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Effect of Transverse Confinement on a Quasi-One-Dimensional Dipolar Bose Gas

Stefania De Palo [1,2], Edmond Orignac [3], Roberta Citro [4] and Luca Salasnich [5,6,*]

[1] CNR-IOM-Democritos, Via Bonomea 265, I-34136 Trieste, Italy
[2] Dipartimento di Fisica Teorica, Università Trieste, Strada Costiera 11, I-34014 Trieste, Italy
[3] Laboratoire de Physique, Université Lyon, Ens de Lyon, CNRS, F-69342 Lyon, France
[4] Dipartimento di Fisica "E. R. Caianiello", Università degli Studi di Salerno, CNR-SPIN, Via Giovanni Paolo II, I-84084 Fisciano, Italy
[5] Dipartimento di Fisica e Astronomia "Galileo Galilei", INFN and QTech, Università di Padova, Via Marzolo 8, I-35131 Padova, Italy
[6] INO-CNR, Unitadi Sesto Fiorentino, Via Nello Carrara 1, I-50019 Sesto Fiorentino, Italy
* Correspondence: luca.salasnich@unipd.it

Abstract: We study a gas of bosonic dipolar atoms in the presence of a transverse harmonic trapping potential by using an improved variational Bethe ansatz, which includes the transverse width of the atomic cloud as a variational parameter. Our calculations show that the system behavior evolves from quasi-one dimensional to a strictly one-dimensional one by changing the atom–atom interaction, or the axial density, or the frequency of the transverse confinement. Quite remarkably, in the droplet phase induced by the attractive dipolar interaction the system becomes sub-one dimensional when the transverse width is smaller than the characteristic length of the transverse harmonic confinement.

Keywords: dipolar interactions; variational method; droplets

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1. Introduction

Trapped ultracold atomic gases offer a convenient and flexible platform to explore the fascinating aspects of many-body physics in one dimension [1,2]. In particular, in recent years the one-dimensional dipolar Bose gas has been largely investigated theoretically, see for instance Ref. [3]. This kind of study is nowadays a vibrant topic of research, triggered by recent observations of self-bound droplets in attractive bosonic mixtures [4–6] and in dipolar atoms [7,8]. In the real experiment, however, the system is not strictly one dimensional: the system made of identical atoms of mass m is usually confined by a transverse harmonic potential of frequency $\omega_\perp$. Lately, we analyzed a more realistic case of finite transverse trapping frequency [3,9,10] by using a variational Bethe ansatz of the ground state energy of a uniform dipolar gas in combination with a generalized Gross–Pitaevskii (GGP) equation. It has been found [11] that the system evolves from a bright soliton-like into a droplet by increasing the atom number or the dipolar interaction strength.

However, when the strength of the transverse trapping is reduced, the transverse width $l_\perp$ of the bosonic cloud could be quite different from the characteristic length $l_0 = \sqrt{\hbar/(m\omega_\perp)}$ of the transverse harmonic confinement. In the case of quasi-one-dimensional bosons with contact interaction, a generalized Lieb–Liniger approach, which takes into account effects of the transverse dynamics, was considered in Refs. [12,13].

In this paper, extending the procedures of Refs. [9–13], we analyze a quasi-one-dimensional dipolar Bose gas by including, in an improved variational Bethe ansatz wave-function, the effect of the transverse confinement. In this way we study the evolution from a quasi-one dimensional dipolar bosonic system, where $l_\perp > l_0$, to an effectively one dimensional configuration, where $l_\perp \simeq l_0$. We find that, by increasing the repulsive short-range interaction, the transverse width $l_\perp$ becomes larger and the effect is stronger for larger axial densities. On the contrary, when the dipolar attractive strength dominates, producing a droplet, the system becomes effectively one dimensional with $l_\perp$ very close to l_0 and, for large densities, it becomes sub-one dimensional with $l_\perp < l_0$.

2. Method: The Variational Approach for the Energy Functional

We start with the interacting dipolar gas of N bosons in three-dimensions, aligned in the $x - z$ plane by an external field along a direction $\hat{d} = \cos\theta\hat{x} + \sin\theta\hat{z}$, in the presence of a transverse harmonic trap of frequency $\omega_\perp$, whose Hamiltonian reads

$$\begin{aligned} H \;&=\; \sum_i^N \left(-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}m\omega_\perp^2 (y_i^2 + z_i^2) \right) + g_{3D} \sum_{i<j} \delta(|\vec{r}_i - \vec{r}_j|) \\ &+ \sum_{i<j} \frac{\mu_0 \mu_d^2}{4\pi |\vec{r}_i - \vec{r}_j|^3} \left(1 - 3\frac{[\hat{d}\cdot(\vec{r}_i - \vec{r}_j)]^2}{|\vec{r}_i - \vec{r}_j|^2} \right) \end{aligned} \tag{1}$$

where m is the mass of the bosons, the contact strength is defined as $g_{3D} = \hbar^2 \frac{4\pi a_{3D}}{m}$ via the three-dimensional scattering length a_{3D}, μ_0 is the vacuum permeability and μ_d is the dipole moment.

The description by means of an effectively one-dimensional system relies on the assumption that the trapping in the transverse direction is sufficiently tight to ensure that the gas behaves as a one-dimensional gas. Here we wish to relax the assumption that the transverse modes are frozen in the ground state of the trapping Hamiltonian and include their effect in the trial wavefunction ansatz [12,13]:

$$\phi(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N) = \psi_{1D}(x_1, x_2 \ldots, x_N) \Pi_{i=1}^N e^{-\frac{z_i^2 + y_i^2}{2\sigma^2 l_0^2}} \tag{2}$$

where ψ_{1D} is the wave function in the one-dimensional space while the wave function in the transverse direction is modelled by the product of Gaussians where σ is the variational parameter that takes care of the spread of the density in the transverse directions. When $\theta = 0$, the dipoles are aligned along the x axis, and the interaction has full rotational symmetry around that axis, thus justifying the choice of an isotropic σ. For $\theta \neq 0$, the model only has a reflection symmetry around the xz and xy planes, and a more general ansatz with a factor $\prod_i \exp[-\frac{z_i^2}{\sigma_z^2 l_0^2} - \frac{y_i^2}{2\sigma_y^2 l_0^2}]$ could be considered. However, in the presence of a tight harmonic trapping with full rotational symmetry, the isotropic ansatz is a good starting point. Within this *ansatz*, the projected one-dimensional Hamiltonian is:

$$\begin{aligned} H_{Q1D} &= -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{(\partial x_i)^2} + N\left(\frac{\hbar^2}{2ml_\perp^2} + \frac{1}{2}m\omega_\perp^2 l_\perp^2 \right) \\ &+ \left[g_{1D} - l_\perp \frac{8}{3} V(\theta, l_\perp) \right] \sum_{i<j} \delta(|x_i - x_j|) + V(\theta, l_\perp) \sum_{i<j} V_{DDI}(|x_i - x_j|/l_\perp) \end{aligned} \tag{3}$$

with [14–16]

$$l_\perp = \sigma l_0 \tag{4}$$

$$g_{1D} = \frac{g_{3D}}{2\pi l_\perp^2} \tag{5}$$

$$a_{1D} = -\frac{l_\perp^2}{a_{3D}} \tag{6}$$

$$V(\theta, l_\perp) = \frac{\mu_0 \mu_d^2}{4\pi} \frac{1 - 3\cos^2\theta}{4 l_\perp^3}. \tag{7}$$

$$V_{DDI}^{1D}\left(\frac{x}{l_\perp}\right) = -2\left|\frac{x}{l_\perp}\right| + \sqrt{2\pi}\left[1+\left(\frac{x}{l_\perp}\right)^2\right]e^{\frac{x^2}{2l_\perp^2}}\,\mathrm{erfc}\left[\left|\frac{x}{\sqrt{2}l_\perp}\right|\right]. \quad (8)$$

In the new Hamiltonian (3) the effective interaction $V_{Q1D}(x) = V(\theta, l_\perp)V_{DDI}(x/l_\perp)$ depends explicitly on σ, at variance with previous derivations [15,16], and its effect can be appreciated in Figure 1: a tighter effective confinement ($\sigma < 1$) leads to a stronger interaction than in the $\sigma = 1$ case and vice versa.

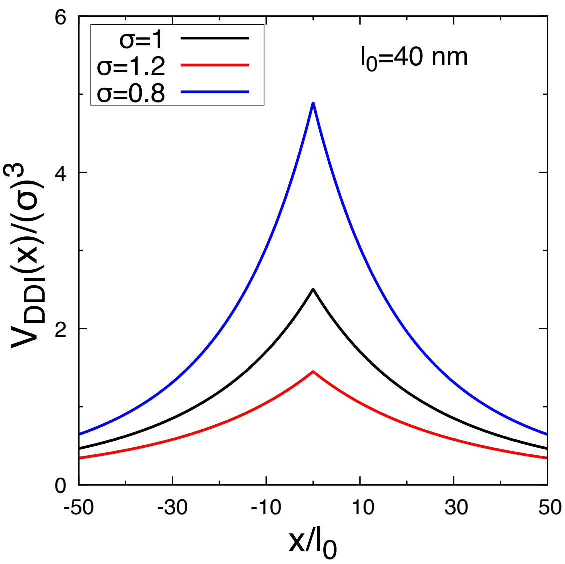

Figure 1. For a fixed $l_0 = 40$ nm we show how $V_{DDI}(x)/\sigma^3$ changes for different values of σ, namely $\sigma = 0.8, 1$ and 1.2.

Finally we estimate the variational ground-state energy of the system by using for ψ_{1D} a Lieb–Liniger ground state wavefunction with dimensionless interaction γ as variational parameter [9]. The trial energy to minimize is

$$\frac{E}{N}\left[\frac{\hbar^2}{2m}n^2\right]^{-1} = \epsilon(\gamma) - \left[\gamma - \frac{\gamma_0}{\sigma^2}\right]\frac{\partial\epsilon(\gamma)}{\partial\gamma} + 2\frac{a_d}{l_\perp}\frac{1-3\cos^2\theta}{nl_\perp}$$
$$\left\{1+\int_0^\infty dq[S(q;\gamma)-1]\left[1-\frac{q^2l_\perp^2}{2}e^{q^2l_\perp^2/2}\Gamma(0;q^2l_\perp^2/2)\right]\right\} + \frac{1}{(nl_0\sigma)^2} + \frac{\sigma^2}{(nl_0)^2} \quad (9)$$

with $q = \pi nq$, $S(a;\gamma)$ the static structure factor [17] and $\Gamma[0,x]$ is the exponential integral function [18],

$$\frac{\gamma_0}{\sigma^2} = \frac{2}{n}\left\{-\frac{1}{a_{1D}} + \frac{a_d}{l_\perp^2}\left[\frac{1-3\cos^2\theta}{4} - \frac{8}{3}\right]\right\} \quad (10)$$

and $a_d = m\mu_0\mu_d^2/(8\pi)$ and where $\epsilon(\gamma)$ is the ground state-energy of the Lieb–Liniger model [19–21]. Using that *ansatz* we have minimized the trial energy with respect to both γ and σ using standard minimization procedure [22].

3. Results and Discussions

Before looking for the variational solution of the full single-mode energy functional (9) we consider a first approximation where the short-range dipolar potential is replaced by an effective contact interaction potential of strength $A = 3.6$ [9,23,24]; within this approximation the Hamiltonian now reads:

$$H_{Q1D} = -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{(\partial x_i)^2} + \left[g_{1D} + l_\perp\left(A - \frac{8}{3}\right)V(\theta, l_\perp)\right]\sum_{i<j}\delta(|x_i - x_j|)$$
$$+\frac{N\hbar^2}{2ml_\perp^2} + \frac{N}{2}m\omega_\perp^2 l_\perp^2 \quad (11)$$

Once we have dropped the short-range dipolar part, we are effectively back to the case already treated in [13]; the minimization of the energy functional with respect to σ gives

$$\frac{\partial E/N}{\partial \sigma} = \sigma^4 + (nl_0)^2\epsilon'\left[\frac{\gamma_0}{\sigma^2}\right] = 0 \quad (12)$$

where now the renormalized interaction is fixed by

$$\gamma_0 = \frac{2}{n}\left\{-\frac{1}{a_{1D}} + \frac{a_d}{l_0^2}\left[\frac{1 - 3\cos^2\theta}{4} + \left(A - \frac{8}{3}\right)\right]\right\} \quad (13)$$

In Figure 2 we show, for a fixed scattering length $a_{1D}/a_0 = -8350$ (a_0 being the Bohr radius) and $l_0 = 57.3$ nm and $a_d = 195a_0$ as from Ref. [23], the optimal σ, i.e., the rescaling parameter for the transverse confinement $l_\perp$. This is obtained by minimizing the full Hamiltonian (3) or minimizing Equation (11) where we consider $A = 3.6$, a constant independent from the longitudinal density n as performed in Ref. [23]. We compare results for the repulsive case ($\theta = \pi/2$, red lines) with the attractive case ($\theta = 0$, black lines), together with a case without dipolar interaction ($a_d = 0$, blue line).

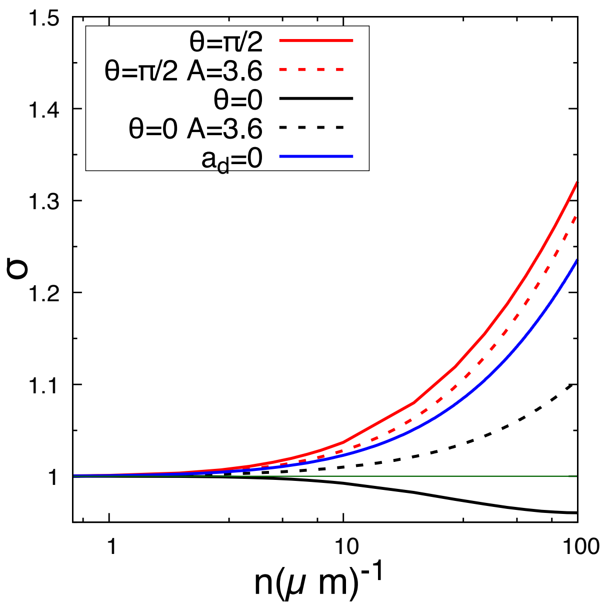

Figure 2. Optimal values for σ obtained with the different approximations as a function of density n. As a point of reference we show σ for the system without dipolar interaction, $a_d = 0$ as a blue solid line. The solid lines show the results obtained minimizing the energy functional (9), σ_{sma}, while the dashed ones correspond to the minimization of the approximated Hamiltonian (11), σ_A. Red lines are for the repulsive case $\theta = \pi/2$ and black lines are for the attractive case $\theta = 0$.

Figure 2 summarises the effect of the transverse confinement. Let us start with a case with pure contact interaction, where, as expected upon increasing the density of the system, the effective transverse width $l_\perp = l_0\sigma$ becomes larger due to the repulsive scattering between particles. When we add the repulsive dipolar interaction that effect becomes more and more pronounced, with the optimal $\sigma_{sma} > \sigma_A$ in the whole range of densities. The situation is different when we move to the attractive case, $\theta = 0$ (we want to stress that for given scattering length and l_0 the variational ground state energy [9] does have a minimum). As shown in Figure 2, indeed, $\sigma_A > 1$ while $\sigma_{sma} < 1$, implying a reduction in the effective transverse width and therefore a tighter, more interacting system, which can be considered sub-one dimensional. We now devote the rest of the section to the quantitative discussion of the effect of including the transverse confinement in the variational approach.

3.1. Repulsive Dipolar Interaction

As already discussed, when the interaction between the particles is repulsive the renormalized transverse confinement felt by the system $l_\perp$ is larger. As expected this effect is more evident for loose confinement, in Figure 3 we show the equation of state, without the transverse energy contribution $E_{tr}/N = \frac{1}{(nl_\perp)^2} + \sigma^2 \frac{1}{nl_0^2}$ for $\sigma = 1$ as a function of density in two cases where the effective interaction is repulsive.

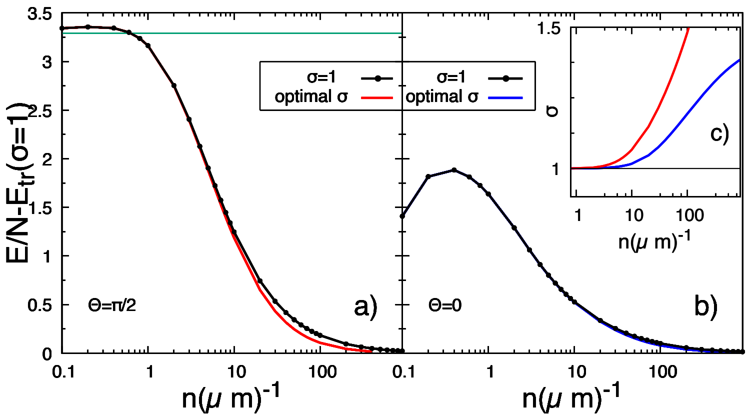

Figure 3. Ground state energy estimates, in $\hbar^2/2mn^2$ units, within variational ansatz for $l_0 = 57.3$ nm and $a_{1D}/a_0 = -2000$ as a function of particles density. The solid black lines are the energies obtained using $\sigma = 1$ [9] while solid red lines are using the optimal σ obtained from variational minimization. We show results for $\theta = \pi/2$ in panel (**a**) and $\theta = 0$ in panel (**b**). We subtracted the transverse energy for $\sigma = 1$ for clarity. In panel (**c**), we show the optimal values of σ as a function of density for the cases reported in panel (**a**), solid red line, and in panel (**b**), solid blue line. The solid green line in panel (**a**) is the limit of the energy in the Tonks–Girardeau limit.

For a quasi-one dimensional system such as the experimental one discussed in Ref. [23], in which typical values of the averaged density at the center of the trap range between 0.8 $(\mu\text{m})^{-1}$ and 3.1 $(\mu\text{m})^{-1}$, the effect of the inclusion of the transverse confinement is small with a the relative change of $\sigma \simeq 5\%$. This justified *a posteriori* the approximation used in Ref. [23].

3.2. Attractive Dipolar Interaction: Droplet Region

When the attractive dipolar interaction becomes more relevant than the repulsive contact interaction in the variational Bethe–Ansatz [9] the estimated ground-state energy develops a deep minimum. Such feature favors the crossover from the gas state towards the liquid-droplet state [11]. The deep minimum occurs for quite large densities and this, together with the variational character of the approach, ensures lower energies when we add another variational parameter, such as σ that governs the transverse confinement. In Figure 4, we assess the effect of varying the transverse trapping length l_0. As expected, reducing the trapping length enhances the interaction between particles and this enhances even more the variational parameter σ.

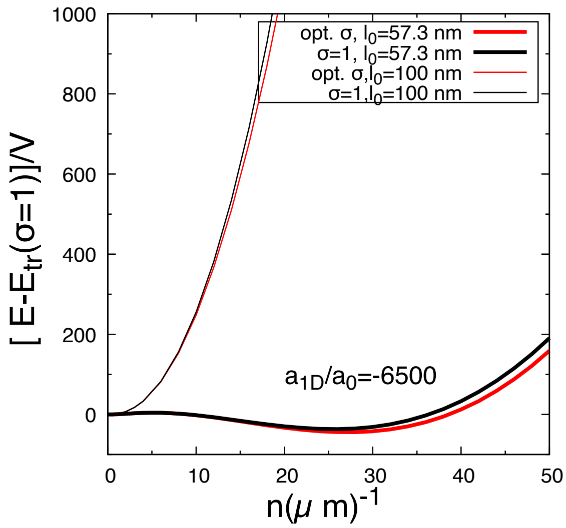

Figure 4. Ground state energy estimates within variational ansatz for $a_{1D}/a_0 = -6500$ for two selected values of l_0, namely $l_0 = 57.3$ nm as from Ref. [23] and $l_0 = 100$ nm. The solid black lines are the trial energies obtained using $\sigma = 1$ while solid red lines are trial energies obtained using the optimal σ from full minimization. The thick solid lines are for $l_0 = 57.3$ nm, while thin ones are for $l_0 = 100$ nm.

In Figure 5, we observe the effect of transverse confinement in a case where the minimum occurs at large densities and the lowering of the energy is sizeable. As a byproduct, the minimum is also shifted to larger values of density. As a combined result the droplet is more stable and less sensitive to the longitudinal harmonic trapping.

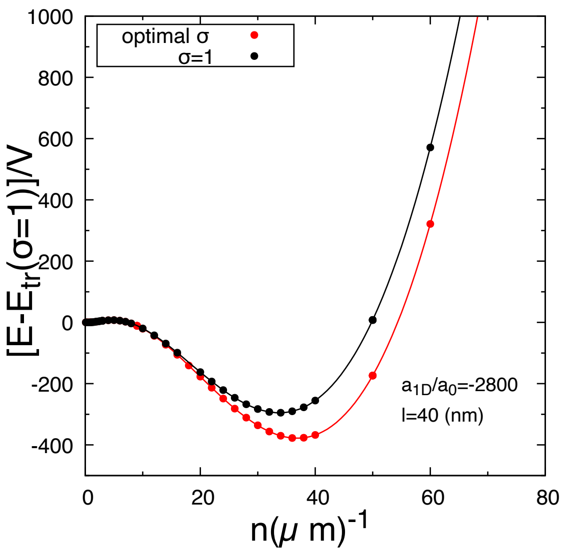

Figure 5. Ground state energy within the variational ansatz for $l_0 = 40$ nm and $a_{1D}/a_0 = -2800$ as a function of particle density. The solid black lines are the trial energies computed using $\sigma = 1$ [9] while the solid red lines are computed with the optimal σ obtained from variational minimization.

4. Conclusions

We used an improved variational Bethe ansatz approach to study a quasi-one dimensional dipolar gas taking care of the effect of transverse confinement. We considered an isotropic variational Gaussian wavefunction that is a good reference choice for a tight confinement. When the interaction between particles is repulsive the effective transverse width of the cloud is increased and the effect is visible for large densities. We found that for densities comparable with the ones of the experiments of Ref. [23] the trapping effect is negligible, thus justifying *a posteriori* the assumptions of a pure one dimensional system ($\sigma = 1$) in Ref. [9], as well as the isotropic ansatz choice with $\sigma_x = \sigma_y$. By contrast, the formation of a droplet liquid state, that occurs when the attractive dipolar attraction prevails over the repulsive contact interaction could be more sensitive to the variation of the transverse trapping length. The extended variational ansatz allows the system to become more tightly trapped in the transverse direction and denser in the longitudinal direction than in the strictly one dimensional case [9]. The net effect is a reinforcement of the stability of the droplet phase.

Our analysis could also be extended to the anisotropic case with Gaussian wavefunction with σ_z, σ_y spreading [25] instead of a single variational parameter σ. This becomes relevant in multi-tube systems [25]. Beyond the static properties, this more accurate ground-state energy description could be used to assess the effect of transverse confinement on non-equilibrium properties, e.g., using a generalized Gross–Pitaevskii equation [11,26–29].

Author Contributions: S.D.P. and E.O. did numerical and analytical computations, R.C. did analytical computations. All the authors discussed the details of the work and contributed to the writing of the paper. All authors have read and agreed to the published version of the manuscript.

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