ULTRACOLD BOSONS IN 1D: FROM BOSE-EINSTEIN CONDENSATE TO TONKS-GIRARDEAU GAS

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(Dated: 15th of January, 2016)

Abstract: We consider an ultracold atomic gas trapped in a one-dimensional harmonic oscillator potential. We study the transition from a Bose-Einstein condensate, in the small atom-atom interaction limit, to a strongly interacting Tonks-Girardeau gas, as the interaction is varied from zero to large values. The response of the system against a monopolar perturbation is characterized by the moments of the dynamic structure function. The calculations have been done by direct diagonalization of the second quantized many-body Hamiltonian in a truncated Fock space. The corresponding virial theorem for the many-body states has been employed to cross-check the validity of our numerical techniques.

I. INTRODUCTION

Bosons are identical particles with integer spin that behave following the Bose-Einstein statistics which, among other things, tell us that more than one boson can be populating the same quantum mechanical state. This property allows the formation of a Bose-Einstein condensate. The latter was first produced in 1995 by E. Cornell and C. Wieman, with ultracold ^{87}Rb gas, and W. Ketterle, with ultracold ^{23}Na gas. They all shared the Nobel Prize in 2001 [1].

Recently, there has been a lot of interest in studying ultracold atomic gases which can not be described by mean-field techniques, thus, far from the Bose-Einstein condensate. Among them, a very interesting case is the Tonks-Girardeau gas [2]. The question behind is what happens if we add a large repulsive atom-atom contact potential. The answer is that one-dimensional bosons, under large interaction, build correlations to avoid the contact [2]. This behaviour is reminiscent of polarized fermions which, due to the Pauli exclusion principle, can not populate the same quantum mechanical state. Therefore, bosons in a Tonks-Girardeau gas are said to fermionize. In the limit of infinite interaction, the ground state for N interacting bosons is the same as the absolute value of the Slater determinant constructed with the lower N single-particle states of non-interacting fermions. [2].

The aim of this document is to study what happens to the system during the transition from a Bose-Einstein condensate to the Tonks-Girardeau gas. Both limits, non-interacting and infinitely interacting, are known and will be used as reference. To this purpose, we have developed a general many-body framework which we particularized to the problem of two interacting bosons trapped in a harmonic oscillator potential with the lowest twenty single-particle states.

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This document is organized in the following way. In Sec. II we present the ground state for both non-interacting bosonic and fermionic one-dimensional gases trapped in a harmonic oscillator potential. In Sec. III we add interaction and study the transition from a Bose-Einstein condensate to a Tonks-Girardeau gas. We focus on characteristics of the system such as the energy spectrum and the density and the pair correlation function of the ground state. The corresponding virial theorem is derived. Then, in Sec. IV, we study the response of the system to a monopolar perturbation and compute the dynamic structure function.

II. NON-INTERACTING BOSONS AND FERMIONS IN A 1D HARMONIC OSCILLATOR POTENTIAL

Let us consider a system of N non-interacting atoms trapped in a 1D harmonic oscillator potential. The many-body Hamiltonian reads,

$$\hat{H}_0 = \hat{T} + \hat{V}_{HO} = \sum_{i=0}^{N} \frac{-\hbar^2}{2m} \frac{d^2}{dx_i^2} + \sum_{i=0}^{N} \frac{1}{2} m\omega^2 x_i^2 . \quad (1)$$

The single-particle eigenfunctions $\psi_i(x)$ and eigenenergies ε_i of the harmonic oscillator Hamiltonian are,

$$\psi_i(x) = \left(\frac{\sqrt{\beta}}{2^i i! \sqrt{\pi}} \right)^{\frac{1}{2}} e^{\frac{-\beta x^2}{2}} \mathcal{H}_i(\sqrt{\beta}x) , \quad (2)$$

$$\varepsilon_i = \hbar\omega \left(\frac{1}{2} + i \right) , \quad i = 0, 1, \ldots, \quad (3)$$

where m is the mass of the atom, $\hbar$ is the Planck constant and ω is the frequency; i denotes the state, $\beta = \frac{m\omega}{\hbar}$ and $\mathcal{H}_i(\sqrt{\beta}x)$ is the Hermite polynomial of order i. From now on, all the results presented in this document are expressed in harmonic oscillator units.

Now we proceed to build the many-body wave function of the ground state of the system. The ground state for

non-interacting bosons is,

$$\Psi_0^{(b)}(x_1,\dots,x_N) = \prod_{i=1}^{N} \psi_0(x_i)\,, \qquad (4)$$

and for non-interacting fermions, the Slater determinant reads,

$$\Psi_0^{(f)}(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_0(x_1) & \dots & \psi_0(x_N) \\ \vdots & \ddots & \vdots \\ \psi_N(x_1) & \dots & \psi_N(x_N) \end{vmatrix}. \quad (5)$$

In first quantization, the density $\rho(x)$ and the pair correlation function $\eta(x,x')$ are given by,

$$\rho(x) = \int dx_2 dx_3 \dots dx_N |\Psi(x,x_2,\dots,x_N)|^2 \qquad (6)$$

$$\eta(x,x') = N(N-1)\int dx_3 \dots dx_N |\Psi(x,x',x_3,\dots,x_N)|^2,$$

with $\int_{-\infty}^{\infty} \rho(x)dx = 1$ and $\int_{-\infty}^{\infty} \eta(x,x')dxdx' = N(N-1)$.

$\rho(x)$ of the ground state of the system for both non-interacting bosons and fermions is shown in Fig. 2. For bosons $\rho(x)$ has one peak in the center of the trap and has the same shape as the single-particle ground state. On the other hand, for fermions we find two peaks as a consequence of the antisymmetry of $\Psi_0^{(f)}$.

$\eta(x,x')$ gives us information about correlations present in the ground state. In particular, it gives the probability of finding an atom at a given position x when another atom is located at x'. For non-interacting bosons, $\rho(x) = |\psi_0(x)|^2$ and $\eta(x,x') = N(N-1)|\psi_0(x)|^2|\psi_0(x')|^2$, see Figs. 2, and 3. This is due to the fact that the bosonic many-body wave function is a product state of single-particle ground states (4). For fermions, the observed behaviour is very different. $\eta(x,x')$ has a 0 whenever $x = x'$ as a consequence of the Pauli exclusion principle.

III. INTERACTING BOSONS IN A HARMONIC OSCILLATOR POTENTIAL

In this section we consider a finite value of the atom-atom interaction. First, in Sec. III A we describe the framework used to study the interacting problem, then, in Sec. III B we derive the corresponding virial theorem, and finally, in Sec. III C we discuss the results obtained when the interaction is increased.

A. Second quantization

In the general case of N bosons it is easier to treat the interacting problem in second quantization. Hence, we work in the Fock space. A Fock vector is written as $|n_0, n_1, \dots, n_M\rangle$, where n_i is the number of atoms in the single-particle state $\psi_i(x)$ from a total of M single-particle states. We refer to these vectors as $|\alpha\rangle$. The dimension of the Fock space is $D = (M+N-1)!/((M-1)!N!)$.

Adding a repulsive atom-atom contact potential $\hat{V}_{int} = \sum_{i<j} g\delta(x_i - x_j)$, the new many-body Hamiltonian $\hat{H}$ in second quantization reads [3, 4],

$$\hat{H} = \hat{H}_0 + \hat{V}_{int} = \sum_{i=0}^{M} \varepsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{g}{2} \sum_{klmn}^{M} I_{klmn} \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_m \hat{a}_n\,, \tag{7}$$

with $I_{klmn} = \int dz \psi_k(x)\psi_l(x)\psi_m(x)\psi_n(x)$, where $[\hat{a}_k^\dagger, \hat{a}_i] = \delta_{ik}$ and $[\hat{a}_k^\dagger, \hat{a}_i^\dagger] = [\hat{a}_k, \hat{a}_i] = 0$, being $\hat{a}^\dagger$ the creation operator: $\hat{a}_k^\dagger |n_0,\dots,n_k,\dots,n_M\rangle = \sqrt{n_k+1}\,|n_0,\dots,n_k+1,\dots,n_M\rangle$; and $\hat{a}$ the destruction operator: $\hat{a}_k |n_0,\dots,n_k,\dots,n_M\rangle = \sqrt{n_k}\,|n_0,\dots,n_k-1,\dots,n_M\rangle$. $\hat{H}_0$ is the harmonic oscillator Hamiltonian (1), ε_i is the single-particle energy (3), $\psi_{k,l,m,n}(x)$ are the single-particle wave functions (2) and g is the interaction strength.

The calculations are done in the following way. First we fix the number of atoms, $N = 2$ in this case, and the number of single-particle states, $M = 20$. Then, we numerically diagonalize the Hamiltonian in the Fock basis. With this procedure we obtain the many-body eigenenergies E_q and eigenstates $|q\rangle$ of the system,

$$\hat{H}|q\rangle = E_q|q\rangle\,, \tag{8}$$

where $|q\rangle = \sum_{\alpha}^{D} C_{\alpha q}|\alpha\rangle$.

Before, in Sec. II, we introduced $\rho(x)$ and $\eta(x,x')$ in first quantization. Now, using the density operator $\hat{\rho}(x) = \sum_{ij}^{M}\langle i|\delta(x-x_1)|j\rangle \hat{a}_i^\dagger \hat{a}_j$ and the pair correlation operator $\hat{\eta}(x,x') = \frac{1}{2}\sum_{ijkl}^{M}\langle ij|\delta(x-x_1)\delta(x'-x_2)|kl\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$, we can rewrite them in second quantization,

$$\rho(x) = \sum_{\alpha\alpha'}^{D}\sum_{ij}^{M} \psi_i^*(x)\psi_j(x)C_{\alpha 0}^* C_{\alpha'0}\langle\alpha|\hat{a}_i^\dagger \hat{a}_j|\alpha'\rangle\,,$$

$$\eta(x,x') = \sum_{\alpha\alpha'}^{D}\sum_{ijkl}^{M} \psi_i^*(x)\psi_j^*(x')\psi_k(x)\psi_l(x') \tag{9}$$
$$C_{\alpha 0}^* C_{\alpha'0}\langle\alpha|\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l|\alpha'\rangle\,,$$

where $|0\rangle = \sum_{\alpha}^{D} C_{\alpha 0}|\alpha\rangle$ is the ground state of the system.

B. Virial theorem

The virial theorem is based on a scaling transformation of a many-body wave function and how the different parts of the Hamiltonian transform [5]. First of all, lets define this new wave function,

$$\Psi_\lambda(x_1,\dots,x_N) = \lambda^{N/2}\Psi(\lambda x_1,\dots,\lambda x_N)\,, \tag{10}$$

where Ψ_λ has the same normalization as Ψ. The energy contributions of the Hamiltonian transform as follows.

The kinetic energy,

$$T(\lambda) = \langle\Psi_\lambda| \sum_{i=1}^{N} -\frac{1}{2}\frac{d^2}{dx_i^2}|\Psi_\lambda\rangle = T(\lambda = 1)\,, \qquad (11)$$

the harmonic oscillator potential energy,

$$V_{HO}(\lambda) = \langle\Psi_\lambda| \sum_{i=1}^{N} \frac{1}{2}x_i^2|\Psi_\lambda\rangle = \frac{1}{\lambda^2}V_{HO}(\lambda = 1)\,, \quad (12)$$

and the interaction potential energy,

$$V_{int}(\lambda) = \langle\Psi_\lambda| \sum_{i<j} g\delta(x_i - x_j)|\Psi_\lambda\rangle = \lambda V_{int}(\lambda = 1)\,.$$
$$(13)$$

These scaling transformations of the energy contributions lead to,

$$E_\lambda = \langle\Psi_\lambda|\hat{H}|\Psi_\lambda\rangle = \lambda^2\langle\hat{T}\rangle + \frac{1}{\lambda^2}\langle\hat{V}_{HO}\rangle + \lambda\langle\hat{V}_{int}\rangle\,, \quad (14)$$

which has a stationary point at $\lambda = 1$ because $\Psi(x_1, \ldots, x_N)$ is taken to be an eigenstate [5],

$$\left.\frac{dE_\lambda}{d\lambda}\right|_{\lambda=1} = 0\,. \qquad (15)$$

Hence, the virial theorem is:

$$0 = 2\langle\hat{T}\rangle - 2\langle\hat{V}_{HO}\rangle + \langle\hat{V}_{int}\rangle\,, \qquad (16)$$

which should be valid for any eigenstate. This equation is a virial theorem for a many-body system.

C. Results

When the interaction strength $g = 0$, we recover the results for non-interacting bosons of Sec. II, as can be seen in Figs. 1, 2, 3, and 4.

In Fig. 1 we show the lower part of the energy spectrum of the system. Increasing the interaction, the lower part of the energy spectrum approaches the energy spectrum of non-interacting fermions in the same confining potential. In particular, the ground-state energy goes from $\varepsilon_0 + \varepsilon_0 = 0.5 + 0.5$ for $g = 0$ to $\varepsilon_0 + \varepsilon_1 = 0.5 + 1.5$ already for $g = 20$.

The transition from small to large interactions can also be seen in $\rho(x)$ and $\eta(x, x')$. In Fig. 2 we depict $\rho(x)$ for different values of g. For $g = 0$ we get back the density from the non-interacting system. For $g = 2$ $\rho(x)$ has changed its shape in a way that the central peak has decreased and its width has become wider. Further increasing g two peaks start to appear approaching the shape of the non-interacting fermionic case. For $g = 20$ we can see that both the interacting bosonic and the non-interacting fermionic density are on top of each other. In a similar way, $\eta(x, x')$ evolves towards the non-interacting fermionic one as we increase g. In Fig. 3 one atom is fixed
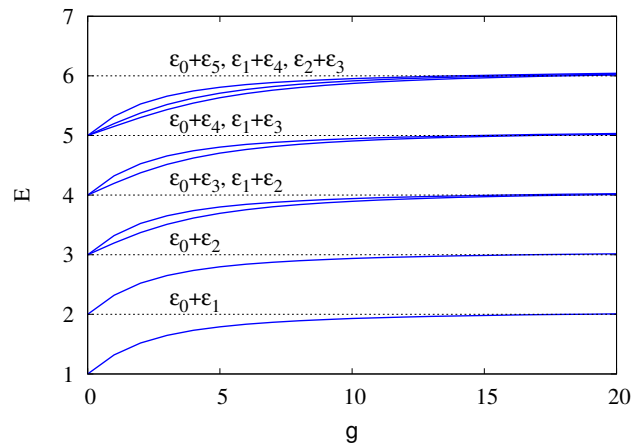

FIG. 1: Lower part of the energy spectrum of two interacting bosons trapped in a harmonic oscillator potential, with the lowest twenty single-particle states, as a function of the interaction strength g. The solid lines are the energies of the two interacting bosons. The dotted lines are the energies of two non-interacting fermions in the same confining potential, for any g.
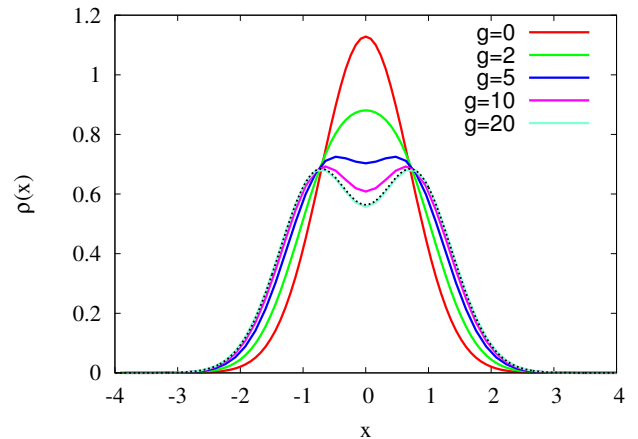

FIG. 2: Density $\rho(x)$ of two interacting bosons trapped in a harmonic oscillator potential, with the lowest twenty single-particle states, for different values of the interaction strength g. The dotted black line is $\rho(x)$ for two non-interacting fermions confined in the same potential.

at the center of the trap. Hence, we see how the central value decreases as g is increased, almost reaching zero for $g = 20$.

The different energy contributions for the ground state, together with the virial theorem, are shown in Fig. 4. E_0 perfectly matches with the ground-state energy shown in Fig. 1. $\langle\hat{V}_{HO}\rangle$ has already reached its value for two non-interacting fermions at $g = 20$. On the other hand, $\langle\hat{T}\rangle$ never reaches its value for the fermionic system. The virial theorem should be fulfilled for any eigenstate of the system (16). Although, it is slightly violated for large values of g.

$\langle\hat{V}_{int}\rangle$ increases for small interaction values. For $g \gtrsim 2$,
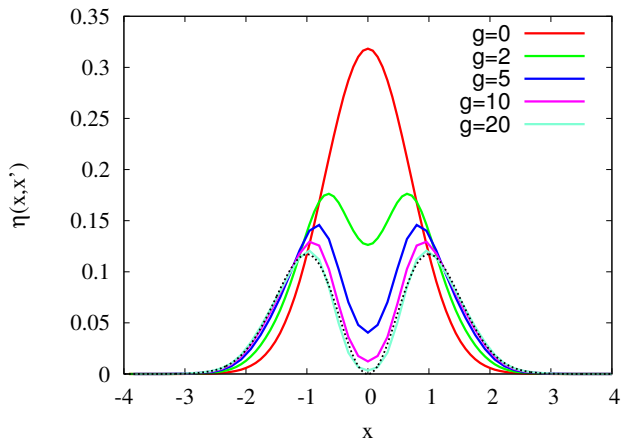
FIG. 3: Pair correlation function $\eta(x,0)$ of two interacting bosons trapped in a harmonic oscillator potential, with the lowest twenty single-particle states, for different values of the interaction strength g. The dotted black line is $\eta(x,0)$ for two non-interacting fermions confined in the same potential. One of the atoms is fixed at the center of the trap.
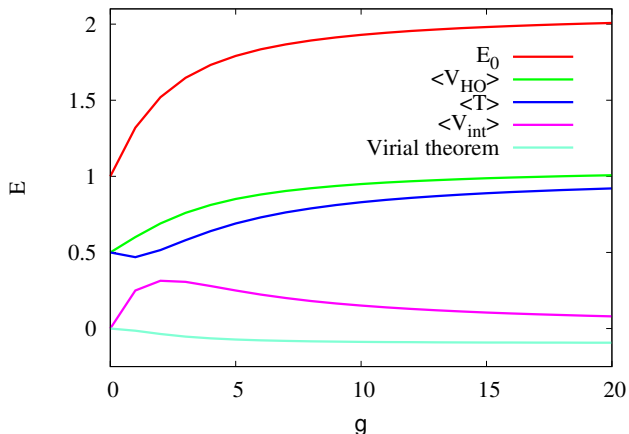

FIG. 4: Total energy, kinetic energy $\langle \hat{T} \rangle$, harmonic oscillator energy $\langle \hat{V}_{HO} \rangle$, interaction energy $\langle \hat{V}_{int} \rangle$ and virial theorem for the ground state of two interacting bosons trapped in a harmonic oscillator potential, with the lowest twenty single-particle states, as functions of the interaction strength g.

$\langle \hat{V}_{int} \rangle$ starts to decrease as g increases. This behaviour is caused by correlations among the interacting bosons. The correlations start to appear when the interaction between bosons gains importance. These correlations make the bosons populate higher single-particle states in order to avoid the atom-atom contact, and thus, minimize the interaction energy of the system. Hence, for an ideal system with infinite number of single-particle states, $\langle \hat{V}_{int} \rangle$ would be zero in the $g \to \infty$ limit. Our numerical calculations have been done with a system with the lower twenty single-particle states, thus, $\langle \hat{V}_{int} \rangle$ never reaches the zero. The inaccuracy in our numerical calculations, due to finite single-particle states, also applies to $\eta(x = x')$ and

$\langle \hat{T} \rangle$. The latter, as well as $\langle \hat{V}_{int} \rangle$, is responsible of the slight violation of the virial theorem.

IV. DYNAMIC STRUCTURE FUNCTION

In this section we study the response of our many-body system to an external monopolar perturbation. We will consider a one-body excitation operator, $\hat{F} = \sum_{i=1}^{N} x_i^2$, to excite the breathing mode. The associated dynamic structure function reads,

$$S_F(E) = \frac{1}{N} \sum_q^D |\langle q|\hat{F}|0\rangle|^2 \delta(E - (E_q - E_0)), \qquad (17)$$

where $\langle q|\hat{F}|0\rangle = \sum_{\alpha'\alpha}^{D} \sum_{kl}^{M} C^*_{\alpha'q} C_{\alpha 0} \langle k|\hat{F}|l\rangle \langle \alpha'|a_k^\dagger a_l|\alpha\rangle$. We can explicitly calculate $S_F(E)$ with the eigenenergies E_q and eigenfunctions $|q\rangle$ of our system. In our truncated space of M single-particle states, we expect the highest part of the energy spectrum to be poorly described. Thus, we truncate the sum for states with $(E_q - E_0) < 20$.

Another way to characterize $S_F(E)$ is calculating its momenta M_n of order n,

$$M_n(E) = \int_0^\infty E^n S_F(E) dE,$$
$$= \frac{1}{N} \sum_q^D (E_q - E_0)^n |\langle q|\hat{F}|0\rangle|^2. \qquad (18)$$

Many times the strength of $S_F(E)$ is concentrated in only one state. Thus, we can write $S_F(E) = Z\delta(E - E_m)$. To determine the monopolar energy E_m, we only require two momenta, e.g.,

$$M_{-1} = \int_0^\infty E^{-1} S_F(E) dE = Z E_m^{-1}, \qquad (19)$$

$$M_1 = \int_0^\infty E S_F(E) dE = Z E_m. \qquad (20)$$

Then, $E_m = \sqrt{M_1/M_{-1}}$.

Furthermore, we can calculate the momenta without knowing $S_F(E)$ with the so-called sum rules [6, 7]. Let us introduce the sum rules for M_1 and M_{-1},

$$M_1 = \frac{1}{2}\frac{1}{N}\langle 0|[\hat{F}^\dagger, [\hat{F}, \hat{H}]]|0\rangle$$
$$= 2\langle 0|x^2|0\rangle = 2\int_{-\infty}^\infty x^2 \rho(x) dx, \qquad (21)$$

with $\int_{-\infty}^\infty \rho(x) dx = 1$.

For the sum rule of M_{-1}, we will build a new Hamiltonian $\tilde{H} = \hat{H} + \lambda\hat{F}$ and perform perturbation theory. The expansion up to second order of the ground-state energy $E_0(\lambda)$, eigenenergy of $\tilde{H}$, reads,

$$E_0(\lambda) = E_0 + \lambda\langle 0|\hat{F}|0\rangle + \lambda^2 \sum_q \frac{|\langle q|\hat{F}|0\rangle|^2}{E_0 - E_q}, \qquad (22)$$
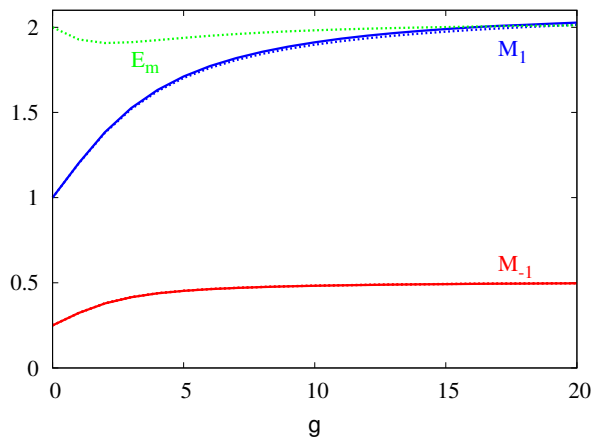
FIG. 5: Momenta M_{-1} and M_1 and the monopolar energy E_m of two interacting bosons trapped in a harmonic oscillator potential, with the lowest twenty single-particle states, as functions of the interaction strength g.

thus, M_{-1} is given by,

$$M_{-1} = -\frac{1}{2}\frac{1}{N}\left.\frac{\partial^2 E_0(\lambda)}{\partial\lambda^2}\right|_{\lambda=0}. \qquad (23)$$

Similar to this procedure, we have a second sum rule for M_{-1},

$$M_{-1} = -\frac{1}{2}\frac{1}{N}\left.\frac{\partial}{\partial\lambda}\langle\tilde{0}|\hat{F}|\tilde{0}\rangle\right|_{\lambda=0}, \qquad (24)$$

where $|\tilde{0}\rangle$ is the ground state of the perturbed Hamiltonian $\tilde{H}$, and $\frac{1}{N}\langle\tilde{0}|\hat{F}|\tilde{0}\rangle = \langle\tilde{0}|x^2|\tilde{0}\rangle = \int_{-\infty}^{\infty} x^2 \rho_\lambda(x)dx$ with $\int_{-\infty}^{\infty} \rho_\lambda(x)dx = 1$.

In our particular case, E_m has very similar values for $g = 0$ and $g = 20$, as recently pointed out in [8], see Fig. 5. The dip of E_m coincides with the peak of the interaction energy at $g \simeq 2$, see Fig. 4. The numerical calculations confirm that (18) and the sum rules coincide for both M_{-1} and M_1. The solid lines are calculated using (18). The dotted lines are calculated using the sum rules (21, 23, 24).

V. SUMMARY AND CONCLUSIONS

We have studied how interacting bosons behave in a 1D harmonic oscillator potential from the non-interacting to a strongly interacting case. For large interaction, the bosonic system resembles a non-interacting fermions system in the same confining potential but we have found that, in a finite space, we can not achieve the theoretical results for some characteristics of the system. Therefore, our conclusions are:

- The ground state of interacting bosons in a 1D harmonic oscillator potential can be mapped by the ground state of non-interacting fermions in the same confining potential in the strongly interacting regime.

- The interaction energy contribution increases in the weakly interacting regime. For large interaction, the bosons correlate and populate higher single-particle states in order to avoid the atom-atom contact. Thus, counter-intuitively, the interaction energy decreases and the energy of the system minimizes.

- The transition from the Bose-Einstein condensate to the Tonks-Girardeau gas makes appear a dip for the monopolar energy in the regime between small and large interaction. In the strongly interacting regime, the correlations among the interacting bosons are responsible for the reentrant behaviour of the monopolar energy.

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