Superfluidity in a gas of strongly-interacting bosons

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Abstract. – We consider small systems of bosonic atoms rotating in a toroidal trap. Using the method of exact numerical diagonalization of the many-body Hamiltonian, we examine the transition from the Bose-Einstein condensed state to the Tonks-Girardeau state. The system supports persistent currents in a wide range between the two limits, even in the absence of Bose-Einstein condensation.

Introduction. – The advances in experimental techniques in the field of cold atoms have made it possible to access experimentally strongly correlated states that had only been part of the mathematical apparatus of quantum theory up to now. A famous recent example is the Tonks-Girardeau limit of bosonic atoms [1] that has been realized in the two experimental studies of Refs. [2]. Confined in elongated, quasi one-dimensional traps – as it nowadays can be realized in many laboratories around the world – at low densities or strong interparticle interactions the boson gas exhibits some properties which resemble those of a fermionic system.

Here, we consider interacting bosonic atoms which rotate in a toroidal trap. We examine the transition from the so-called Gross-Pitaevskii limit of weak interactions, where the gas forms a Bose-Einstein condensate, to the Tonks-Girardeau limit. In this transition, while Bose-Einstein condensation disappears, superfluidity persists in a much wider region. “Superfluidity”, throughout this paper, means the metastability of currents, or in other words, the existence of persistent currents [3–6], which is defined more precisely below.

The whole question of superfluidity is based upon two crucial issues: firstly, that there is an energy barrier between the current-carrying state and the current-free state. Secondly that no single-particle operator \(\Delta V\) connects the two states, at least to some order. In this case the decay rate of the current due to some weak perturbation that dissipates angular momentum and energy, if necessary, is highly suppressed. In the present problem the criterion we use is that no single-particle operator connects the two states at least to \textit{first-order} in this perturbation. As we will see, the two states are connected via \(\Delta V\) to lower and lower order, as the system goes from the Gross-Pitaevskii to the Tonks-Girardeau regimes. As a result, the characteristic timescale of the decay decreases in the transition between these two limits. Still, a transition that is not allowed even to first-order, will take a very long timescale (compared to the lifetime of these gases) for sufficiently weak perturbations. This approach is equivalent to examining the dynamic structure factor, as in Refs. [3, 4].
It is known that Bose-Einstein condensation is neither a necessary, nor a sufficient condition for superfluidity [7]. The problem investigated here provides an example where: (i) for Bose-Einstein condensation to imply superfluidity, interactions are necessary, and (ii) superfluidity exists in a much wider region between the two limits, even in the absence of Bose-Einstein condensation.

Assuming the usual contact interactions between the atoms, the many-body Hamiltonian is

\[
\hat{H} = -\frac{\hbar^2}{2M} \int \psi^\dagger(r) \nabla^2 \psi(r) \, dr + \frac{U_0}{2} \int \psi^\dagger(r) \psi^\dagger(r) \psi(r) \psi(r) \, dr.
\]

Here \( M \) is the atom mass and \( U_0 = 4\pi \hbar^2 a / M \), where \( a \) is the scattering length for elastic atom-atom collisions. Since we assume that the atoms are confined in a toroidal trap, we express the bosonic annihilation operator \( \psi \) in terms of the annihilation operators \( c_m \) of an atom with angular momentum \( m \), \( \psi(r) = \sum_m c_m e^{im\theta} / \sqrt{V} \). Here \( V = 2\pi RS \) is the volume of the torus with \( R \) its radius and \( S \) its cross section, with \( \sqrt{S} \ll R \). Measuring the energy in units of \( E_0 = \hbar^2 / (2MR^2) \) we thus find [8,9]

\[
\hat{H} = \sum_{l} l^2 c_l^\dagger c_l + \frac{g}{2} \sum_{k,l,m,n} c_k^\dagger c_l^\dagger c_m c_n \delta_{k+l,m+n},
\]

where the dimensionless constant \( g \) equals \( 4aR / S \).

**Transition between the Gross-Pitaevskii and the Tonks-Girardeau regimes.** In the Gross-Pitaevskii limit one has a Bose-Einstein condensate. In this case, the typical kinetic energy per atom is \( \hbar^2 / (2MR^2) \), and the typical interaction energy per atom is \( nU_0 \). Here \( n = N/V \) is the atom density and \( N \) is the atom number. From these two energy scales, we see that in this limit \( g \) should not exceed \( g_{\text{GP}} \sim 1/N \). In the opposite Tonks-Girardeau extreme, the typical kinetic energy per atom is on the order of \( \hbar^2 k_F^2 / (2M) \) (just like the Fermi energy in a Fermi gas), with \( k_F = \sigma \pi \) and \( \sigma = N / (2\pi R) \) the density per unit length. The interaction energy is still on the order of \( nU_0 \), and thus the characteristic value of \( \sigma \) is of order \( a / S \). Therefore, the coefficient \( aR / S \) is of order \( N \) in the Tonks-Girardeau limit, \( g \geq g_{\text{TG}} \sim N \). The parameter \( \gamma \) in the Lieb-Liniger model [8] is \( (\pi / 2)g / N \). Then, for \( g \sim N \), \( \gamma \) is indeed of order unity. The above estimates are in agreement with the two higher curves of Fig. 2, as explained below.

**Gross-Pitaevskii limit and persistent currents.** Although the results of the numerical diagonalization that we present below are much more general, it is instructive to start with a mean-field variational calculation that is valid in the Gross-Pitaevskii extreme. The existence of persistent currents can be seen easily in the following way [7,10,11]. Let us start with the usual basis states of angular momentum \( m \hbar, \phi_m(\theta) = \sqrt{N} e^{im\theta} / \sqrt{2\pi R} \) (normalized to \( N \)), and consider a linear superposition of \( \phi_0 \) and \( \phi_1 \), \( \psi_{\text{var}}(\theta) = c_0 \phi_0 + c_1 \phi_1 = \sqrt{1-I} \phi_0 + e^{i\phi} \sqrt{I} \phi_1 \). Here \( \phi \) is an arbitrary phase, and \( I \) is a parameter, being equal to the expectation value of the angular momentum per particle, \( l = L / N \). For \( l = 1 \), \( \psi_{\text{var}} \) describes a vortex located at its center, while for \( l = 0 \) the vortex is at an infinite distance away from the torus.

Because of the extra kinetic energy, the expectation value of the energy in the above state is higher for \( l = 1 \) than for \( l = 0 \). The first decisive question is whether there exists an energy barrier for some intermediate value of \( l \). Such a barrier is expected to be present for sufficiently strong repulsive interatomic interactions for the following reason: As \( l \) decreases, at some intermediate value between zero and unity, the vortex passes through the torus, which implies that a node forms in the atom density. This, however, costs interaction energy, since
for \( l = 0 \) and \( l = 1 \) the density is homogeneous, which is the configuration with the lowest interaction energy. Therefore, for sufficiently strong interactions, such a barrier is expected to develop.

Quantitatively, the expectation value of the Hamiltonian in the state \( \psi_{\text{var}} \) above is the Gross-Pitaevskii energy \( E_{\text{GP}} \), which is (in units of \( E_0 \))

\[
E_{\text{GP}}/N - \delta/2 = (1 + \delta)l - \delta l^2 + O(g),
\]

with \( \delta = (N - 1)g \) [12]. According to Eq. (3), \( E_{\text{GP}} \) develops a local maximum at \( l = (1 + \delta)/(2 \delta) \). In order for this to appear at a value of \( l \) smaller than unity, \( \delta > 1 \), or \( g > 1/(N - 1) \). Therefore, this is the critical value of \( \delta \) (and of \( g \)) above which an energy barrier develops in the dispersion relation \( E_{\text{GP}} = E_{\text{GP}}(l) \). Equation (3) also coincides with the excitation spectrum calculated by Lieb [9] in the limit \( N \to \infty \) and \( R \to \infty \), with \( N/(2\pi R) = \sigma \), finite, and for small \( \gamma \), i.e., \( E_{\text{GP}}/N - 4\pi \gamma = 8\pi \gamma (l - l^2) \) in the units of energy of Refs. [8, 9], \( \hbar^2 \sigma^2/2M \).

In order for our argument for the persistent currents to be complete, we need to consider the possibility of connecting the many-body states \( \Psi_0 \) with \( L = 0 \) and \( \Psi_N \) with \( L = N \) via some single-particle operator \( \Delta V \) of the form \( \Delta V = V_0 \delta(\theta) \). Only one Fourier component of the delta function connects the two states and provides the difference in the angular momentum between them, thus

\[
\Delta V = V_0 \sum_{j=1}^{N} e^{iN\theta_j} + c.c. \tag{4}
\]

The above operator is precisely the one that enters in the calculation of the dynamic structure factor \( S(k, \omega) \) for \( k = 2k_F \) (or \( L = N \) in our model). In Ref. [4] it has been argued that the vanishing of \( S(k = 2k_F, \omega = 0) \) implies that the decay rate of persistent currents is suppressed, in agreement with the present study, as we discuss below.

The state \( \Psi_{L=N} \) results from \( \Psi_{L=0} \) as \( \Psi_{L=N} = \left[ \prod_{j=1}^{N} e^{i\theta_j} \right] \Psi_{L=0} \), (i.e., by exciting the center of mass) [13], and thus

\[
\langle \Psi_{L=0} | \Delta V | \Psi_{L=N} \rangle = NV_0 \int |\Psi_{L=0}|^2 e^{i[-N\theta_1 + \theta_1 + \ldots + \theta_N]} d\theta_1 \ldots d\theta_N. \tag{5}
\]

In the Gross-Pitaevskii limit \( |\Psi_{L=0}\rangle \) is independent of \( \theta_j \), and the matrix element vanishes; only high-order perturbation theory in \( \Delta V \) then connects the states \( |\Psi_{L=0}\rangle \) and \( |\Psi_{L=N}\rangle \).

**Exact results from numerical diagonalization of the Hamiltonian.** To go beyond the mean-field approximation (which breaks down far away from the Gross-Pitaevskii limit of weak interactions), we have performed numerical diagonalization of the full many-body Hamiltonian \( \hat{H} \). We thus evaluate numerically the eigenstates of \( \hat{H} \), which are also eigenstates of the momentum operator \( \hat{L} \), and of the number operator \( \hat{N} \), for various values of \( g \).

Although “exact” (apart from the naturally necessary truncation of the Hilbert space), this method is quite restrictive in the values of \( N \), \( L \), and \( g \) that can be considered. More specifically, the number of the basis states that need to be included increases as one approaches the Tonks-Girardeau regime. In the Gross-Pitaevskii limit for a non-rotating cloud the dominant contribution to the many-body state comes from the \( m = 0 \) single-particle state. In the opposite extreme of the Tonks-Girardeau limit, even for a non-rotating cloud, the dominant contribution comes from the single-particle states with \( |m| < m_{\text{max}} \sim N/2 \), since in this limit the many-body wavefunction has to build correlations of characteristic length \( R/N \). Furthermore, for a given interaction strength \( U_0 \) and a given density \( n \), \( \hbar^2 m_{\text{max}}^2/(2MR^2) \sim nU_0 \), or \( m_{\text{max}}^2 \sim Ng \). Thus, more generally, \( m_{\text{max}} \sim \max(N/2, \sqrt{Ng}) \).
The points show the lowest eigenenergies of the Hamiltonian $E = E(L)$ for $L = 0, \ldots, 5$ and $N = 5$. Also $g = 0.1$ (top), $g = 1$ (middle), and $g = 10$ (bottom). The curves show the energy as given by the mean-field approximation $E_{GP}$ [Eq. (3)] in the top graph and $E_{TG}$ [Eq. (6)] in the bottom graph.

In Fig. 1 we consider $N = 5$ atoms, and $L = 0, \ldots, 5$, with $m_{\text{max}} = 20$, which gives a change of the lowest eigenenergy that is less than 1% between $m_{\text{max}} = 19$ and $m_{\text{max}} = 20$, for the highest value of $g = 10$ that we used. For $N = 5$, $g_{GP} \sim 1/N = 0.2$, while $g_{TG} \sim N = 5$. Figure 1 shows the lowest eigenenergy $E$ of the Hamiltonian as function of the total angular momentum $L$, for $g = 0.1$, $g = 1$, and $g = 10$. As argued above, for $g = 0.1$ the system is essentially in the Gross-Pitaevskii limit. Furthermore, there is no maximum in $E = E(L)$, since the interaction is not strong enough (the mean-field approximation predicts that the critical value of $g$ is 0.25 for 5 atoms). The dashed curve in the upper graph of Fig. 1 shows the result of the mean-field approximation. Clearly, it is possible to improve the mean-field energies by including states with higher $|m|$ in $\psi_{\text{var}}$. For $g = 1$, there is a maximum in $E = E(L)$ at $L = 4$. Finally, for $g = 10$, the system is closer to the Tonks-Girardeau limit, and there is still a maximum in $E = E(L)$. The dashed curve in the lower graph of Fig. 1 is the energy predicted in the Tonks-Girardeau limit [9],

$$E_{TG} = \frac{N^3}{12} - L^2 + NL,$$

plus corrections of order $N$. Such corrections are seen clearly in this graph. For $L = 0$ the leading-order term in the energy is $N^3/12$, which is the total energy of a Fermi gas in
one dimension, \(N \sigma \pi / 3\) (with \(\sigma \pi\) the Fermi energy), for a value of the Fermi momentum \(k_F = \sigma \pi = N/(2R)\). The expression for \(E_{\text{TFG}}\) implies that the energy barrier in \(E = E(L)\) [i.e., the difference between the maximum in \(E(L)\) and \(E(L = N)\)] scales quadratically with \(N\) in the Tonks-Girardeau limit, in agreement with our numerical results. On the other hand, in the Gross-Pitaevskii limit, the maximum of the energy barrier scales linearly with \(N\). This is the reason for the emergence of this barrier as one goes from the one limit to the other.

An exact result. – The eigenenergies calculated above satisfy an exact formula, valid for any value of \(g\), which is in agreement with the study of Felix Bloch [13]. More specifically, \(E(L') - E(L) = L' - L\), which also implies that \(E(L = N) - E(L = 0) = N\), or more generally \(E(L = qN) - E(L = 0) = q^2 N\), \(q = 0, 1, 2, \ldots\). Geometrically \(E(L') - E(L) = L' - L\) implies that all the lines connecting the points with \(L\) and \(L' = N - L\) are parallel.

To see this result, we recall that any state \(|L\rangle\) is related to the state \(|L' = N - L\rangle\) via some collective excitation of the system. The state \(|L\rangle\) is a linear superposition of Fock states of the form \(|(-m)^{N_m}, \ldots, 0^{N_0}, \ldots, m^{N_m}\rangle\), with \(\sum_m N_m = N\), and \(\sum_m m N_m = L\). Then, the state that consists of the Fock states \(|(-m+1)^{N_m}, \ldots, (-1)^{N_2}, 0^{N_1}, 1^{N_0}, \ldots, m^{N_{m+1}}, (m+1)^{N_{m-1}}\rangle\) with the same amplitudes as \(|L\rangle\) is \(|L' = N - L\rangle\), since it has \(N\) atoms, \(L' = \sum_m (-m+1) N_m = N - L\), and a total energy which is higher than that of \(|L\rangle\) by \(\sum_m ((-m+1)^2 - m^2) N_m = L' - L\) purely because of the kinetic energy; the interaction energy is the same in \(|L\rangle\) and \(|L'\rangle\), since all the matrix elements of the interaction are the same, independent of \(m\). Similar arguments apply in all the branches with \(pN \leq L, L' \leq (p + 1)N\), with \(p = 1, 2, 3, \ldots\).

Persistent currents close to the Tonks-Girardeau limit. – In this last part of our study we examine the lifetime of the current-carrying state with \(L = N\) close to the Tonks-Girardeau limit. Due to the Bose-Fermi mapping [1], for \(\gamma \rightarrow \infty\) the matrix element \(\langle \Psi_{L=0} | \Delta V | \Psi_{L=N} \rangle\) is identical to the one for non-interacting fermions and equal to \(V_0\). The two lower curves in Fig. 2 show \(\langle | \Psi_{L=0} | \Delta V | \Psi_{L=N} \rangle | / V_0 \rangle^2\), for \(N = 3\) and \(N = 6\), which indeed tend to unity for large \(g\). Therefore, for \(\gamma \rightarrow \infty\) there is a single-particle operator that connects the two states and destroys the persistent current for \(L = N\). In addition, the difference in the energy associated with the transition between the states \(\Psi_{L=N}\) and \(\Psi_{L=0}\) is zero to leading order in \(N\): for \(\gamma \rightarrow \infty\), the occupation of some “quasi-momenta” states of quantum number \(\tilde{m}\) is a flat, Fermi-Dirac-like distribution, with \(\langle \tilde{m} - \tilde{m} \rangle \leq N/2\) for \(L = 0\) [8]. To get to the state with \(L = N + \mathcal{O}(1)\), one has to promote the atom from the single-particle state with \(\tilde{m} = -N/2\) to the one with \(\tilde{m} = N/2 + 1\). The difference between the energy of the two states

![Fig. 2 – Two higher curves: the function \(1 - g^{(2)}(0)\), for \(N = 3\) and \(N = 6\) atoms. Two lower curves: the matrix element \(| \langle \Psi_{L=0} | \Delta V | \Psi_{L=N} \rangle | / V_0 \rangle^2\) for \(N = 3\) and \(N = 6\) atoms.](image)
is \((N/2 + 1)^2 - (-N/2)^2 = N + 1\), which is indeed zero to leading order in \(N\) (which is \(N^2\)).

For large but finite \(\gamma\) the width of the Fermi-Dirac-like distribution within the Lieb-Liniger model – shown in the higher graph of Fig. 3 – is \(\Delta L = N\gamma/(\gamma + 2) + \mathcal{O}(1)\) \[8\], or

\[
\Delta L \approx N - 2\frac{N}{\gamma} + \mathcal{O}(1),
\]

(7)

neglecting terms of order \(N/\gamma^2\) [which is self-consistent with the final result, that implies that \(\gamma \sim \mathcal{O}(N)\)]. If the single-particle operator \(\Delta V\) acts on the state \(|\Psi_{L=N}\rangle\) once, similar arguments to the ones mentioned in the previous paragraph (for \(\gamma \to \infty\)) imply that the change of the total angular momentum which does not alter the energy of the system to leading order in \(N\), is again equal to the width \(\Delta L\).

However, in order for the transition to be allowed to first order in \(\Delta V\), \(\Delta L\) has to be larger than the width of the energy barrier \(W\) shown in the lower graph of Fig. 3 [defined as \(W = N - L_b\), where \(\mathcal{E}(L = L_b) = \mathcal{E}(L = N)\)]. Since for large \(\gamma\) the speed of sound for \(L = 0\) is \(c_s = \partial \mathcal{E} / \partial L = N\gamma^2/(\gamma + 2)^2\) \[9\], therefore \(\mathcal{E}(L_b) \approx \mathcal{E}(0) + c_s L_b\), and \(L_b = 1 + \mathcal{O}(1/\gamma)\), or

\[
W = N - 1 + \mathcal{O}(1/\gamma).
\]

(8)

In order for \(W < \Delta L\) (and the decay rate of persistent currents to be allowed to first order in \(\Delta V\)), Eqs. \[7\] and \[8\] imply that the corresponding typical value of \(\gamma\), denoted as \(\gamma_{\text{decay}}\), can be as large as \(N\), [or \(g_{\text{decay}}\) can be as large as \(\mathcal{O}(N^2)\)]. In other words, the decay rate of persistent currents is highly suppressed up to a value of \(g_{\text{decay}} \sim \mathcal{O}(N^2)\), far beyond the coupling \(g_{\text{TG}} \sim \mathcal{O}(N)\) for which the system gets in the Tonks-Girardeau regime. Over the large window of couplings \(g_{\text{TG}} \leq g \leq g_{\text{decay}}\) the system is very close to the Tonks-Girardeau limit and on the same time it supports persistent currents.

To get numerical evidence about these estimates, we have calculated the pair correlation
function, defined as
\[ g^{(2)}(\theta - \theta') = \frac{\langle \Psi_{L=0} \left| \sum_{i \neq j} \delta(\theta - \theta_i) \delta(\theta' - \theta_j) \right| \Psi_{L=0} \rangle}{(N-1)\langle \Psi_{L=0} | \sum_i \delta(\theta - \theta_i) | \Psi_{L=0} \rangle}, \] (9)
as function of the coupling \( g \). Figure 2 shows \( 1 - g^{(2)}(0) \) (two higher curves in Fig. 2) for \( N = 3 \), and \( 6 \). The proximity of \( 1 - g^{(2)}(0) \) to zero/unity gives the extent to which the system is in the Gross-Pitaevskii/Tonks-Girardeau limit. These results are consistent with the previous estimates \( g_{\text{TG}} \sim \mathcal{O}(N) \), and \( g_{\text{decay}} \sim \mathcal{O}(N^2) \). Furthermore, for a given \( g \sim \mathcal{O}(N) \), the matrix element decreases with increasing \( N \), and probably approaches a step-like function for very large \( N \), that reflects the Fermi-Dirac-like distribution. Figure 2 provides a specific example in this very small system, in which for \( g_{\text{TG}} \leq g \leq g_{\text{decay}} \) the system is close to the Tonks-Girardeau limit, while the decay rate of persistent currents is suppressed.

Summary. – In conclusion, we considered bosonic atoms which rotate in a toroidal trap and examined the transition between the Gross-Pitaevskii and the Tonks-Girardeau limits. For any coupling \( \mathcal{E}(L' = N - L) - \mathcal{E}(L) = L' - L \), and thus \( \mathcal{E}(N) - \mathcal{E}(0) = N \). The energy barrier that the system has to overcome in order to get from the \( l = 1 \) to the \( l = 0 \) state and the corresponding distribution function of the atoms imply that persistent currents exist all the way between the Gross-Pitaevskii limit – above some critical coupling constant – up to a much higher critical coupling constant, close to the Tonks-Girardeau limit. Our model provides an example of a system where Bose-Einstein condensation is neither a necessary, nor a sufficient condition for superfluidity.

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