One-Dimensional Bosons in Three-Dimensional Traps

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Recent experimental and theoretical work has indicated conditions in which a trapped, low density Bose gas ought to behave like the 1D delta-function Bose gas solved by Lieb and Liniger. Up until now, the theoretical arguments have been based on variational/perturbative ideas or numerical investigations. There are four parameters: density, transverse and longitudinal dimensions, and scattering length. In this paper we explicate five parameter regions in which various types of 1D or 3D behavior occur in the ground state. Our treatment is based on a rigorous analysis of the many-body Schrödinger equation.

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It appears to be possible to do experiments in highly elongated traps on ultracold Bose gases that are effectively 1D. More precisely, the 1D Bose gas with a delta-function two-body interaction, analyzed long ago [1,2], should be visible, with its quasifermionic behavior [3], the absence of Bose-Einstein condensation (BEC) in a dilute limit [4], and an excitation spectrum different from that predicted by Bogoliubov's theory [2,5]. Several theoretical investigations on the transitions from 3D to an effective 1D behavior were triggered by [6]. See, e.g., [7–9]. Systems showing indications of such a transition have recently been prepared experimentally [10].

The theoretical work on the dimensional crossover for the ground state in elongated traps has so far been based either on variational calculations, starting from a 3D delta potential [6,9], or on numerical quantum Monte Carlo studies [11] with more realistic, genuine 3D potentials, but particle numbers limited to the order of 100. This work is important and has led to valuable insights, in particular about different parameter regions [7], but a more thorough theoretical understanding is clearly desirable since this is not a simple problem. In fact, it is evident that for a potential with a hard core the true 3D wave functions do not approximately factorize in the longitudinal and transverse variable (otherwise the energy would be infinite) and the effective 1D potential cannot be obtained by simply integrating out the transverse variables of the 3D potential (that would immediately create an impenetrable barrier in 1D). It is important to be able to demonstrate rigorously, and therefore unambiguously, that the 1D behavior really follows from the fundamental Schrödinger equation. It is also important to delineate, as we do here, precisely what can be seen in the different parameter regions. The full proofs of our assertions are long and will be given elsewhere [12], but we emphasize that everything can be rigorously derived from first principles. In this Letter we state our main results and outline the basic ideas for the proofs.

We shall always be concerned with the ground state and with large particle number, $N \gg 1$, which is appropriate for the consideration of actual experiments. Other parameters of the problem are the scattering length, a, of the two-body interaction potential and two lengths, r and L, describing the transverse and the longitudinal extension of the trap potential, respectively.

It is convenient to write the Hamiltonian in the following way (in units where $\hbar = 2m = 1$):

$$H_{N,L,r,a} = \sum_{j=1}^{N}[-\nabla_j^2 + V_r^\perp(\mathbf{x}_j^\perp) + V_L(z_j)] + \sum_{1\le i<j\le N} v_a(|\mathbf{x}_i - \mathbf{x}_j|), \quad (1)$$

with $\mathbf{x} = (x, y, z) = (\mathbf{x}^\perp, z)$ and with

$$V_r^\perp(\mathbf{x}^\perp) = r^{-2}V^\perp(\mathbf{x}^\perp/r), \qquad V_L(z) = L^{-2}V(z/L),$$
$$v_a(|\mathbf{x}|) = a^{-2}v(|\mathbf{x}|/a). \quad (2)$$

Here, r, L, a are variable scaling parameters while $V^\perp$, V, and v are fixed. The interaction potential v is supposed to be non-negative, of finite range, and have scattering length 1; the scaled potential v_a then has scattering length a. The external trap potentials V and $V^\perp$ confine the motion in the longitudinal (z) and the transversal ($\mathbf{x}^\perp$) directions, respectively, and are assumed to be continuous and tend to ∞ as $|z|$ and $|\mathbf{x}^\perp|$ tend to ∞. To simplify the discussion we find it also convenient to assume that V is homogeneous of some order $s > 0$, namely $V(z) = |z|^s$, but weaker assumptions, e.g., asymptotic homogeneity [13], would in fact suffice. The case of a simple box with hard walls is realized by taking $s = \infty$, while the usual harmonic approximation is $s = 2$. It is understood that the lengths associated with the ground states of $-d^2/dz^2 + V(z)$ and $-(\nabla^\perp)^2 + V^\perp(\mathbf{x}^\perp)$ are both of the order of 1 so that L and r measure, respectively, the longitudinal and the transverse extensions of the trap.

We denote the ground state energy of (1) by $E^{\rm QM}(N, L, r, a)$ and the ground state particle density by $\rho^{\rm QM}_{N,L,r,a}(\mathbf{x})$.

In parallel with the 3D Hamiltonian we consider the Hamiltonian for n bosons in 1D with delta interaction and coupling constant $g \geq 0$ (denoted $2c$ in [1]); i.e.,

$$H^{\rm 1D}_{n,g} = \sum_{j=1}^{n} -\partial^2/\partial z_j^2 + g \sum_{1\leq i<j\leq n} \delta(z_i - z_j). \qquad (3)$$

We consider the Hamiltonian for the z_j in an interval of length ℓ in the thermodynamic limit, $\ell \to \infty$, $n \to \infty$, with $\rho = n/\ell$ fixed. The ground state energy per particle in this limit is independent of boundary conditions and can, according to Lieb and Liniger [1], be written as

$$e^{\rm 1D}_0(\rho) = \rho^2 e(g/\rho), \qquad (4)$$

with a function $e(t)$ determined by a certain integral equation. Its asymptotic form is $e(t) \approx \frac{1}{2}t$ for $t \ll 1$ and $e(t) \to \pi^2/3$ for $t \to \infty$. Thus

$$e^{\rm 1D}_0(\rho) \approx \frac{1}{2} g\rho \quad \text{for } g/\rho \ll 1, \qquad (5)$$

$$e^{\rm 1D}_0(\rho) \approx (\pi^2/3)\rho^2 \quad \text{for } g/\rho \gg 1. \qquad (6)$$

These two situations correspond to high 1D density (weak interaction) and low 1D density (strong interaction), respectively. The latter case is usually referred to as the Girardeau-Tonks regime. Physically, the main difference is that in the strong interaction regime the motion of the particles in the longitudinal direction is highly correlated, while in the weak interaction regime it is not.

Taking $\rho e^{\rm 1D}_0(\rho)$ as a local energy density for an inhomogeneous 1D system we can form the energy functional

$$\mathcal{E}[\rho] = \int_{-\infty}^{\infty} [|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))]dz. \qquad (7)$$

The gradient term represents additional kinetic energy associated with the inhomogeneity of the gas that is not accounted for by the "local" kinetic energy included in the last term. The ground state energy of this functional is defined to be $E^{\rm 1D}(N, L, g) = \inf\{\mathcal{E}[\rho]: \rho(z) \geq 0, \int \rho(z)dz = N\}$. By standard methods (cf., e.g., [14]) one can show that there is a unique minimizer, i.e., a density $\rho_{N,L,g}(z)$ with $\int \rho_{N,L,g}(z)dz = N$ and $\mathcal{E}[\rho_{N,L,g}] = E^{\rm 1D}(N, L, g)$. We define the mean 1D density of this minimizer to be $\bar{\rho} = N^{-1}\int_{-\infty}^{\infty}(\rho_{N,L,g}(z))^2dz$. In the rigid box, i.e., for $s = \infty$, $\bar{\rho}$ is simply N/L (except for boundary corrections), but in more general traps it depends also on g besides N and L. The order of magnitude of $\bar{\rho}$ in various regions of the parameters will be described below.

Our main result relates the 3D ground state energy of (1), $E^{\rm QM}(N, L, r, a)$, to the 1D density functional energy $E^{\rm 1D}(N, L, g)$ in the large N limit with $g \sim a/r^2$ provided r/L and a/r are sufficiently small. To state this precisely, let $e^{\perp}$ and $b(\mathbf{x}^{\perp})$, respectively, denote the ground state energy and the normalized ground state wave function of $-(\nabla^{\perp})^2 + V^{\perp}(\mathbf{x}^{\perp})$. The corresponding quantities for $-(\nabla^{\perp})^2 + V^{\perp}_r(\mathbf{x}^{\perp})$ are $e^{\perp}/r^2$ and $b_r(\mathbf{x}^{\perp}) = (1/r)b(\mathbf{x}^{\perp}/r)$. In the case that the trap is a cylinder with hard walls b is a Bessel function; for a quadratic $V^{\perp}$ it is a Gaussian.

Define g by

$$g = \frac{8\pi a}{r^2}\int |b(\mathbf{x}^{\perp})|^4 d^2\mathbf{x}^{\perp} = 8\pi a \int |b_r(\mathbf{x}^{\perp})|^4 d^2\mathbf{x}^{\perp}. \qquad (8)$$

THEOREM: *Let $N \to \infty$ and simultaneously $r/L \to 0$ and $a/r \to 0$ in such a way that $r^2\bar{\rho}\cdot\min\{\bar{\rho}, g\} \to 0$. Then*

$$\lim \frac{E^{\rm QM}(N, L, r, a) - Ne^{\perp}/r^2}{E^{\rm 1D}(N, L, g)} = 1. \qquad (9)$$

Moreover, if we define the 1D quantum-mechanical density by averaging over the transverse variables, i.e.,

$$\hat{\rho}^{\rm QM}_{N,L,r,a}(z) \equiv \int \rho^{\rm QM}_{N,L,r,a}(\mathbf{x}^{\perp}, z)d^2\mathbf{x}^{\perp}, \qquad (10)$$

then $\hat{\rho}^{\rm QM}_{N,L,r,a}(z)/\rho_{N,L,g}(z) \to 1$ in a suitable sense.

Note that because of (5) and (6) the condition $r^2\bar{\rho}\cdot\min\{\bar{\rho}, g\} \to 0$ is the same as $e^{\rm 1D}_0(\bar{\rho}) \ll 1/r^2$, i.e., the average energy per particle associated with the longitudinal motion should be much smaller than the energy gap between the ground and first excited state of the confining Hamiltonian in the transverse directions. Thus, the basic physics is highly quantum mechanical and has no classical counterpart. The system can be described by a 1D functional (7), even though the transverse trap dimension is much larger than the range of the atomic forces.

The domain of the parameters can be divided into subregions characterized by specific restrictions on the size of the ratio $g/\bar{\rho}$ as $N \to \infty$. It turns out that there are five regions altogether, each described by a limiting case of the general density functional (7), but there is a basic dichotomy between the regions that can be regarded as limits of 3D Gross-Pitaevskii theory and those that cannot be reached in that way. The former (regions 1–3 below) are characterized by the condition that the 3D ground state energy per particle, which is proportional to a times the three dimensional density $\rho^{\rm 3D} \sim N/(r^2L)$ for a dilute gas [15], is much smaller than the energy given by the formula (6). This means that $g/\bar{\rho} \ll 1$ with g given by (8). In the latter regime (regions 4 and 5 below) the energy (6) is comparable to or smaller than the 3D energy. In both regimes the internal energy of the gas is small compared to the energy of transversal confinement which is of the order N/r^2. However, this in itself does not imply a specifically 1D behavior. (If a is sufficiently small it is satisfied in a trap of any shape.) 1D behavior, when it occurs, manifests itself by the fact that the transverse motion of the atoms is uncorrelated while the longitudinal motion is correlated (very roughly speaking) in the same way as pearls on a necklace. Thus, the true criterion for 1D behavior is that $g/\overline{\rho}$ is of the order unity or larger, and not merely the condition that the energy of confinement dominates the internal energy.

We shall now briefly describe the division of the two regimes into the five subregions. We always assume $N \to \infty$ and $r/L \to 0$.

REGION 1: *The ideal gas case.*—$g/\overline{\rho} \ll N^{-2}$, with $\overline{\rho} \sim N/L$, corresponding to the trivial case where the interaction is so weak that it effectively vanishes in the large N limit and everything collapses to the ground state of $-d^2/dz^2 + V(z)$ with ground state energy $e^{\|}$. The energy E^{1D} in (9) can be replaced by $Ne^{\|}/L^2$. Note that $g/\overline{\rho} \ll N^{-2}$ means that the 3D interaction energy $\sim \rho^{3D} a \ll 1/L^2$.

REGION 2: *The 1D GP case.*—$g/\overline{\rho} \sim N^{-2}$, with $\overline{\rho} \sim N/L$, described by a 1D Gross-Pitaevskii energy functional

$$\mathcal{E}^{\rm GP}[\rho] = \int_{-\infty}^{\infty} [|\nabla\sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \frac{1}{2} g\rho(z)^2] dz, \tag{11}$$

corresponding to the high density approximation (5) of the interaction energy in (7). Its ground state energy, $E^{\rm GP} = \inf\{\mathcal{E}^{\rm GP}[\rho]: \rho(z) \geq 0, \int \rho = N\}$, has the scaling property $E^{\rm GP}(N, L, g) = NL^{-2} E^{\rm GP}(1, 1, NgL)$.

REGION 3: *The 1D TF case.*—$N^{-2} \ll g/\overline{\rho} \ll 1$, with $\overline{\rho} \sim (N/L)(NgL)^{-1/(s+1)}$, where s is the degree of homogeneity of the longitudinal confining potential V. This region is described by a Thomas-Fermi type functional

$$\mathcal{E}^{\rm TF}[\rho] = \int_{-\infty}^{\infty} [V_L(z)\rho(z) + \frac{1}{2} g\rho(z)^2] dz. \tag{12}$$

It is a limiting case of region 2 in the sense that $NgL \sim NaL/r^2 \to \infty$, but a/r is sufficiently small so that $g/\overline{\rho} \sim (aL/Nr^2)(NaL/r^2)^{1/(s+1)} \to 0$; i.e., the high density approximation in (5) is still valid. In this limit the gradient term in (11) becomes vanishingly small compared to the other terms.

REGION 4: *The LL case.*—$g/\overline{\rho} \sim 1$, with $\overline{\rho} \sim (N/L)N^{-2/(s+2)}$, described by an energy functional

$$\mathcal{E}^{\rm LL}[\rho] = \int_{-\infty}^{\infty} [V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))] dz. \tag{13}$$

This region corresponds to the case $g/\overline{\rho} \sim 1$, so that neither the high density (5) nor the low density approximation (6) is valid and the full LL energy (4) has to be used, but, as in region 3, the gradient term in (7) is negligible. The scaling of the ground state energy of (13) is $E^{\rm LL}(N, L, g) = N\gamma^2 E^{\rm LL}(1, 1, g/\gamma)$ with $\gamma = (N/L)N^{-2/(s+2)}$.

REGION 5: *The GT case.*—$g/\overline{\rho} \gg 1$, with $\overline{\rho} \sim (N/L)N^{-2/(s+2)}$, described by a functional with energy density $\sim\rho^3$, corresponding to the Girardeau-Tonks limit of the LL energy density. It corresponds to impenetrable particles, i.e., the limiting case $g/\overline{\rho} \to \infty$ and hence formula (6) for the energy density. The energy functional is

$$\mathcal{E}^{\rm GT}[\rho] = \int_{-\infty}^{\infty} [V_L(z)\rho(z) + (\pi^2/3)\rho(z)^3] dz, \tag{14}$$

with minimum energy $E^{\rm GT}(N, L) = N\gamma^2 E^{\rm GT}(1, 1)$.

We note that the condition $g/\overline{\rho} \sim 1$ means that region 4 requires the gas cloud to have aspect ratio $r/\overline{L}$ of the order $N^{-1}(a/r)$ or smaller, where $\overline{L} \sim LN^{2/(s+2)}$ is the length of the cloud. Experimentally, such small aspect ratios are quite a challenge and the situations described in [10] are still rather far from this regime. It may not be completely out of reach, however.

Regions 1–3 can be reached as limiting cases of a 3D Gross-Pitaevskii theory [12]. In this sense, the behavior in these regions contains remnants of the 3D theory, which also shows up in the fact that the proof of BEC in the 3D Gross-Pitaevskii limit in [16] can be carried over to regions 1 and 2 [12]. Heuristically, these traces of 3D can be understood from the fact that in regions 1–3 the 1D formula (5) for energy per particle, $g\rho \sim aN/(r^2 L)$, gives the same result as the 3D formula [15], i.e., $a\rho^{3D}$. This is no longer so in regions 4 and 5.

We now comment on the main steps in the proof of the theorem, referring to [12] for full details. The different parameter regions have to be treated by different methods, a watershed lying between regions 1–3 on the one hand and regions 4–5 on the other. In regions 1–3, similar methods as in the proof of the 3D Gross-Pitaevskii limit theorem in [14] can be used. This 3D proof needs considerable modifications, however, because in [14] the external potential is fixed and the estimates are not uniform in the ratio r/L.

To prove (9) one has to establish upper and lower bounds, with controlled errors, on the QM many-body energy in terms of the energies obtained by minimizing the energy functionals appropriate for the various regions. The limit theorem for the densities can be derived from the energy estimates in a standard way by variation with respect to the external potential V_L. As usual, the upper bounds for the energy are easier than the lower bounds, but nevertheless not simple, in particular, not for "hard" potentials v.

The upper bound in regions 1–3 is obtained from a variational ansatz of the form $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = F(\mathbf{x}_1, \ldots, \mathbf{x}_N) \prod_{k=1}^{N} b_r(\mathbf{x}_k^{\perp}) \sqrt{\rho^{\rm GP}(z_k)}$, with $F(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{k=1}^{N} f(\mathbf{x}_k - \mathbf{x}_{j(k)})$, where $\mathbf{x}_{j(k)}$ is the nearest neighbor of $\mathbf{x}_k$ among the points $\mathbf{x}_j$, $j < k$, $b_r(\mathbf{x}^{\perp})$ is the lowest eigenfunction of $-(\nabla^{\perp})^2 + V_r^{\perp}$, and $\rho^{\rm GP}(z)$ the minimizer of the 1D GP functional (11). The function f is, up to a cutoff length that has to be chosen optimally, the zero energy scattering solution for the two-body Hamiltonian with interaction v_a. The form of F, inspired by [17], is chosen rather than a Jastrow ansatz $\prod_{i<j} f(\mathbf{x}_i - \mathbf{x}_j)$, because it is computationally simpler for the purposes of obtaining rigorous estimates.

For an upper bound in regions 4–5 a natural variational ansatz would appear to be $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = F(\mathbf{x}_1, \ldots, \mathbf{x}_N) \prod_{k=1}^N b_r(\mathbf{x}_k^\perp)\psi(z_1, \ldots, z_N)$, where ψ is the ground state of $H_{N,g}^{1D}$ with the external potential V_L added. However, in order to make a link with the exact solution (4) for a homogeneous gas, but also to control the norm of the trial function, it turns out to be necessary to localize the particles by dividing the trap into finite "boxes"(finite in z direction), with a finite particle number in each box and making the ansatz with the boundary condition $\Psi = 0$ for each box individually. The particles are then distributed optimally among the boxes to minimize the energy. This box method, but with the boundary condition $\nabla\Psi = 0$, is also used for the lower bounds to the energy. Another essential device for the lower bounds is *Dyson's lemma* that was also used in [14–16]. This lemma, which goes back to Dyson's seminal paper [17] on the hard-core Bose gas, estimates the kinetic and potential energy for a Hamiltonian with a hard potential v of finite range from below by the potential energy of a "soft" potential U of larger range but essentially the same scattering length as v. Borrowing a tiny part of the kinetic energy it is then possible to do perturbation theory with the soft potential U and use Temple's inequality [18] to bound the errors. A direct application of perturbation theory to the original potential v, on the other hand, is in general not possible.

A core lemma for regions 4–5 is a lower bound on the 3D ground state energy in a finite box in terms of the 1D energy of the Hamiltonian (3) both with the boundary condition $\nabla\Psi = 0$. Denoting the former energy by E_{box}^{3D} and the latter by E_{box}^{1D}, this bound for n particles in a box of length ℓ in the z direction reads

$$E_{\text{box}}^{3D} - \frac{ne^\perp}{r^2} \geq E_{\text{box}}^{1D}\left\{1 - Cn\left(\frac{a}{r}\right)^{1/8}\left[1 + \frac{nr}{\ell}\left(\frac{a}{r}\right)^{1/8}\right]\right\},$$

with a constant C. To prove this bound the ground state wave function is first written as a product of $\prod_k b_r(\mathbf{x}_k^\perp)$ and a function $G(\mathbf{x}_1, \ldots, \mathbf{x}_n)$. This subtracts $ne^\perp/r^2$ from E_{box}^{3D} but the resulting minimization problem for G involves the weighted measure $\prod_k b_r(\mathbf{x}_k^\perp)^2 d^3\mathbf{x}_k$ in place of $\prod_k d^3\mathbf{x}_k$. Nevertheless, Dyson's lemma can be used, and after the hard potential v has been replaced by the soft potential U, it is possible to integrate the transverse variables away and obtain a minimization problem for a 1D many-body Hamiltonian with interaction $d(z_i - z_j) = a \int\int b_r(\mathbf{x}_i^\perp)^2 b_r(\mathbf{x}_j^\perp)^2 U(\mathbf{x}_i - \mathbf{x}_j) d^2\mathbf{x}_i^\perp d^2\mathbf{x}_j^\perp$. In the limit considered this converges to a delta interaction with the coupling constant (8). The error terms in the estimate for E_{box}^{3D} arise both from Temple's inequality and the replacement of d by a delta function, among other things. When the particles are distributed optimally among the boxes to obtain a global lower bound, superadditivity of the energy and convexity of the energy density $\rho^3 e(g/\rho)$ are used, generalizing corresponding arguments in [15].

In conclusion, we have reported a rigorous analysis of the parameter regions in which a Bose gas in an elongated trap may or may not be expected to display 1D behavior in its ground state. We also present a 1D energy functional, analogous to the Gross-Pitaevskii functional, that correctly describes the energy and density in all the five parameter regions considered here.

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