Beyond Mean-Field Theory for Attractive Bosons under Transverse Harmonic Confinement

Luca Salasnich

CNR-INFM and CNISM, Unità di Milano Università, c/o Dipartimento di Fisica, Università di Milano,

Via Celoria 16, 20133 Milano, Italy

We study a dilute gas of attractive bosons confined in a harmonic cylinder, i.e. under cylindric confinement due to a transverse harmonic potential. We introduce a many-body wave function which extends the Bethe ansatz proposed by McGuire (J. Math. Phys. 5, 622 (1964)) by including a variational transverse Gaussian shape. We investigate the ground state properties of the system comparing them with the ones of the one-dimensional (1D) attractive Bose gas. We find that the gas becomes ultra 1D as a consequence of the attractive interaction: the transverse width of the Bose gas reduces by increasing the number of particles up to a critical width below which there is the collapse of the cloud. In addition, we derive a simple analytical expression for the simmetry-breaking solitonic density profile of the ground-state, which generalize the one deduced by Calogero and Degasperis (Phys. Rev. A **11**, 265 (1975)). This bright-soliton analytical solution shows near the collapse small deviations with respect to the 3D mean-field numerical solution. Finally, we show that our variational Gauss-McGuire theory is always more accurate than the McGuire theory. In addition, we prove that for small numbers of particles the Gauss-McGuire theory is more reliable than the mean-field theory described by the 3D Gross-Pitaevskii equation.

PACS Numbers: 03.75.Kk

I. INTRODUCTION

A three-dimensional (3D) dilute Bose gas is well described by the mean-field Gross-Pitaevskii theory [1,2], while in the 1D regime quantum fluctuations become important and an appropriate theoretical treatment requires beyond mean-field approaches [3]. Recently, we have investigated, for a bosonic cloud of atoms, the crossover from 3D to 1D induced by a strong harmonic confinement in the transverse cylindric radial direction [4–7]. In particular, by using a generalized Lieb-Liniger theory [8,7], based on a variational treatment of the transverse width of the repulsive Bose gas, we have analyzed the transition from a 3D Bose-Einstein condensate to a 1D Tonks-Girardeau gas of impenetrable bosons.

In this paper we consider the case of an attractive Bose gas under cylindric transverse harmonic confinement. We introduce a trial wave fuction that is a variational extension of the 1D exact Bethe ansatz [10] proposed by McGuire [11] for the 1D gas of bosons with attractive contact interaction. We show that, contrary to the 1D theory where the transverse width is constant and equal to the characteristic length of harmonic confinement, our theory predicts that the transverse width of the gas reduces by increasing the interatomic strength up to a critical value for which there is the collapse of the system. We investigate also the solitonic axial density profile of the Bose gas with a fixed center of mass, comparing it to the 1D profile and also to the 3D mean-field Gross-Pitaevskii theory.

II. TRANSVERSE GAUSSIAN ANSATZ

The Hamiltonian of a gas of N interacting identical Bose atoms confined in the transverse cylindric radial direction with a harmonic potential of frequency ω_{\perp} is given by

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2} \nabla_i^2 + \frac{1}{2} (x_i^2 + y_i^2) \right) + \sum_{i < j=1}^{N} V(\mathbf{r}_i, \mathbf{r}_j) , \quad (1)$$

where $V(\mathbf{r}_i, \mathbf{r}_j)$ is the inter-atomic potential. In the Hamiltonian we use scaled units: energies are in units of the energy $\hbar\omega_{\perp}$ of the transverse confinement and lengths in units of the characteristic harmonic length $a_{\perp} = (\hbar/(m\omega_{\perp}))^{1/2}$.

The determination of the N-body wave function $\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$ that minimizes the energy

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \int \Psi^* \hat{H} \Psi \ d^3 \mathbf{r}_1 ... d^3 \mathbf{r}_N \tag{2}$$

of the system is a very difficult task. Nevertheless, due to the symmetry of the problem, a variational trial wave function can be written in the form

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = f(z_1, ..., z_N) \prod_{i=1}^N \frac{\exp\left(-\frac{x_i^2 + y_i^2}{2\sigma^2}\right)}{\pi^{1/2}\sigma} , \quad (3)$$

where σ is a variational parameter of the Gaussian transverse wave function [13], that gives the effective transverse length of the Bose gas. In addition, by considering a dilute gas with a mean particle spacing much larger than the interaction radius we set

$$V(\mathbf{r}_i, \mathbf{r}_j) = \Gamma \,\delta^{(3)}(\mathbf{r}_i - \mathbf{r}_j) \,, \tag{4}$$

where $\Gamma = 4\pi a_s/a_{\perp}$, with a_s the s-wave scattering length of the inter-atomic potential. This pseudo-potential gives the correct dilute gas limit and a well-posed variational problem by choosing a smooth trial wave function. Under transverse harmonic trapping a confinement-induced resonance has been predicted by Olshanii [9] at $|a_s|/a_{\perp} \simeq 1$, i.e. when the absolute value of the highest bound-state energy of a realistic inter-atomic potential approaches the confining transverse energy. Therefore the pseudopotential of Eq. (4) can be used in the range $|a_s|/a_{\perp} \ll 1$, a regime where the effects of confinement-induced resonance are negligible.

By inserting Eq. (3) into Eq. (2), using Eq. (4) and integrating over x and y, the total energy reads

$$E = E_z + E_\perp , \qquad (5)$$

where the longitudinal axial energy is

$$E_z = \langle f | \sum_{i=1}^N -\frac{1}{2} \frac{\partial^2}{\partial z_i^2} + \frac{\Gamma}{2\pi\sigma^2} \sum_{i< j=1}^N \delta(z_i - z_j) | f \rangle . \quad (6)$$

It is important to stress that the 1D Hamiltonian that appears in the previous expression is exactly the Hamiltonian studied by Lieb and Liniger [8] for positive interaction strength ($\Gamma/(2\pi\sigma^2) > 0$) and by Mc Guire [11] and by Calogero and De Gasperis [12] for negative interaction strength ($\Gamma/(2\pi\sigma^2) < 0$). The transverse radial energy is instead given by

$$E_{\perp} = \frac{1}{2} (\frac{1}{\sigma^2} + \sigma^2) N .$$
 (7)

As previously stressed, with the ansatz of Eq. (3) we have recently analyzed [6] the repulsive case $(a_s > 0)$ by using the Lieb-Liniger exact result [8] for the longitudinal axial energy. Here we consider the attractive case $(a_s < 0)$ and set $\Gamma/2\pi\sigma^2 = -\gamma/\sigma^2$ with $\gamma = 2|a_s|/a_{\perp}$.

III. GAUSS-MCGUIRE ANSATZ

McGuire [11] proposed the following Bethe ansatz [10] for the axial many-body wave function

$$f(z_1, \dots z_N) = C_N \prod_{1 \le i < j \le N} \exp\left(-\frac{1}{2}\frac{\gamma}{\sigma^2}|z_i - z_j|\right), \quad (8)$$

where C_N is the normalization constant and γ/σ^2 is the strength of the contact δ interaction in the 1D Hamiltonian of Eq. (6). According to the exact result of Mcguire [11] the axial energy E_z of Eq. (6) reads

$$E_z = -\frac{1}{24} \frac{\gamma^2}{\sigma^4} N(N^2 - 1) .$$
 (9)

Using this expression the total energy E of our 3D system can be rewritten as

$$E = -\frac{1}{24}\frac{\gamma^2}{\sigma^4}(N^2 - 1)N + \frac{1}{2}(\frac{1}{\sigma^2} + \sigma^2)N.$$
 (10)

In the weak-coupling 1D limit, where the transverse width $\sigma \simeq 1$, one recovers the 1D result obtained by McGuire [11] plus the constant transverse energy, that is 1 in units of $\hbar\omega_{\perp}$.

In our approach the energy depends on the variational parameter σ . The minimization of the energy E with respect to σ gives the equation

$$\sigma^6 - \sigma^2 + \frac{1}{6}\gamma^2(N^2 - 1) = 0.$$
 (11)

One easily finds that this algebric equation admits real solutions with $d^2E/d\sigma^2 > 0$ if and only if

$$\frac{1}{3^{1/4}} \le \sigma \le 1$$
 . (12)

Below the value $\sigma = 1/3^{1/4}$ there are no stable solutions and the ground state becomes the collapsed state, i.e. the configuration with $\sigma = 0$ and energy $E = -\infty$. The critical strength, corresponding to $\sigma = 1/3^{1/4}$, is

$$\gamma (N^2 - 1)^{1/2} = \frac{2}{3^{1/4}} \simeq 1.52$$
 (13)



FIG. 1. Comparison between our variational Gauss-McGuire theory (GMG) and the McGuire theory (MG) for the attractive Bose gas in a harmonic cylinder. Upper panel: transverse width σ . The unstable branch $(d^2E/d\sigma^2 < 0)$ of Eq. (11) is shown as a dotted line. Lower panel: energy per particle E/N. $\gamma = 2|a_s|/a_{\perp}$ is the inter-atomic strength and N is the number of particles.

In the upper panel of Fig. 1 we plot the transverse width σ obtained from Eq. (11) as a function of $\gamma (N^2 - 1)^{1/2}$ (solid line). While in the 1D case σ is

constant (dashed line), our variational Gauss-McGuire (GMG) method shows that the attractive Bose gas is actually ultra 1D: the width σ decreases by increasing the interaction strength up to the collapse. In the lower panel of Fig. 1 we plot the energy per particle E/N as a function of $\gamma (N^2 - 1)^{1/2}$. We compare our variational energy given by Eqs. (10,11) with the McGuire (MG) energy given by Eq. (10) and $\sigma = 1$. As expected the variational GMG energy is lower than the MG energy giving a better determination (upper bound) of the true ground state of the many-body system.

It is important to observe that the axial McGuire wave function is invariant by a global translation of the positions of the particles. As shown by Calogero and Degasperis [12], and also by Castin and Herzog [14], the wave function of Eq. (8) can be normalized by imposing that its center of mass z_{cm} is fixed, namely

$$\int \delta(z - z_{cm}) |f|^2 \, dz_1 ... dz_N = N \,. \tag{14}$$

The density of particles with respect to z_{cm} is then given by

$$\rho(z) = \int \delta(z_{cm}) \delta(z_1 - z) |f|^2 \, dz_1 \, \dots \, dz_N \, . \tag{15}$$

Following Calogero and Degasperis [12] we immediately find

$$\rho(z) = \frac{\gamma}{\sigma^2} \sum_{l=1}^{N-1} \frac{(-1)^{l+1} l(N!)^2 \exp\left(-\gamma l N |z|/\sigma^2\right)}{(N+l-1)!(N-l-1)!} \,. \tag{16}$$

For $N \gg 1$ this formula can be approximated by

$$\rho(z) = \frac{\gamma N^2}{4\sigma^2} \operatorname{sech}^2\left(\frac{\gamma N}{2\sigma^2}z\right) , \qquad (17)$$

that is the first term in a 1/N expansion of the previous expression. Obviously, only for $\sigma = 1$ the Eq. (16) gives the 1D solitonic profile predicted by Calogero and Degasperis [12]. In our variational GMG scheme σ is not constant and must be determined using the Eq. (11).

IV. COMPARISON WITH THE 3D GPE

Here we compare the GMG wave function with the fully 3D Hartree wave function, from which one obtains the 3D Gross-Pitaevskii equation (GPE). The 3D Hartree approximation is obtained by setting

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = N^{1/2} \prod_{i=1}^N \psi(\mathbf{r}_i) .$$
 (18)

Inserting this many-body wave function into Eq. (2) with Eq. (4), after integration one finds the Gross-Pitaevskii energy functional

$$E[\psi(\mathbf{r})] = N \int \psi^* \left[-\frac{1}{2} \nabla^2 + \frac{1}{2} (x^2 + y^2) \right]$$

$$-\frac{1}{2}2\pi\gamma(N-1)|\psi|^2 \bigg]\psi \ d^3\mathbf{r} \ . \tag{19}$$

By minimizing this energy functional with respect to $\psi(\mathbf{r})$ with the constraint of the normalization $\int |\psi|^2 d^3 \mathbf{r} = 1$ one finds the familiar mean-field 3D GPE given by

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}(x^2 + y^2) - 2\pi\gamma(N-1)|\psi|^2\right]\psi = \mu \ \psi \ , \ (20)$$

where μ is the chemical potential fixed by the normalization. We solve the stationary GPE by using a finitedifference Crank-Nicolson predictor-corrector algorithm with imaginary time [15].



FIG. 2. Density profile $\rho(z)$ of the bright soliton solution obtained with three different theories: Gauss-McGuire (GMG), McGuire (MG) and the Gross-Pitaevskii equation (GPE).Four values of the interaction strength: (a) $\gamma(N-1) = 0.7$; (b) $\gamma(N-1) = 0.9$; (c) $\gamma(N-1) = 1$; (d) $\gamma(N-1) = 1.2$. N is the number of particles and $\gamma = 0.001$.

In Fig. 2 we plot the solitonic density profile of the GPE and compare it with the profile of GMG theory, i.e. Eq. (16) with σ given by Eq. (11). We insert also the solitonic profile of the MG theory, i.e. Eq. (16) with $\sigma = 1$. Up to the collapse our GMG solitionic profile is close to the GPE one; there are instead relevant deviations with respect to the MG soliton (which does not collapse). Our numerical integration of the GPE gives the collapse for $\gamma(N-1) \simeq 1.35$ in agreement with previous computations [16] and not too far from the analytical prediction of Eq. (13). The GPE critical strength is very close to the analytical prediction $\gamma(N-1) = 4/3 \simeq 1.33$ of the non-polynomial Schrodinger equation (NPSE) [4,5]. However the NPSE is not an exact variational equation: it was obtained from the GPE by neglecting some space derivatives (for details see [4] and [17]).

The results of Fig. 2 are obtained by setting $\gamma = 0.001$. In Fig. 3 we use the same value of γ , that is relevant for the experiments performed with Bose-Einstein condensates of ⁷Li atoms [18,19]. Fig. 3 shows the energy per particle E/N, the chemical potential μ , the density per particle $\rho(0)/N$, and also the transverse width σ of the soliton as a function of the number N of bosons. The GMG energy (solid line) is always close to the GPE energy (dotted line) and near the collapse the energy difference slightly increases. Chemical potentials and densities have a similar behavior. Fig. 3 shows that for a large number N of bosons the MG theory (dashed lines) differs with respect to the other two theories: for N > 750deviations are clearly visible.



FIG. 3. Bright soliton properties. Comparison among different theories: Gauss-McGuire (solid line), McGuire (dashed line) and the Gross-Pitaevskii equation (dotted line). (a) Energy per particle E/N. (b) Chemical potential μ . (c) Axial density per particle $\rho(0)/N$ at the origin. (d) Transverse width σ at z = 0. N is the number of particles and $\gamma = 0.001$.

The panel (d) of Fig. 3 shows that the transverse width σ decreases by increasing N for both the GPE and the GMG theory; however σ stays always of the order of one up to the collapse. Note that the transverse width σ obtained by using the GPE depends on the axial coordinate z. In the plot we choose σ at z = 0, that is the lower value of the transverse width.

The variational principle says that the lowest energy indicates the most accurate solution. The variational principle applies when different variational solutions for the same Hamiltonian are compared. In our case, the Hamiltonian is given by Eq. (1) with Eq. (4) and the three variational solutions are: the GMG one given by Eq. (3) and Eq. (8), the MG one given by Eq. (3) with $\sigma = 1$ and Eq. (8), and the GPE one given by Eq. (19). For N = 1 the three theories give the same value of energy: E/N = 1. The top panel of Fig. 3 shows that for a large N the GPE gives the lowest energy. We expect that for a small N the GMG theory and the MG theory are more reliable than the GPE. To verify this prediction we choose a larger value of γ , namely $\gamma = 0.01$, and calculate numerically the GPE energy of Eq. (19) for all integer values of N up the the collapse. The results are shown in Fig. 4 where we plot the energies for increasing values of N.



FIG. 4. Energy per particle E/N as a function of the number N of bosons. Comparison among different theories: Gauss-McGuire (solid line), McGuire (dashed line) and the Gross-Pitaevskii equation (filled circles). Here $\gamma = 0.01$.

For 1 < N < 40 the GMG energy (solid line) and the MG energy (dashed line) are indistinguishable but both lower than the GPE energy (filled circles). Around N = 60 the GPE energy becomes lower then the MG energy but still higher than the GMG energy. Only around N = 100 the GPE energy becomes smaller than the GMG energy. At N = 136 there is the collapse of the GPE solitonic solution while the GMG soliton collapses at N = 153. Just before the collapse of the GPE solution, i.e. for N = 135, the relative difference Δ_R between GPE energy and GMG energy is 0.79%, while Δ_R between GPE energy and MG energy is 2.68% (see also the upper panel of Fig. 5).



FIG. 5. Energetic relative difference Δ_R (percentual) as a function of the number N of bosons. Circles: Δ_R between McGuire and Gauss-McGuire. Filled squares: Δ_R between Gross-Pitaevskii equation and Gauss-McGuire. Triangles: Δ_R between Gross-Pitaevskii equation and McGuire.

Similar results are obtained by setting $\gamma = 0.001$. Here the energetic relative difference Δ_R between GPE and MG theory changes sign around N = 270. Instead Δ_R between GPE and GMG theory changes sign around N =480. Just before the collapse of the GPE solution, i.e for N = 1334, Δ_R is 2.86% and 1.00% respectively.

To better study beyond mean-field effects we perform numerical calculations for various values of γ in the interval [0.01, 0.1]. The results are reported in Fig. 5, where we plot the energetic relative difference Δ_R for three values of the inter-atomic strength γ . The figure shows that the energy of the GMG theory is always smaller than the energy of the MG theory; in fact, their relative difference Δ_R (curves with circles) is always positive. The behavior of the curves in the three panels reveals that by growing γ the range of N reduces and the range of Δ_R increases. The curves with triangles (GPE energy minus GMG energy) and also the curves with filled squares (GPE energy minus MG energy) show that by fixing the number N of particles and increasing the strength γ , the beyond mean-field effects become more important. Fig. 5 shows that for $\gamma = 0.05$ and $\gamma = 0.1$ the GMG theory gives a lower energy than the GPE up to the collapse. We find that the critical strength γ_s beyond which the GMG theory is better than the GPE for all N is $\gamma_s = 0.044$; in this regime the critical number N_c of particles for the collapse predicted by the GMG theory is more reliable than the GPE one.

V. CONCLUSIONS

We have introduced a beyond mean-field many-body wave function which describes dilute attractive bosons under transverse harmonic confinement. This variational approach, that we have called Gauss-McGuire theory, gives simple analytical formulas for the ground-state energy and the solitonic density profile. These formulas are in good agreement with the numerical results of the 3D mean-field theory. By comparing the ground-state energies, we have verified that for small numbers of particles the Gauss-McGuire theory is better than the 3D mean-field theory while the 3D mean-field theory is more reliable for a large number of particles and a small interatomic strength.

ACKNOWLEDGEMENTS

We thank A. Parola, L. Reatto, Y. Castin and A. Recati for useful discussions.

- [1] E.P. Gross, Nuovo Cimento **20**, 454 (1961).
- [2] L.P. Pitaevskii, Sov. Phys. JETP 13, 451 (1961).
- [3] See, for instance, G.E. Astrakharchik, D. Blume, S. Giorgini, and B.E. Granger, J. Phys. B: At. Mol. Opt. Phys. 37, S205 (2004).
- [4] L. Salasnich, Laser Phys. **12**, 198 (2002); L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A **65**, 043614 (2002).
- [5] L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A 66, 043603 (2002).
- [6] L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. Lett. **91**, 080405 (2003); L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A **69**, 045601 (2004).
- [7] L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A 70, 013606 (2004); L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A 72, 025602 (2005).
- [8] E.H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).
- [9] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
- [10] H.A. Bethe, Z. Physik **71**, 205 (1931).
- [11] J.B. McGuire, J. Math. Phys. 5, 622 (1964).
- [12] F. Calogero and A. Degasperis, Phys. Rev. A 11, 265 (1975).
- [13] V.M. Perez-Garcia, H. Machinel, and H. Herrero, Phys. Rev. A 57, 3837 (1998); L. Salasnich, Int. J. Mod. Phys. B 14, 1 (2000).
- [14] Y. Castin and C. Herzog, Comptes Rendus de l'Academie des Sciences de Paris, tome 2, serie IV, 419-443 (2001).
- [15] E. Cerboneschi, R. Mannella, E. Arimondo, and L. Salasnich, Phys. Lett. A **249**, 495 (1998); L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A **64**, 023601 (2001).
- [16] A. Gammal, L. Tomio and T. Frederico, Phys. Rev. A 66, 043619 (2002).

- [17] A.M. Kamchatnov and V.S. Shchesnovich, Phys. Rev. A 70, 023604 (2004).
- [18] K.E. Strecker, G.B. Partridge, A.G. Truscott, and R.G. Hulet, Nature 417, 150 (2002).
- [19] L. Khaykovich, F. Schreck, G. Ferrari, T. Bourdel, J. Cubizolles, L.D. Carr, Y. Castin, and C. Salomon, Science 296, 1290 (2002).