Solitary waves and yrast states in Bose-Einstein condensed gases of atoms

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Abstract – Considering a Bose-Einstein condensed gas confined in one dimension with periodic boundary conditions, we demonstrate that, very generally, solitary-wave and rotational excitations coincide. This exact equivalence allows us to establish connections within a number of effects that are present in these two problems, many of which have been studied in the mean-field approximation and in the Tonks-Girardeau limit of hard-core bosons.

Introduction. – Remarkable experimental developments in the field of cold atomic gases now permit the realization of systems previously not accessible. One example is the recent fabrication of toroidal traps that realize periodic boundary conditions [1–5]. Tight, elongated traps now allow us to realize quasi–one-dimensional motion of the atoms, since the energy associated with transverse excitations is much higher than the interaction energy [6]. A very tight toroidal trap is expected soon and will permit the study of periodic motion in a quasi–one-dimensional system.

Such advances will make it possible to study many of the interesting phenomena predicted by the various non-linear models of such systems that have been studied in recent decades. In the case of bosonic atoms, for example, even the ground state is non-trivial. When the effective interaction is attractive, a localized density maximum forms for sufficiently strong coupling [7,8]. When the effective interaction is weakly repulsive, the density is homogeneous. As the interaction strength increases, however, the gas eventually enters the Tonks-Girardeau state of hard-core bosons, in which the bosons resemble fermions in many respects [9,10].

Another interesting aspect of bosonic atoms confined by a ring potential is their excitation spectrum [11–13]. Two fundamental forms of excitations, solitary-wave excitations and rotational excitations, have been investigated. In the first case, one is interested in travelling-wave solutions for which the wave propagates around the ring with a constant velocity and without change of form. In the second case, one is interested in the lowest-energy state of the system for a given angular momentum, which is the so-called “yrast” state.

Clearly, both are excited states of the system, and it is interesting to investigate if and how they are related. Bloch’s theorem [14] implies that states of different values of the winding number are connected via excitation of the center of mass. As a result, the dispersion relation, i.e., the energy of the system as a function of the angular momentum, is a periodic function on top of a parabolic envelope function due to center-of-mass excitations. The yrast state is (by definition) the lowest-energy state for a fixed angular momentum. Therefore, the naive expectation is that the dispersion relation appropriate for solitary-wave excitation should have a structure similar to that of the yrast spectrum, but with a higher energy. However, in a recent study [15], Kanamoto, Carr, and Ueda have provided numerical evidence that “quantum solitons in the Lieb-Liniger Hamiltonian are precisely the yrast states”.

The first goal of the present study is to demonstrate analytically, using simple arguments, that “solitary-wave” states (to be defined more precisely below) and yrast states are identical for all interaction strengths. A second goal of our study is to explore the effects of this equivalence on various physical quantities in the language of solitary-wave and of rotational excitation.
The present study contributes to the long-standing problem of the excitation spectrum of a one-dimensional Bose gas with periodic boundary conditions. In his seminal work Lieb [13] demonstrated that this spectrum has two branches. The usual Bogoliubov spectrum which is linear for long wavelengths and quadratic (i.e., single-particle like) for higher energies. It is shown here that the other branch, which has been identified as corresponding to solitary-wave excitations [16,17], can also be regarded as the lowest-energy state of the gas for a fixed value of the angular momentum.

In the following we first demonstrate the equivalence of yrast states and solitary-wave states for the case of an axially symmetric ring. This result is completely general and makes no assumption about the explicit form of the many-body state. We then examine the limit of weak interactions, where the mean-field approximation is an excellent description of both states, and discuss the links among various effects that appear in these two seemingly different problems. Finally, we consider the Tonks-Girardeau limit of strong interactions.

The equivalence of rotational and solitary-wave excitations. – Let us start with the yrast states. For a given Hamiltonian, \( \hat{H} \), the constraints of a fixed particle number and a fixed angular momentum can be imposed with the introduction of two Lagrangian multipliers, \( \mu \) and \( \Omega \), which can be interpreted physically as the chemical potential and the angular velocity of the trapping potential. (We assume here that the gas has equilibrated in the rotating trap.) If \( \Psi_y(x_1, x_2, \ldots, x_N) \) is the yrast many-body state, variations of the energy functional,

\[
E(\Psi_y, \Psi_y^*) = \int \Psi_y^* \hat{H} \Psi_y \, dx_1 \ldots \, dx_N
\]

\[
-\mu \int \Psi_y^* \Psi_y \, dx_1 \ldots \, dx_N - \Omega \int \Psi_y^* \hat{L} \Psi_y \, dx_1 \ldots \, dx_N,
\]

with respect to \( \Psi_y^* \) yield

\[
\hat{H} \Psi_y - \mu \Psi_y - \Omega \hat{L} \Psi_y = 0. \tag{2}
\]

We stress that the single-particle density distribution corresponding to the states \( \Psi_y \) is axially symmetric, because of the axial symmetry of the Hamiltonian, \( \hat{H} \). On the other hand, in the limit of the mean-field approximation, \( \Psi_y \) is well approximated by a product state that breaks the axial symmetry but has the same energy as that of \( \Psi_y \) to leading order in \( N \) \[18,19\].

We now turn to travelling-wave solutions which propagate unaltered with a velocity \( u \). In the limit of the mean-field approximation and the case of contact interactions the many-body state is a product state, which is the solution of the Gross-Pitaevskii equation [20]. This state has a density distribution that is not axially symmetric and is the well-known solitary wave, with a localized density depression or elevation. More generally, we can write this travelling-wave solution as

\[
\Psi_s(x_1, x_2, \ldots, x_N, t) = \Psi_s(z_1, z_2, \ldots, z_N) e^{-iut/\hbar}, \tag{3}
\]

with \( z_i = x_i - ut \), where \( u \) corresponds to the velocity of propagation of the solitary wave. Since \( i\hbar \partial \Psi_s/\partial t = \hat{H} \Psi_s \),

\[
\hat{H} \Psi_s - \mu \Psi_s - u \hat{P} \Psi_s = 0, \tag{4}
\]

where \( \hat{P} \) is the momentum operator. Comparison of eqs. (2) and (4) reveals that \( \Psi_y \) and \( \Psi_s \) satisfy the same differential equation and the same boundary conditions. They are thus identical with the obvious equality \( u = \Omega R \), where \( R \) is the radius of the ring.

This equivalence is extremely general and requires only that the Hamiltonian is invariant under the transformation \( x_i \rightarrow z_i \). While the kinetic energy and the two-body interaction evidently meet this requirement, this is not always the case in the presence of an external one-body potential, \( V(x) \). The above results apply when \( V(x) \) is axially symmetric and time independent. As mentioned also above, the imposition of strict axial symmetry has important effects on the exact wave functions \( \Psi_y \) and \( \Psi_s \).

It forces them to have an axially symmetric single-particle density distribution, and it also implies that the condensed state is, in general, fragmented. However, these conclusions do not necessarily reflect the behaviour of real physical systems. In practice, it is impossible to avoid weak anisotropies in the trapping potential. Such symmetry-breaking anisotropies, even those which are vanishingly small in the limit of large atom numbers, are sufficient to break the axial symmetry of the single-particle density and to restore an unfragmented condensate [21–26].

Mean-field limit. – In the following, we first focus on the mean-field approximation, which is valid for sufficiently weak interactions. At mean-field level, we seek yrast states with a constrained average value of \( \hat{L} \), rather than insisting on having eigenstates of \( \hat{L} \). It should be noted that although the yrast state and its corresponding solitary-wave state are rotationally symmetric, this rotational symmetry breaks within the mean-field approximation for both of them. As mentioned also above, it has been shown that in the limit of weak interactions the energies of the axially symmetric and broken-symmetry yrast states are identical to leading order in \( N \), with differences of order \( 1/N \) \[18,19\].

In the case of solitary-wave solutions we seek travelling-wave solutions, which propagate with a constant velocity. As shown more generally above, both problems reduce to the same differential equation for the order parameters, with the result that \( \psi_y = \psi_s = \psi \). Specifically,

\[
-ih \frac{\partial \psi}{\partial x} = -\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial x^2} + (U_0 |\psi|^2 - \mu) \psi. \tag{5}
\]

In this equation we have assumed contact interactions, where \( U_0 \) is the matrix element for zero-energy elastic atom-atom collisions (in one dimension), and where
\( u = \Omega R \) as above. We now examine the consequences of this equivalence.

The solitary-wave solutions for a Bose-Einstein condensate confined to a ring potential with a repulsive effective interatomic interaction, \( U_0 > 0 \), are known to be Jacobi elliptic functions \([27,28]\) with density

\[
\begin{align*}
n(z) &= n_{\text{min}} + (n_{\text{max}} - n_{\text{min}}) \sin^2 \left( \frac{K(m)z}{\pi R} \right) m, \\
\end{align*}
\]

where \( \sin(x|m) \) are the Jacobi elliptic functions, \( n_{\text{min}} \) and \( n_{\text{max}} \) are the minimum and maximum values of the density, and \( K(m) \) is the elliptic integral of the first kind. The details of this calculation may be found in refs. [27,28]. According to the above argument, the yrast states in mean-field approximation are given exactly by the same expressions.

**Dispersion in the mean-field limit.** We turn now to the dispersion relation, i.e., the energy as a function of momentum, appropriate for both solitary-wave and yrast states. Given the solitary-wave order parameter in the form \( \psi(z) = \sqrt{n} e^{i \phi} \), one can determine the energy and momentum per particle according to the following formulas:

\[
E = \frac{1}{N} \int_{-\pi R}^{\pi R} \left[ \frac{\hbar^2}{2M} \left( \left( \frac{\partial \sqrt{n}}{\partial z} \right)^2 + n \left( \frac{\partial \phi}{\partial z} \right)^2 \right) + \frac{U_0}{2} n^2 \right] dz,
\]

and

\[
p = \frac{\hbar}{N} \int_{-\pi R}^{\pi R} n \left( \frac{\partial \phi}{\partial z} \right) dz.
\]

The analytic form of \( \phi(z) \), which is somewhat complicated, is given in ref. [28]. The desired \( E(p) \) follows immediately given \( E(u) \) and \( p(u) \). Figure 1 shows the results of this calculation for two different situations. Only the first two branches of this function are shown. Note that \( E(-p) = E(p) \). Clearly, the dispersion relation has the structure expected from Bloch’s theorem as stated above.

It is worth mentioning that the periodicity is incorporated in the expression for the density and the phase that is used in calculating the energy and momentum. An alternate approach is to consider the solution for the solitary waves on an infinite line [29]. In this case, however, it is necessary to impose the periodicity by using a modified expression for the momentum and also to evaluate the free energy. Furthermore, the resulting dispersion relation gives the limiting case of a ring of infinite radius. The advantages of the calculation above are that it is physically more transparent and, in addition, it gives the general dispersion relation for a ring of arbitrary radius.

It is convenient to introduce the dimensionless quantity \( g = NU_0 M R / (\pi \hbar^2) \), which is the ratio between the interaction energy \( n_0 U_0 \), with \( n_0 \) being the homogeneous density \( n_0 = N / (\pi R) \), and the kinetic energy, \( E_0 = \hbar^2 / (2 M R^2) \). In fig. 1 the value of \( g \) has been chosen to be \( 120/\pi^2 \) in the upper curve, and \( 3/4 \pi^2 \) in the lower curve. In this plot the energy is measured in units of \( E_0 = \hbar^2 / (2 M R^2) \), and the momentum is measured in units of \( p_0 = \hbar / (2 \pi R) \). When \( p = 0 \), the energy \( E(p = 0) \) comes purely from the interaction energy, which is \( U_0 N / (4 \pi R) \) or \( g/2 \) in units of \( E_0 \). The maximum value of the momentum per atom in each “quasi-periodic” interval is \( 2 \pi p_0 \). Finally, the energy difference \( E(p = 2 \pi p_0) - E(p = 0) = E_0 \), and \( E(p = 4 \pi p_0) - E(p = 2 \pi p_0) = (2^2 - 1) E_0 \). More generally, these energy differences are all the odd multiples of \( E_0 \), due to the excitation of the center of mass, as expected from Bloch’s theorem. In the non-interacting limit, the energy consists of straight line segments with slopes of \( E_0, 3E_0, 5E_0 \), etc. For this reason in the lower plot of fig. 1, where the interaction energy is small compared to the kinetic energy, the spectrum is almost linear in each interval. For larger interaction strengths, the slopes at the end points of each interval are unaltered, but the energy is no longer a straight line.

In the physics of solitary waves, it is well known that the velocity of propagation, \( u \), of a solitary wave satisfies the equation \( u = \partial E / \partial p \). This equality can also be viewed from the point of view of the yrast states in mean-field approximation. Assume that \( E(l) \) is the yrast energy per particle as a function of the angular momentum per particle \( l \) and that \( E' \) is the energy in a rotating frame of reference for which the density distribution of the yrast state is stationary. Given that \( E' = E - l \Omega \) and that \( \partial E' / \partial l = 0 \), it follows that \( \Omega = \partial E / \partial p \), which is the formula given above.

In ref. [28] it was argued that, when the winding number \( q \) is zero, the velocity of propagation of a solitary wave cannot vanish. This is obvious from the dispersion

![Fig. 1: The dispersion relation \( E(p) \), for \( g = 120/\pi^2 \) (a), and \( g = 3/4 \pi^2 \) (b). The energy is measured in units of \( E_0 = \hbar^2 / (2 M R^2) \), and the momentum in units of \( p_0 = \hbar / (2 \pi R) \). In the two curves both \( N/R \) and \( U_0 \) have the same value; however, in the lower curve the radius is 40 times smaller than in the upper one.](image)
relations of fig. 1. The region from \( p = 0 \) to \( p = \pi p_0 \) (given by the left solid points in the two plots of fig. 1) corresponds to \( q = 0 \). The smallest possible value of \( u \) (for \( q = 0 \)) is attained at \( p = \pi p_0 \) where its value is \( u = \hbar/(2MR) \). At this value of \( p \) the density develops a node, and a “dark” solitary wave forms. The density is relatively insensitive to changes in the momentum in the vicinity of this point, but there is a violent and discontinuous change in the phase of the order parameter that is associated with the change of the winding number. More generally, the solitary waves become dark and the winding number changes whenever \( p \) is an odd multiple of \( \pi p_0 \). The first two such points, where \( q \) changes from 0 to \(-1\) and from \(-1\) to \(-2\), are given as solid points in the two plots of fig. 1.

It is also interesting to note that the interaction energy (which scales like \( N/R \)) decreases relative to the zero-point energy (which scales like \( \hbar^2/(MR^2) \)) as the radius of the ring decreases for a fixed value of \( N/R \). The ratio of these energies is the parameter \( g \), which is \( \propto (N/R)^2 \). As \( R \) decreases for fixed \( N/R \), the interaction energy becomes less important, and the gas approaches the limit of a non-interacting system. In the limit of small \( R \), (i.e., \( g \ll 1 \)), the quasi-periodic intervals of the dispersion relation become linear with a discontinuous first derivative between them. The velocity of propagation of the solitary wave thus approaches constant values, given as odd multiples of \( v = \hbar/(2MR) \), set by the non-interacting problem \[32\]. This effect is clearly seen in the lower plot of fig. 1.

From the above remarks it is obvious that, as \( R \) decreases, there is a minimum value of the radius below which \( u \) cannot vanish \[27\]. The condition for this is \( R/\xi = \sqrt{6}/2 \), where \( \xi \) is the coherence length corresponding to a density \( n_0 = N/(2\pi R) \). In the language of the states, this says that there is a critical coupling of \( g = 3/2 \) for having a metastable minimum at \( L/N = l = \hbar/(2MR) \) (or equivalently at \( p = 2\pi p_0 \) \[7,8\]. For smaller values of \( g \), the slope of the dispersion relation is positive as \( l \rightarrow 0^- \) (or \( p \rightarrow 2\pi p_0^- \)), and the possible metastable minimum at this point disappears.

**Energetic stability in the mean-field limit.**– The creation of solitary waves in ring-like potentials will be of considerable interest. The intimate connection between solitary-wave and yrast states discussed here enables us to draw a number of conclusions about the possible generation of solitary waves and their energetic stability. The most obvious of these is that the lowest-energy state with a given \( \langle L \rangle \) will also be a solitary-wave state. Ideally, one would like to observe a family of solitary-wave solutions much like those observed in harmonic traps \[30,31\], i.e., density depressions travelling with a velocity which is less than that of sound and which decreases as the depression becomes deeper.

In the case of a repulsive effective interatomic interaction, the curvature of the dispersion relation is negative (as shown also in fig. 1) \[32\]. The “kink” states with a momentum per particle which is equal to an integer multiple of \( 2\pi p_0 \) are the only possible local minima in the absence of rotation of the trap. The occupation of these states will give rise to persistent currents. Since these states have a homogeneous density distribution and a non-zero circulation, they would be difficult to observe experimentally\(^1\). The same conclusion applies to a rotating trap. One way to overcome this difficulty would be to consider systems with attractive effective interactions \[15\].

In this case the curvature of the dispersion relation is positive \[32\], and persistent currents cannot be stable. In contrast, solitary waves can be stabilized by rotating the trap. The energy in a frame rotating with angular velocity \( \Omega \) is \( E' = E - \Omega p \), and \( E' \) can have local minima for a continuous range of \( l \) which is determined by \( \Omega \).

**Tonks-Girardeau limit.** – As was mentioned above, the equivalence of yrast states and travelling-wave states is general, given that the Hamiltonian is rotationally invariant. This implies that this equivalence persists as the interaction strength increases to the Tonks-Girardeau limit \[9,10\].

In the Tonks-Girardeau limit, the equivalence between the two kinds of excitation allows us to draw the following conclusions: in this limit the energy per particle of a Bose gas of a momentum per particle \( 0 \leq p \leq 2\pi p_0 \) is given by \[13\]

\[
E_{TG}(p) = E_0 \frac{N^2}{12} + \frac{N\hbar p}{2MR} - \frac{Np^2}{2M}. \tag{8}
\]

The first term on the right of eq. (8) is simply the Fermi energy of a Fermi gas in one dimension, \( E_F/3 \), for the value of the Fermi momentum, which is equal to \( N/2R \). Equation (8) is valid in the limit of \( N \) and \( R \) tending to infinity with \( N/R \) finite.

In a finite ring there are corrections to \( E_{TG}(p) \) of order \( E_0 = \hbar^2/(2MR^2) \), which result from center-of-mass excitations, as Bloch’s theorem implies \[14\]. The corresponding dispersion relation in a small system can be found in ref. \[33\] and has the same structure as that shown in the upper plot of fig. 1. More specifically, the only change is on the energy axis, since the energy scale is of order \( NE_0 \), rather than \( E_0 \). This observation allows us to make various physical statements which resemble those which are valid also within the mean-field approximation.

The fact that \( E_{TG}(p) \) is also the yrast energy, i.e., the lowest possible energy for some angular momentum \( l = pR \) allows us to evaluate the critical angular velocity \( \Omega_c \) for rotational excitation of the system. The above expression implies that this critical frequency is simply the derivative \( R^{-1}(\partial E_{TG}/\partial p) \) at \( p = 0 \), i.e., \( \Omega_c = N\hbar/(2MR^2) \). Actually, \( \Omega_cR \) may be identified as the speed of sound \[10\].

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\(^1\)Since a necessary (but not sufficient) condition for metastability is that the density distribution is homogeneous, while repulsive interactions are necessary to create persistent currents, the metastability of superflow works against the observation of the solitary waves with an inhomogeneous density distribution.
The velocity of propagation $u$ of solitary-wave excitation (defined earlier) also follows trivially, $u = (\partial E_{TG}/\partial p) = Nh/(2MR)$ $(1-2R/R_0)$. A “dark soliton” solution in the Tonks-Girardeau limit was investigated in ref. [34], which corresponds to $u = 0$, where the momentum is $p = h/(2R) = \pi p_0$, very much like the case of the mean-field approximation (in the limit of an infinite ring).

Since the single-particle density distribution is axially symmetric (because of the axial symmetry of the Hamiltonian) the authors of ref. [34] broke this symmetry by assuming that the cloud is pierced at some point. This solution has $u = 0$ in a infinite ring, whereas in a finite ring $u$ has a finite, non-zero minimum value for the reasons already mentioned in the mean-field limit. Furthermore, the curvature of the parabolic dispersion relation $E_{TG}(p)$ is still negative, which implies that the only yrast states(solitary-wave states which are energetically stable are those with a momentum per particle which is an integer multiple of $2\pi p_0$, as in the case of the mean-field approximation.

Summary. – In the present study we have presented a unified picture of two seemingly different forms of excitation of a Bose gas moving in one dimension with periodic boundary conditions, namely rotational and solitary-wave excitation. We have shown that yrast states and solitary-wave states are identical whenever the Hamiltonian is axially symmetric. This result is a simple consequence of the more general observation that the problem of finding wave functions that propagate with a fixed velocity is equivalent to the problem of minimizing the energy subject to a constraint of fixed angular momentum.

The only necessary condition for this equivalence, which holds for all functional forms of the wave function, is the rotational invariance of the Hamiltonian. This equivalence permits the consideration of such systems from two distinct points of view, and we have noted certain aspects of a unified picture that result from this observation in the mean-field regime, that is valid for sufficiently weak interactions, as well as in the opposite limit of hard-core bosons, i.e., in the Tonks-Girardeau limit.

This connection between solitary-wave and yrast states has been suggested previously [15] and the arguments offered here are admittedly elementary. It would appear, however, that the rigorous equivalence demonstrated here is neither generally known, nor adequately appreciated.

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