 0)\) in one dimension, the integrable Lieb-Liniger-(McGuire) Hamiltonian [28, 29] is a very useful model

\[
\hat{H} = -\sum_{j=1}^{N} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N-1} \sum_{n=j+1}^{N} g_{1D} \delta(x_j - x_n), \quad -\frac{L}{2} \leq x_j \leq \frac{L}{2},
\]

where \(x_j\) denotes the position of particle \(j\) of mass \(m\), and the interaction strength \(g_{1D} = 2\hbar \omega_a \mathcal{a} < 0\) is set by the \(s\)-wave scattering length \(a\) and the perpendicular angular trapping-frequency \(\omega_a\) [30]. For sufficiently large \(L\) [31] we have the ground state energy [29]

\[
E_0(N) = -\frac{1}{24} \frac{mg^2_{1D}}{\hbar^2} N(N^2 - 1) - \frac{1}{24} \frac{mg^2_{1D}N^2}{\hbar^2},
\]

and all excited energies [32]

\[
E_{\text{total}} = \sum_{r=1}^{R} \left( E_0(N_r) + N_r \frac{\hbar^2 k_r^2}{2m} \right), \quad \sum_{r=1}^{R} N_r = N, \quad N_r \geq 1,
\]

corresponding to the intuitive picture of solitonlets of size \(N_r\) and their respective center-of-mass kinetic energies.

The ground state wave function

\[
\Psi(x_1, x_2, \ldots, x_N) \propto \exp \left( -\frac{mg_{1D}}{2\hbar^2} \sum_{j \neq \nu} |x_j - x_\nu| \right); \quad (5)
\]
is translationally invariant and corresponds to a quantum bright soliton — a weakly bound molecule with delocalized center-of-mass wave function and localized relative wave function. It also helps to quantify what a sufficiently large $L$ is [31]. The size of the molecule can also be characterized by the single particle density (after replacing the delocalized center-of-mass wave function by a delta function at $X_0$ [32, 33], which is identical to the mean-field result [34])

$$|\varphi(x)|^2 \propto \frac{1}{\cosh[(x-X_0)/(2\xi_N)]^2}, \quad \xi_N \equiv \frac{\hbar^2}{m(N-1)g_{1D}}. \quad (6)$$

In order to ensure that a finite-temperature phase transition does not violate the (Hohenberg-)Mermin-Wagner theorem [4, 5], we use the thermodynamic limit [26, 27]

$$N \to \infty, \quad L \to \infty, \quad g_{1D} \to 0, \quad \frac{N}{L} = \text{const.}, \quad \xi_N = \text{const.}, \quad (7)$$

where the particle number $N$, system length $L$, interaction strength $g_{1D}$ and soliton length $\xi_N$ are defined in Eqs. (1), (2) and (6).

We note that there is no off-diagonal long-range order\(^1\) for bright solitons in the limit (7). The many-particle ground state can be viewed as consisting of a relative\(^2\) wave-function given by a Hartree product state with $N$ particles occupying the mean-field-bright-soliton mode $\varphi(x) \propto \cosh[(x-X_0)/(2\xi_N)]^{-1}$ [see Eq. (6)]; and a center-of-mass wave function for the variable $X_0$ (cf. [32, 33]). The one-body density matrix [36] then is $\propto \cosh[(x-X_0)/(2\xi_N)]^{-1} \cosh[(x'-X_0)/(2\xi_N)]^{-1}$ which vanishes in the limit $|x-x'| \to \infty$ even after integrating over $X_0$. Thus, there is no off-diagonal long range order in our system [27]; the existence of bright solitons at low but non-zero temperatures in the thermodynamic limit (7) therefore does not violate the (Hohenberg-)Mermin-Wagner theorem [4, 5].

However, there is a severe problem with the canonical description of the attractive Lieb-Liniger gas in 1D: the scaling of the specific heat [27]. The average energy $\langle E \rangle$ changes sign at the transition temperature from a negative value (3) — which scales $\propto N$ in the limit (7) — to a positive value $\propto N$ within a temperature range $\delta T \propto 1/N$. By using the textbook results for calculating the specific heat [25] we thus obtain

$$C_{L,N} \propto \Delta E^2 \propto \frac{\partial \langle E \rangle}{\partial T} \approx \frac{\delta E}{\delta T} \propto N^2. \quad (8)$$

near the transition temperature. Ensemble equivalence between MCE and CE would usually require a scaling not faster than $N$ (rather than $N^2$) — as is the case outside the transition region [27]. Thus a complete description will require a micro-canonical treatment with fixed total energy (possibly including some very small energy uncertainty) within the MCE, which is the most suitable ensemble for state-of-the-art bright soliton experiments [6–15]. Nevertheless we can profit from the CE result as we know what happens both at high temperatures ($N$ single atoms) and at low temperatures (a single bright soliton containing all $N$ atoms) [26, 27]. We only have to identify the energy regimes which correspond to these two phases. Note that the disagreement between MCE and CE only happens in the transition region of size $\delta T$ which vanishes in the limit (7) and thus appears to be negligible for practical purposes. However, as we will see below, this region covers a huge energy scale and covers all experimentally accessible cases of realizing bright solitons in a one-dimensional wave guide — as long as 3D effects can be discarded.

For very low total energies [$E_{\text{total}} \geq E_0(N)$], when approaching the internal ground state energy [$E_{\text{total}} \to E_0(N)$], only the internal ground state (plus some non-degenerate kinetic energy of the big soliton) is energetically accessible — as long as

$$E_0(N-1) > E_{\text{total}}.$$  

For slightly higher (less negative) total energy, the only energetically accessible states are the $N$-particle soliton or, alternatively, an $N-1$-particle soliton and a single unbound particle. Naively applying the Landau hypothesis\(^3\) suggests that it must be the former as the only “allowed” options seem to be either the $N$ single atoms or an $N$-particle soliton. However, when counting possible configurations the $N$-particle soliton will always lose compared to distributing the kinetic energy among two or more smaller solitons or solitons and single particles.

We hasten to add that there is of course no error in the derivation of the Landau hypothesis (footnote 3; page 2) as given in what is frequently considered to be an authoritative text on theoretical physics [37]. However, its powerful statement is based on assumptions that, while fulfilled by a huge class of models, are not fulfilled by the attractive Lieb-Liniger model. One example is that the size of many objects scales with the number of particles $N$ the object is composed of; like neutron stars, bright solitons become smaller with larger particle numbers [Eq. (6)].

Here, as long as the total energy is negative, $0 > E_{\text{total}}$, within the MCE the configuration consisting of $N$ single atoms is simply not energetically accessible (the $N$ single atom case has a positive total energy) and the configuration of an $N$-atom soliton is in most cases statistically irrelevant. A summary of the three energy regimes can be found in Table I.

In order to gain a better understanding of what would happen in an experiment within the co-existence region

$$0 \geq E_{\text{total}} > E_0(N-1), \quad (9)$$

\(^1\) There is, however, long-range order in the limit investigated in addition to the limit (7) in Ref. [26]. Thus, given the (Hohenberg-)Mermin-Wagner theorem [4, 5] one should expect the characteristic temperature to approach zero for the infinite system. This is indeed the case [35].

\(^2\) The wave-function described in terms of the relative motional degrees of freedom — which we call the relative wave-function.

\(^3\) According to the textbook series by Landau and Lifshitz (the very end of Ref. [37]), the co-existence of single unbound atoms with one bound state or several bound states is excluded in a large class of 1D systems.
we will distribute a negative energy that is proportional to the ground state energy:

$$E_{\text{total}} \equiv \gamma E_0(N), \quad 0 > \gamma \geq -1.$$  \hfill (10)

The number of possibilities to distribute \(N\) atoms among up to \(N\) solitonlets for the distinct energy eigenstates (4) is given by the number partitioning problem which asymptotically reads \cite{38}

$$\Omega_{\text{number partitioning}}(N) \sim \frac{\exp \left( \frac{\pi \sqrt{2/3} \sqrt{N}}{4N^{3/2}} \right)}{\sqrt{\pi}}.$$  \hfill (11)

When there is no kinetic energy, all energies of the type given in Eq. (4) lie between 0 and the ground-state energy as \((\sum_j N_j^3) \geq \sum_j N_j^3\) for \(N_j \geq 0\). Thus, for typical energies distributing all particles into all possible solitonlets would give an exponentially growing number of states (11) — but this grows only to the power \(\sqrt{N}\) and as we show below is thus not the leading order contribution.

So far, the above considerations ignore distribution of the kinetic energy. For \(N\) single atoms and large enough kinetic energy \(E_{\text{kin}}\), the accessible number of states scales as for the classical gas. We note that quantum corrections are negligible as there is no condensation temperature for non-interacting Bose-gases in a one-dimensional translationally invariant wave-guide. Thus, all possible quantum corrections must vanish in the limit (7) because the transition temperature remains finite in the canonical calculations \cite{26,27}. Hence, the leading contribution to the total number of configurations reads \cite{25}

$$\Omega_{1D \text{ gas}}(N) \sim \left( \frac{4\pi L^2 m E_{\text{kin}}}{3h^2 N} \right)^{N/2}.$$  \hfill (12)

If \(E\) is (at least) extensive \((\propto N)\), this thus grows considerably faster with \(N\) than the number partitioning problem (11).

Outside the crossover region there are no differences between the canonical and micro-canonical ensemble [see text below Eq. (8)], thus we can use the canonical predictions as a basis for our micro-canonical calculations. This confirms that the most probable outcome consists of solitonlets of size \(N_s = 1\) at high enough total energies. For positive total energies, all particles can be in such a state. However, for negative total energies this is no longer the case.

The large exponential growth (12) clearly suggests that we should have as many single atoms as possible. Thus, the negative total energy should be carried by one large soliton and there should be many solitonlets of unit size carrying kinetic energy:

$$E_{\text{total}} = E_0(N_1) + \sum_{j=1}^{N-N_1} E_{\text{kin}}^{(j)}.$$  

It would of course be possible to increase the kinetic energy by adding a further larger solitonlet and reducing the number of single unbound atoms. But the scaling of Eq. (12) and the canonical treatment of the high-temperature phase \cite{26,27} clearly shows that these configurations are not statistically relevant. Thus, the leading contribution to the number of possible configurations is

$$\Omega(N) \sim \left( \frac{4\pi L^2 m E_{\text{total}} - E_0(N_1)}{3h^2 N} \right)^{(N-N_1)/2}.$$  \hfill (13)

Taking the leading order approximation \(E_{\text{total}} = E_0(N_1^{(0)}) \propto N_1^{(0)}\) \(\left[(N_1^{(0)})^2 - 1\right] \sim (N_1^{(0)})^2\),

$$N_1^{(0)} \sim (-\gamma)^{1/3} N, \quad 0 > \gamma \geq -1,$$  \hfill (14)

and then using

$$N_1 = N_1^{(0)} + \delta N_1,$$  \hfill (15)

we can show that \(\delta N_1/N_1\) is indeed small for negative \(E_{\text{total}}\). With \(E_{\text{total}} - E_0(N_1) = -E_{\text{kin}}^{(0)}\delta N_1 > 0\) the “maximum finding condition”

$$\frac{\partial \ln[\Omega(N)]}{\partial \delta N_1} = 0$$

then implies in leading order

$$\frac{N - N_1^{(0)} - \delta N_1}{\delta N_1} = \ln \left( \frac{4\pi L^2 m}{3h^2 N} \right) \approx 0.$$  \hfill (16)

In the limit (7) and for \(E_{\text{total}} \propto E_0(N)\), \(E_0^{(0)}(N_1^{(0)})\) is independent of \(N\) (as is \(m\)). All other quantities (including \(L\)) are proportional to \(N\). This yields the leading-order behaviour \cite{39}

$$\delta N_1 = \frac{\left(1 - \sqrt{-\gamma}\right) N}{W \left( \frac{N^4 \pi g_{1D}^2 m^2 \left(\left(-\gamma\right)^{2/3} + \gamma\right)}{6h^4 g_0^2 \left(1 - \sqrt{-\gamma}\right)} \right) + 1} \sim \frac{\left(1 - \sqrt{-\gamma}\right) N}{2 \ln(N)}.$$  \hfill (17)

in the limit (7) where \(g_0 = N/L\) and \(g_{1D}\) are constants. The Lambert function \(W(x)\) solves the equation \(W(x) \exp[W(x)] = x\).

Repeating the above calculation for \(E_{\text{total}} > 0\) we have as our starting point

$$N_1 = 1, \quad \gamma > 0,$$  \hfill (18)

and we have again that \(\delta N_1 \rightarrow 0\) in the limit (7).

\begin{table}[h]
\begin{center}
\begin{tabular}{|c|c|c|c|}
\hline
regime & \(E_{\text{total}} \geq 0\) & \(0 \geq E_{\text{total}} > E_0(N - 1)\) & \(E_0(N - 1) > E_{\text{total}}\) \\
\hline
MCE & \(N\) atoms & coexistence & one large soliton \\
\hline
\end{tabular}
\end{center}
\caption{For positive total energies, the micro-canonical ensemble (MCE) agrees with the canonical prediction that there are \(N\) single atoms \cite{26,27}. Contrary to the canonical predictions, the regime for which single atoms and solitons co-exist survives the thermodynamic limit (7), thus indicating that the general assumptions of the Landau hypothesis do not directly apply to the Lieb-Linger model when treated in the MCE. The only way to on average obtain an \(N\)-particle soliton is for very negative \(E_{\text{total}} < E_0(N - 1)\) and thus \(E_{\text{total}}/E_0(N) \rightarrow 1\) in the limit (7).}
\end{table}
Figure 1 shows the size of the largest soliton as predicted by the MCE. Parameters near $E_{\text{total}} \approx 0$ are consistent with soliton trains [40–42] which were observed in the experiment of Ref. [7]: for, say, five solitons of equal size, the total ground state energy would be only $1/25$ of $E_0$ (in the absence of kinetic energy).

To conclude, the statistical ensembles MCE and CE are not equivalent for the Lieb-Liniger model with attractive interactions. The violation of ensemble equivalence is indicated by anomalous (canonical) energy fluctuations. We note that the existence of anomalous fluctuations — that have been discussed for condensate fluctuations [43–45], both for non-interacting Bose-Einstein condensates [46–48] and for interacting models [49, 50] — has been questioned for state-of-the-art bright soliton experiments in BECs [6–15]. Given that the temperature barely changes over the energy regime relevant for the existence of bright solitons, it seems to be easier to simply approximately give it as the transition temperature [26, 27] and calculate it for the experimentally relevant parameters, the result being practically identical for 73% of all particles occupying one large soliton or, say, 42%. As the corresponding energy difference is rather large, getting from one to the other requires more experimental effort than the tiny temperature difference might suggest. This behaviour is similar to water freezing or ice melting without any change of temperature. For bright solitons in the presence of a harmonic trap, classical field theory has been used to investigate the statistics of an attractive 1D Bose gas [54], an approach that might help to investigate the open question about the statistics near $E_{\text{total}} \approx 0$.

The data presented in this paper are available online [55].

ACKNOWLEDGMENTS

We thank T. P. Billam, L. D. Carr, Y. Castin, J. Tempere and T. P. Wiles for discussions. C.W. and S.A.G. thank the UK Engineering and Physical Sciences Research Council (Grant No. EP/L010844/1) for funding. B.G. thanks the European Union for funding through FP7-PEOPLE-2013-IRSES Grant Number 605096.

[1] T. P. Meyrath, F. Schreck, J. L. Hanssen, C.-S. Chuu, and M. G. Raizen, “Bose-Einstein condensate in a box,” Phys. Rev. A 71, 041604 (2005).
[2] A. L. Gaunt, T. F. Schmidutz, I. Gol'tubovych, R. P. Smith, and Z. Hadzibabic, “Bose-Einstein condensation of atoms in a uniform potential,” Phys. Rev. Lett. 110, 200406 (2013).
[3] C. Herzog and M. Olshanii, “Trapped bose gas: The canonical versus grand canonical statistics,” Phys. Rev. A 55, 3254 (1997).
[4] N. D. Mermin and H. Wagner, “Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models,” Phys. Rev. Lett. 17, 1133 (1966).
[5] P. C. Hohenberg, “Existence of long-range order in one and two dimensions,” Phys. Rev. 158, 383 (1967).
[6] L. Khaykovich, F. Schreck, G. Ferrari, T. Bourdel, J. Cubizolles, L. D. Carr, Y. Castin, and C. Salomon, “Formation of a matter-wave bright soliton,” Science 296, 1290 (2002).
[7] K. E. Strecker, G. B. Partridge, A. G. Truscott, and R. G. Hulet, “Formation and propagation of matter-wave soliton trains,” Nature (London) 417, 150 (2002).
[8] S. L. Cornish, S. T. Thompson, and C. E. Wieman, “Formation of bright matter-wave solitons during the collapse of attractive Bose-Einstein condensates,” Phys. Rev. Lett. 96, 170401 (2006).
[9] A. L. Marchant, T. P. Billam, T. P. Wiles, M. M. H. Yu, S. A. Gardiner, and S. L. Cornish, “Controlled formation and reflection of a bright solitary matter-wave,” Nat. Commun. 4, 1865 (2013).
(Europhys. Lett.) 96, 10011 (2011).

[55] C. Weiss, S. A. Gardiner, and B. Gertjerenken, https://collections.durham.ac.uk/files/vt150j26r, http://dx.doi.org/10.15128/vt150j26r (2016), “Temperatures are not useful to characterise bright-soliton experiments for ultra-cold atoms: Supporting data”.