Finite-temperature phase transition in a homogeneous one-dimensional gas of attractive bosons

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(Dated: Submitted: August 16, 2013; current version October 29, 2016)

In typical one-dimensional models the Mermin-Wagner theorem forbids long range order, thus preventing finite-temperature phase transitions. We find a finite-temperature phase transition for a homogeneous system of attractive bosons in one dimension. The low-temperature phase is characterized by a quantum bright soliton without long range order; the high-temperature phase is a free gas. Numerical calculations for finite particle numbers show a specific heat scaling as $N^2$, consistent with a vanishing transition region in the thermodynamic limit.

PACS numbers: 05.70.Fh, 03.75.Lm, 05.30.Jp, 03.75.Hh

Keywords: phase transition, one dimension, finite temperatures, bright solitons, Bethe ansatz, Lieb-Liniger model, attractive interactions, Mermin-Wagner theorem, Bose-Einstein condensation

Bright solitons generated from attractively interacting Bose-Einstein condensates in quasi-one-dimensional wave guides are investigated experimentally in an increasing number of experiments[1–10]. As experiments do not truly take place in one dimension but rather in quasi-one-dimensional wave guides, providing a thermalization mechanism [11, 12], this leads to the question whether or not these bright solitons can be stable in the presence of thermal fluctuations.

The Mermin-Wagner theorem [13] proves that in many models long-range order in one or two dimensions cannot exist at finite temperatures [13, 14]; this excludes the existence of many phase transitions. Finite-temperature transitions are fundamentally different from quantum phase transitions (cf. [15, 16]); one-dimensional quantum phase transitions can be found, e.g., in Refs. [17–19]). While there are some finite temperature phase transitions in low-dimensional systems like the Berezinsky-Kosterlitz-Thouless transition in two dimensions [20] or the phase transition in the two-dimensional Ising model [21], the generic case is that low-dimensional models to not undergo finite-temperature phase transitions [22]. Indeed, a book on “thermodynamics of one-dimensional solvable models” does not include the word “phase transition” in its index [23]. For a disordered system displaying Anderson-localization [24], a finite-temperature phase transition for weakly interacting bosons in one dimension has been found in Ref. [25].

A quasi one-dimensional system of attractively interacting bosons can be modeled [26–29] by the solvable Lieb-Liniger model [30–32]. One of the challenges for bright-soliton experiments [1–7, 33] is to realize true quantum behavior predicted, so far, with zero-temperature calculations [34–40]. For the Lieb-Liniger model, investigations of thermal effects on the many-body level for bosons in one dimension have so far focused on the more extensively studied case of repulsive interactions (Ref. [23] and references therein); for finite systems classical field methods have been applied [41]. In other soliton models, thermodynamics with interacting solitons has been investigated [42, 43].

In this Letter we show that attractive bosons in the Lieb-Liniger model undergo a finite-temperature phase transition; a bright soliton – no-soliton transition. As bright solitons do not display long-range order, this does not violate the Mermin-Wagner theorem. Although bright solitons do not display long-range order, quantum bright solitons are fundamentally different from localized states cf. [25]: For the Lieb-Liniger model, the energy eigenfunction describing a soliton of $N$-particles has to obey the symmetry of the Hamiltonian and is thus translationally invariant.

For $N$ identical bosons on a one-dimensional line of length $L$, corresponding to the experimentally realizable [44] box potential, the Lieb-Liniger Hamiltonian reads [30–32]

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

where $g_{1D} < 0$ quantifies the contact interactions between two particles, $m$ is the mass, and $x_j$ the position of the $j$th particle. Contrary to the phenomenological model used in [45] for a harmonically trapped one-dimensional gas of attractive bosons, we use the complete set of energy-eigenvalues which are known analytically for large $L$ [27, 46],

$$E_{LL}\left(\{n_r,k_r\}_{r=1,R}\right) = \sum_{r=1}^{R} \left( E_0(n_r) + \frac{\hbar^2 K_r^2}{2n_r m} \right), \quad \sum_{r=1}^{R} n_r = N, \quad (1)$$

where the $R$ natural numbers $n_r$ correspond to either free particles, if $n_r = 1$, or matter-wave bright solitons, if $n_r > 1$ (cf. the energy-eigenfunctions discussed in Ref. [27]); for experiments with more than two solitons see Refs. [2, 3], cf. [34, 38]). Each soliton has kinetic energy (proportional to the square of the single-particle momentum $\hbar k_r$, shared by all particles belonging to this soliton) and ground-state energy [27, 31]

$$E_0(n_r) = -\frac{1}{24} \frac{m g_{1D}^2}{\hbar^2} n_r (n_r^2 - 1). \quad (2)$$

1 The precise limit, which was not discussed in Refs. [30, 31], will be defined in Eq. (4) after the necessary physical requirements on this limit are stated.
We choose periodic boundary conditions (cf. [46]) which lead to $KL$ having to be an integer multiple of $2\pi$, thus

$$K_r = \frac{2\pi}{L} v_r, \quad v_r = \ldots, -2, -1, 0, 1, 2, \ldots$$

As we are dealing with indistinguishable particles, many-particle wave functions [27] are unambiguously defined by only considering configurations with

$$n_1 \geq n_2 \geq n_3 \ldots \geq n_R.$$ 

Because of Eq. (1), the total number of possibilities to distribute $N$ particles among up to $N$ parts is thus given by the number partitioning problem [47]

$$p(N) \sim \frac{1}{4N \sqrt{\pi}} \exp\left(\frac{\pi \sqrt{\frac{3}{2}}}{\sqrt{N}}\right), \quad N \gg 1. \quad (3)$$

The $N^3$-dependence of the ground-state energy (2) is a problem for the treatment of the thermodynamic limit ($N \to \infty, L \to \infty$ such that $N/L = \text{const.}$) [23]: the Lieb-Liniger model with repulsive interaction is thus normally used to do thermodynamics [23]. However, for attractive interactions treating the limit $N \to \infty$ at fixed interaction would lead to infinite densities, cf. [27]. We thus combine the thermodynamic limit with vanishing interaction – as used in the mean-field (Gross-Pitaevskii) theory of bright solitons [48].

$$N \to \infty, \quad L \to \infty, \quad g_{1D} \to 0, \quad \varrho = \text{const.}, \quad \mathcal{G} = \text{const.},$$

where $\varrho \equiv N/L$ and $\mathcal{G} \equiv N g_{1D}$. When approaching the limit (4), the energy-gap $E_{\text{gap}} \equiv E_0(N-1) - E_0(N)$ is an $N$-independent energy scale which will turn out to be the relevant energy scale for thermodynamics; we can express characteristic temperatures as

$$k_B T_0 = AE_{\text{gap}},$$

and subsequently investigate if the prefactor $A$ remains non-zero in the limit (4). The ground state energy (2) now reads

$$E_0(n_r) = -\frac{E_{\text{gap}}}{3N(N-1)} n_r(n_r^2 - 1);$$

in the limit (4) the energy gap is given by

$$E_{\text{gap}} = \frac{1}{8} \frac{mg^2}{\hbar^2} = \text{const.} > 0.$$ 

Before we choose the canonical ensemble (characterized by temperature $T$ and particle number $N$ [49]) to do thermodynamics, we should quantify the requirement that $L$ has to be large in order for the energy-eigenvalues (1) to be correct within the limit (4). The ground-state wave function for $N$ bosons is given by

$$\psi_0 \propto \exp\left[-\frac{mg_{1D}}{2\hbar^2} \sum_{1 \leq j, k \leq N} |x_j - x_k|\right];$$

the size of an $N$-particle soliton $\sigma \approx 1/(|g_{1D}|N)$ [27] and thus remains a non-zero constant in the limit (4), leading to a single particle density $\propto \cosh(\chi/\sigma)^{-2}$ and thus also to a vanishing off-diagonal long-range order.\footnote{The many-particle ground state can be viewed as consisting of a relative wave-function given by a Hartree product state with $N$ particles occupying the GPE-soliton mode $\cosh((x - x_0)/\sigma)^{-1}$ and a center-of-mass wave function for the variable $x_0$ (cf. [27, 50]). The one-body density matrix [48] then is $\propto \cosh((x - x_0)/\sigma)^{-1} \cosh((x' - x_0)/\sigma)^{1}$ which vanishes in the limit $|x - x'| \to \infty$ after integrating over $x_0$. Thus, there is no off-diagonal long range order in our system.}

In order for the energy eigenvalues given by Eq. (1) to be valid, the system has to be larger than the size of a $N = 2$ soliton (the more particles are in a soliton, the smaller it gets [27]). To be on the safe side we ask the wave function to be below $e^{-100}$ for particle separation greater than $L$, that is

$$\frac{m|g_{1D}|}{2\hbar^2} L \gtrsim 100.$$ 

For the two relevant energy scales of Eq. (1) this gives an energy ratio

$$\mathcal{E}(N) \equiv \frac{E_{\text{gap}}}{E_{\text{lim}}(v_r = 1)} = BN^2,$$

$$B \equiv \left(\frac{mg_{1D}}{2\hbar^2}\right)^2 \frac{1}{(2\pi)^2};$$

(6)

the eigenvalues (1) are therefore a very good approximation to the true eigenvalues of the Lieb-Liniger model (for all temperatures) if

$$B \gtrsim B_0 = \frac{100^2}{(2\pi)^2} \approx 253.$$ 

(7)

For any choice of $\{n_r\}_{r=1,R}$, the canonical partition function will depend on how often solitons of exactly size $n_r$ occur. We thus rewrite these configurations, now listing them using distinct integers $n'_r$ with $n'_r > n'_{r+1}$ and the multiplicity $\#(n'_r)$ with which the value $n_r$ had occurred:

$$\{n_r\}_{r=1,R} \longrightarrow \{(n'_r, \#(n'_r))\}_{r=1,R'}, \quad \sum_{r=1}^{R'} n'_r \#(n'_r) = N.$$ 

Note that replacing $\{n_r\}_{r=1,R}$ by $\{(n'_r, \#(n'_r))\}_{r=1,R'}$ is bijective, that is, to each set of $n_r$ there is exactly one set of $\{(n'_r, \#(n'_r))\}$ (and vice versa); in the following we can thus always use the notation which is more convenient. The total canonical partition function is the sum

$$Z_{N,\text{total}}(\beta) \equiv \sum_{\{n_r\}_{r=1,R}} Z_{N'}(\{(n'_r, \#(n'_r))\}_{r=1,R'}) (\beta)$$

(8)

over the partition functions for fixed $\{n_r\}_{r=1,R}$

$$Z_{N'}(\{(n'_r, \#(n'_r))\}_{r=1,R'}) (\beta) = \prod_{r=1}^{R'} e^{-\#(n'_r)B E_0(n'_r) \#(n'_r) k_B T},$$

(9)
The soliton partition function is given by
\[ Z_{n_1, \theta(n_1), \text{kin}}(\beta) = \frac{1}{\#(n_1)} \sum_{l=1}^{\#(n_1)} Z_{n_1, \text{kin}}(l\beta) Z_{n_1, \theta(n_1)-l, \text{kin}}(\beta), \] (10)

with \( Z_{n_0, \text{kin}}(\beta) = 1 \) and the kinetic energy part of the single-soliton partition function is given by
\[ Z_{n_1, \text{kin}}(\beta) = \sum_{\nu=\infty}^{\infty} \exp\left(-\beta \frac{E_{\text{gap}}}{n_1 B N^2} \nu^2 \right) \]
\[ \simeq \int_{-\infty}^{\infty} \nu \exp(-\beta \frac{E_{\text{gap}}}{n_1 B N^2} \nu^2) = \left( \frac{\pi n_1 B N^2}{\beta E_{\text{gap}}} \right)^{\frac{1}{2}}. \] (11)

Rather than having to explicitly do sums over a large number of configurations, for larger particle numbers it is preferable to calculate the partition function again via a recurrence relation, starting with \( R = 1 \) and \( Z_{M_0, \theta(n_0)}(\beta) \), \( M = 1, 2, \ldots N \) given by Eq. (9). The step \( R \to R + 1 \) then yields the case \( n_{R+1} = n_R \) with
\[ Z_{M+\#(n_1), \theta(n_1)+1, \text{kin}}(\beta) = \frac{e^{-\beta E(n_1)+1}}{Z_{M, \theta(n_1), \text{kin}}(\beta)} \]
\[ \times Z_{R}^{\text{(1)}}(M_{\theta(n_1), \theta(n_1)+1}, \beta) \] (12)

as well as
\[ Z_{M+\#(n_1), \theta(n_1)+1}^{\text{(1)}}(\beta) = e^{-\beta E(n_1)} Z_{n_1, \text{kin}}(\beta) \]
\[ \times \sum_{n_{R+1} = \#(n_1)+1}^{M} \sum_{\#(n_R) = 1} Z_{M_{\theta(n_1), \theta(n_1)+1}}(\beta), \] (13)

where \( [x] \) denotes the largest integer \( \leq x \).

From the total canonical partition function (8) we obtain the specific heat (at fixed particle number \( N \) and system size \( L \), which is proportional to the variance of the energy) as
\[ C_{N,L}(T) = \frac{\partial}{\partial T} \langle E \rangle = -\frac{\partial}{\partial T} \frac{\partial}{\partial \beta} \ln[Z_{N,\text{total}}(\beta)] \]
\[ = \frac{1}{k_B T^2} \frac{\partial^2}{\partial \beta^2} \ln[Z_{N,\text{total}}(\beta)] = \frac{1}{k_B T^2} \left( \langle E^2 \rangle - \langle E \rangle^2 \right); \] (14)

the number of atoms in the largest soliton is given by
\[ \langle n_1 \rangle(T) = \frac{1}{Z_{N,\text{total}}(\beta)} \sum_{n_1=1}^{N} n_1 Z_{N,\{n_1, \theta(n_1)\}}(\beta). \] (15)

For analytic calculations Eq. (11) leads to
\[ \frac{1}{\#(n_1)} \left( \frac{n_1 B N^2}{\beta E_{\text{gap}}} \right)^{n_1+1} \leq Z_{n_1, \theta(n_1), \text{kin}}(\beta) \]
\[ \leq e^{\theta(n_1)+1} \left( \frac{n_1 B N^2}{\beta E_{\text{gap}}} \right)^{n_1}, \]
\[ c_1 \equiv \ln(2), \] (16)

the lower bound being (for temperatures large compared to the center-of-mass first excited state) the largest term involved in the sum (10); to obtain the upper bound we choose the value for \( c_1 \) such that all \( 2^{\theta(n_1)+1} < e^{\theta(n_1)+1} \) addends in the sum (10) (treated separately) are of the same order as the highest term.

In order to define a characteristic temperature (5), we now use the temperature below which finding a single soliton with \( N \) particles is more probable than finding \( N \) single particles. Both partition functions, evaluated at \( T = T_0 \), are thus the same,
\[ Z_{N,\text{kin}}(\beta_0) e^{-\beta_0 E(N)} = Z_{N,\theta(n), \text{kin}}(\beta_0), \]
\[ \beta_0 \equiv \frac{1}{k_B T_0}. \] (17)

While the left-hand side is known exactly \( [Z_{N,\text{kin}}(\beta)] \) is given by Eq. (11), the right-hand side of Eq. (17) lies between the bounds given by Eq. (16). Taking the \( N \)th root of Eq. (17) for each of these bounds leads [55], in the thermodynamic limit (4), to two characteristic, \( N \)-independent temperatures
\[ T_1^{(\infty)} = \frac{2 E_{\text{gap}}}{3 k_B} W \left( \frac{5 \pi B \exp(2)}{2} \right), \] (18)
\[ T_2^{(\infty)} = \frac{2 E_{\text{gap}}}{3 k_B} W \left( \frac{5 \pi B \exp(2)}{2} \right), \] (19)

where \( W(x) \) is the Lambert W function which solves \( W(x) \exp[W(x)] = x \) [55]. In the thermodynamic limit (4), the temperature for which it is equally probable to find \( N \) single particles and one bright soliton is lies in the range
\[ 0 < T_1^{(\infty)} \leq T_0^{(\infty)} \leq T_2^{(\infty)} < \infty \]

For numerical finite-size investigations we focus on particle numbers \( N \approx 100 \) relevant for generation of Schrödinger-cat states on timescales shorter than characteristic decoherence times [35]; \( T_2^{(\infty)} \) turns out to be a characteristic temperature scale already for these particle numbers (see Fig. 1).

Figure 1 shows that the numerical data obtained via exact recurrence relations for the canonical partition function [Eqs. (9)-(13)] at the transition many solitons are involved (Fig. 1 d). Near \( T_2^{(\infty)} \), the numerical data is consistent with both the specific heat and the temperature-derivative of \( \langle n_1 \rangle \) scaling \( \propto N^2 \) for \( N \approx 100 \).

To demonstrate that we indeed have a phase transition let us start by focusing on cases where we have \( N-n \) particles in one soliton and \( n \) free particles; \( n = O(N) \) and \( N \gg 1 \). Using Eq. (17) to express the partition function for \( n \) free particles corresponds to a system with fewer atoms \( \hat{n} \) but the same \( \beta \) thereby rescaling \( E_{\text{gap}} \) and therefore also \( T_1^{(\infty)} \) by a factor

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1 When approximating the sum \( \sum_{\nu=\infty}^{\infty} \exp(-\nu^2) \) by the integral \( \int_{-\infty}^{\infty} \nu \exp(-\nu^2) \), the error lies below \( 10^{-40} \) for \( 0 < x < 0.1 \) [55]. When approaching the limit (4), \( x \rightarrow 0 \) and Eq. (11) thus becomes exact.
we thus have

Thus, using the canonical ensemble [49] we have shown the existence of a phase transition in the thermodynamic limit (4) [cf. Fig. 2].

The $N$-dependence of the specific heat shows that both in the high-temperature phase [Fig. 1 (b),(c)] and in the low-temperature phase [Fig. 1 (b)] predictions of the canonical and the microcanonical ensemble [49] agree [49]. As the mean energy is a monotonously increasing function of temperature [Eq. (14)] and as furthermore, the choice of the thermodynamic limit (4) leads to a mean energy $\propto N$ and an $N$-independent temperature scale, the $\propto N^2$ behavior displayed by the specific heat in Fig. 1 (d) can only occur in a small ($\propto 1/N$) temperature range in which both ensembles no longer are equivalent.

To conclude, we find the existence of a finite-temperature many-particle phase transition in a one-dimensional quantum many-particle model, the homogeneous Lieb-Liniger gas with attractive interactions [Eqs. (21) and (22); Fig. 2]. The low temperature phase consists of a macroscopic number of atoms being one large quantum matter-wave bright soliton with delocalized center-of-mass wave function (which does not display long-range order thus not violating the Mermin-Wagner theorem [13, 14]; the Landau criterion [56] which argues against the co-existence of two distinct phases is also not violated); the high temperature phase is a free gas. As a harmonic trap would facilitate soliton formation [58], we conjecture that the existence of a finite-temperature phase transition remains true for weak harmonic traps. In experiments, even the integrable Lieb-Liniger gas can thermalize as the wave guides are quasi-one-dimensional (cf. [11, 12]).

Via exact canonical recurrence relations we also numerically investigate the experimentally relevant case of some 100 atoms (cf. [5, 35, 36]) with the (experimentally realizable [44]) box potential. The spike-like specific heat provides further insight: the specific heat ($\propto N^2$) is the derivative (14) of an energy scaling not faster than $\propto N$ (4). At low temperatures all atoms form one soliton; the size of the soliton thus is an ideal experimental signature (cf. [1–10]).
I thank T. P. Billam, Y. Castin, S. A. Gardiner, D. I. H. Holdaway, N. Proukakis and T. P. Wiles for discussions and the UK EPSRC for funding (Grant No. EP/L010844/1 and EP/G056781/1). The data presented in this paper will be available online [59].

Note added: Recently, a related work appeared [60].

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