Speed of sound in a Bose-Einstein condensate

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In the present work we determine the speed of sound in a Bose–Einstein condensate confined by an isotropic harmonic oscillator trap. The deduction of this physical parameter is done resorting to the N–body Hamiltonian operator. The single–particle eigenfunctions that have been employed in this formalism are those stemming from the corresponding harmonic oscillator potential, and an expression for the dependence of this speed on the temperature is also deduced. These functions are used in the calculation of the scattering length, etc. The situation for a Bose–Einstein condensate of sodium is evaluated and the corresponding speed of sound is obtained and compared against the known experimental outcomes. The possibility that the solution, to the existing discrepancy between experiment and theoretical predictions, could be given by the Zaremba–Nikuni–Griffin formalism is also explored.

I. INTRODUCTION

A fundamental aspect in the context of quantum gases is related to the analysis of their collective excitations. Collective modes in uniform quantum fluids can be categorized in two different realms, namely, collisionless and hydrodynamic modes. The former are associated to the dynamic self–consistent mean fields, whereas, the latter emerge as a consequence of the properties of the interactions [1]. The study of collective excitations could provide a deep insight into some physical characteristics of these systems. In other words, the study of the excitations in a Bose–Einstein condensate (BEC) opens up a new realm in the comprehension of the structure of quantum fluids, at least in the regime of dilute quantum fluids. Clearly, in this direction there are several properties to be considered; among them we may find the role that trapping potentials and interactions among the constituents of the system play in the determination of certain features of a BEC. At this point let us focus our attention on the consequences of binary interactions upon some features of a BEC. In some cases, for instance, $^{87}\text{Rb}$ or $^{23}\text{Na}$, the size of the corresponding condensate suffers an enlargement due to the presence of the two–body repulsive forces. A further effect of these repulsive interactions is the fact that the central density of a non–ideal BEC at very low temperatures can be two or three orders of magnitude higher than the one associated to an ideal BEC [2], i.e., when the interaction among the particles of the gas is switched off.

A knowledge of the speed of sound opens up several possibilities. For instance, the study of correlated momentum excitations in the many–body condensate wave function [3, 4]. As a further comment let us mention that the dispersion relation for elementary excitations has a very different form when the possibility of an interaction among the particles is considered or not [5]. Since binary collisions are not a frequent event in a BEC it is a little bit surprising that the concept of interaction plays a primordial role in the determination of some physical features. The answer to this interrogant stems from the large coherent mean field associated to a BEC [6]. These comments lead us to conclude that the comprehension of the speed of sound in a condensate defines an issue that bears an important physical relevance. In this context let us mention that it is believed that Gross–Pitaevskii mean field formalism captures the most essential properties associated to the ground state of a BEC [7]. Of course, the comparison of the theoretical predictions against the experimental outcomes provides a test of the validity of the mean field formalism, at least indirectly.

Usually the deduction of the speed of sound in a BEC is done resorting to the linearized time–independent Gross–Pitaevskii equation in the so–called Tomas–Fermi limit. Afterwards, this expression is cast in the form of two quantum hydrodynamic equations (one for the density fluctuations and the second one for the velocity). Finally, the velocity is eliminated from the aforementioned equations and a differential equation for the density fluctuations is obtained [8]. Clearly, the aforementioned procedure does not exhaust all the possible manners in which the speed of sound can be deduced. Another way starts from the N–body Hamiltonian in the second quantization formalism, introduces the Bogoliubov approximation and the resulting Hamiltonian is diagonalized by means of the Bogoliubov canonical transformation. The energy of the ground state of this diagonalized Hamiltonian allows us to calculate the pressure and speed of sound of the corresponding BEC [9]. A crucial point in all these approaches is the Mean Field Theory (MFT) [10]. This formalism requires the use of several assumptions, one of them is related to the introduction of single–particle wave functions, a fact that can be tracked down to the Gibbs–Bogoliubov–Feynman equation [11, 12]. The choice of these aforementioned single–particle eigenfunctions is a consequence of a minimization procedure, nevertheless, in some cases free–particles eigenfunctions [9], in other situations the eigenfunctions related to the particular trapping potential are employed [9], without proving if they are the minimizing case.

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In the present work we determine the speed of sound in a Bose–Einstein condensate confined by an isotropic harmonic oscillator trap. The deduction of this physical parameter is done resorting to the \(N\)-body Hamiltonian operator. The single–particle eigenfunctions that have been employed in this formalism are those stemming from the corresponding harmonic oscillator potential, and an expression for the dependence of this speed on the temperature is also deduced. These functions are used in the calculation of the scattering length, etc. The situation for a Bose–Einstein condensate of sodium is evaluated and the corresponding speed of sound is obtained and compared against the known experimental outcomes. Finally, we must mention that there is a discrepancy, the one emerges from the comparison between some of the extant theoretical predictions against the experimental outcomes. Here we discuss also the possibility that the solution to this discrepancy could be given by the Zaremba–Nikuni–Griffing formalism.

II. MEAN FIELD THEORY AND SPEED OF SOUND IN A BEC

Our starting point is the \(N\)-body Hamiltonian operator, in addition we assume that the collisions in the gas are, mainly, two–body interactions, this result is a consequence of the fact that we introduced, as additional condition, a dilute gas \([9]\). Under these restrictions the aforementioned Hamiltonian reads

\[
\hat{H} = -\frac{\hbar^2}{2m} \sum_{\alpha, \beta} \langle \alpha | \nabla^2 | \beta \rangle \hat{a}^\dagger_\alpha \hat{a}_\beta
\]

\[
\frac{1}{2} \sum_{\alpha, \beta, \gamma, \epsilon} \langle \alpha, \beta | V|\gamma, \epsilon \rangle \hat{a}^\dagger_\alpha \hat{a}_\beta \hat{a}_\gamma \hat{a}_\epsilon 
+ \sum_{\alpha} \langle \alpha | V(\vec{r})|\beta \rangle \hat{a}^\dagger_\alpha \hat{a}_\beta. \tag{1}
\]

In this last expression we have the following terms

\[
\langle \alpha \rangle \langle \nabla^2 | \beta \rangle = \int u^*_\alpha(\vec{r})\nabla^2 u_\beta(\vec{r}) d^3r, \tag{2}
\]

\[
\langle \alpha, \beta \rangle V|\gamma, \epsilon \rangle = \int u^*_\alpha(\vec{r}) u^*_\beta(\vec{r}) V(\vec{r}) u_\gamma(\vec{r}) u_\epsilon(\vec{r}) d^3r \tag{3}
\]

\[
\langle \alpha | V(\vec{r})|\beta \rangle = \int u^*_\alpha(\vec{r}) V(\vec{r}) u_\beta(\vec{r}) d^3r. \tag{4}
\]

Here \(V(\vec{r})\) denotes the two–body potential, whereas \(V(\vec{r})\) depicts the trapping potential. Clearly, we have, explicitly, assumed that only two–body interactions are relevant for our case. An explanation for this approximation is related to the fact that the systems employed in condensation are always, sufficiently, dilute. Let us explain this fact; usually, particle separations, in the case of alkali atom vapours, have an order of magnitude of, approximately, \(10^2 nm\), whereas, the scattering length (here denoted by \(a\)) is two orders of magnitude smaller, \(a \approx 100 a_0\), being \(a_0\) the Bohr radius \([13]\). These comments entail that an \((n + 1)\)-body collision is less probable than an \(n\)-body collision, i.e., we may keep only two–body collisions.

At this point no restriction upon the two–body interaction has been imposed. The next step, in this direction, concerns the introduction of some of the postulates of MFT. Indeed, the assumption of very low temperature implies that the \(s\)-wave approximation can be used and the interatomic potential can be described by the so–called pseudo–potential. At low temperatures one of the features of two–body interactions is the emergence of the concept of scattering length as a fundamental idea \([13]\). This last comment does not allow us to evaluate (3). Indeed, we must know the set of single–particle functions, i.e., \(\{u_\beta(\vec{r})\}\). It has to be stressed that the introduction of single–particle wavefunctions in (1) already implies the introduction, at least partially, of MFT. This last assertion can be understood noting that MFT assumes that the \(n\)-body symmetrized wavefunction can be replaced by a 1–body case where the bridge between these two cases is given by the deduction (via a mini–mization process stemming from the Gibbs–Bogoliubov–Feynmann equation) of a set of single–particle wavefunctions which lead to the definition of the so–called Mean Field Hamiltonian \([11]\).

In the context of the calculations about the speed of sound in BEC usually two choices are made, namely, (i) The eigenfunctions of a three–dimensional harmonic oscillator \([8]\); (ii) Free particle wavefunctions \([9]\). These choices are made without checking if they correspond to the minimum required by the Gibbs–Bogoliubov–Feynmann formalism. Of course, the first choice, for the case of a BEC trapped by a three–dimensional harmonic oscillator, seems to be a good conjecture since it reflects the symmetry of the trap.

III. SPEED OF SOUND AND NON–VANISHING TEMPERATURE

In the present work our trap will be an isotropic three–dimensional harmonic oscillator (with a frequency equal to \(\omega\)) and the corresponding eigenfunctions will be our choice for single–particle wavefunctions to be introduced in \([11]\). Since we consider the limit of very low temperatures we assume that only the first excited state is populated. In other words, ground state and first excited state are the only states populated. For an ideal BEC (no interactions among the particles of the gas) the number of particles in excited states (for temperatures below the condensation temperature) is a function of the trapping potential, namely, \(N_e = N \left[1 - \left(\frac{T_c}{T_c}\right)^6\right]\), here the poten-
potential is represented by $\alpha$ [13]. If we consider the presence of repulsive two–body interactions, then the number of particles in the ground and first excited state, $N_0$ and $N_e$, respectively, for temperatures below the condensation temperature ($T_c$), are given by

$$N_0 = N \left[ 1 - \left( \frac{T}{T_c} \right)^3 + \frac{8}{3} \sqrt{\frac{a^3 N}{V \pi}} \right]. \quad (5)$$

$$N_e = N \left[ \left( \frac{T}{T_c} \right)^3 - \frac{8}{3} \sqrt{\frac{a^3 N}{V \pi}} \right]. \quad (6)$$

In this last expression $a$ denotes the scattering length, and $V$ the volume of the BEC. In the present case, in which there is no container of volume $V$, but a trap confines the gas, the definition of $V$ requires a sound explanation. In this context we recall that a one–dimensional harmonic oscillator, whose frequency reads $\omega$, acting upon a quantum particle of mass $m$ defines a length parameter

$$l = \sqrt{\frac{\hbar}{m\omega}}. \quad (7)$$

The ground state wavefunction reads

$$\psi(x) = \sqrt{\frac{1}{l \sqrt{\pi}}} \exp\{-\frac{x^2}{2l^2}\}. \quad (8)$$

The size of this one–dimensional system will be defined by the value $x = x_1$ such that $\psi(x_1) = \psi(x = 0)e^{-1}$, i.e., $x_1 = 2l$.

Under these conditions a three–dimensional system has a volume given by [11]

$$V = 2^{3/2}l^3. \quad (9)$$

With these arguments we now proceed to calculate [11].

The first term to be addressed involves the kinetic energy. In order to do this we cast the operator $\hat{p}^2$ as a function of the creation and annihilation operators [14]

$$\frac{\hat{p}^2}{2m} = \frac{\hbar \omega}{4} \left[ \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger - (\hat{a}^\dagger)^2 - (\hat{a})^2 \right]. \quad (10)$$

The corresponding term $<\alpha|\nabla^2|\beta>$ has to be calculated over all the possibilities for $\alpha$ and $\beta$. Since, by hypothesis, we have assumed that only the ground and first excited states are populated, then $<\alpha|\nabla^2|\beta>$ does not vanish if and only if the following two conditions are fulfilled: (i) $\alpha$ or $\beta$ represent the ground or first excited states; (ii) $\alpha = \beta$. This is no new restriction. Indeed, according to the rules that the annihilation and creation operators satisfy notice that $<\alpha|\hat{a}^\dagger \hat{a}|\beta> = \gamma \delta_{(\alpha+1, \beta-1)}$, where $\gamma$ is a real number. It is readily seen that this last expression does not vanish if the following two conditions are fulfilled: (i) $\gamma \neq 0$, and (ii) $\alpha - 1 = \beta + 1 \Rightarrow \alpha = \beta + 2$. This last conclusion entails, since only the ground and first excited states are populated, that $<\alpha|\hat{a}^\dagger \hat{a}|\beta> = 0$ if $\alpha \neq \beta$. These arguments allow us to deduce, very easily, that if $|\psi_N>$ denotes the wave function of our $N$–body system then

$$<\psi_N|\frac{\hat{p}^2}{2m}|\psi_N> = \frac{3\hbar \omega}{4} N_0 + \frac{5\hbar \omega}{4} N_e. \quad (11)$$

Resorting to [11] we may cast this last expression in the following form

$$<\psi_N|\frac{\hat{p}^2}{2m}|\psi_N> = \frac{3\hbar \omega}{4} N \left[ 1 - \left( \frac{T}{T_c} \right)^3 + \frac{8}{3} \sqrt{\frac{a^3 N}{V \pi}} \right]$$

$$+ \frac{5\hbar \omega}{4} N \left[ \left( \frac{T}{T_c} \right)^3 - \frac{8}{3} \sqrt{\frac{a^3 N}{V \pi}} \right].$$

This last result provides us with an expression that shows a temperature dependence, for the case in which $T \leq T_c$. We now consider [11]. In the calculation of this term we will assume that the involved particles are in the ground state. Clearly, energy has to be conserved. This condition entails that if we denote by a superindex the values of the occupation numbers before and after the collision, $b$ and $a$, respectively, then energy conservation entails for our two involved particles

$$\sum_{i=1}^{2} \left[ n_{x}^{(i)} + n_{y}^{(i)} + n_{z}^{(i)} \right] =$$

$$\sum_{i=1}^{2} \left[ n_{x}^{(b)} + n_{y}^{(b)} + n_{z}^{(b)} \right]. \quad (13)$$

In the case in which the eigenfunctions of single–particle are the free–particle functions, the evaluation of the corresponding integral is done resorting to momentum conservation [9]. In this direction we find our sought term

$$<0, 0|V|0, 0> = \frac{32}{\sqrt{\pi} \lambda^3} \int_0^{\infty} r^2 V(r) \exp\{-\frac{r^2}{\lambda^2}\} dr. \quad (14)$$

Here $r$ denotes the relative distance between the involved particles. This last expression leads us to the definition of the concept of scattering length

$$a = \frac{m}{4\pi \hbar^2} \int_0^{\infty} r^2 V(r) \exp\{-\frac{r^2}{\lambda^2}\} dr. \quad (15)$$

The usual situation is proportional to the integral of the interaction potential [13]. We now deduce the energy
of this system, as a function of the temperature, in the usual manner \[1\]

\[E(T) = \frac{3h^2}{2mV^{2/3}}N \left[ 1 - \left( \frac{T}{T_c} \right)^3 + \frac{8}{3} \sqrt{\frac{a^3N}{V\pi}} \right] + \frac{5h^2}{2mV^{2/3}}N \left[ \left( \frac{T}{T_c} \right)^3 - \frac{8}{3} \sqrt{\frac{a^3N}{V\pi}} \right] + \frac{2\pi a h^2}{mV} N^2 \left[ 3 - \frac{4}{3} \sqrt{\frac{a^3N}{V\pi}} \right]. \tag{16}\]

The pressure \(P(T)\) reads

\[P(T) = \frac{kT}{mV^{2/3}}N + \frac{2h^2}{3mV^{2/3}}N \left[ \left( \frac{T}{T_c} \right)^3 - \frac{17}{3} \sqrt{\frac{a^3N}{V\pi}} + \frac{2\pi a h^2}{mV} N^2 \left[ 3 - \frac{2}{3} \sqrt{\frac{a^3N}{V\pi}} \right] \right]. \tag{17}\]

The speed of sound \((c_s(T))\) is given by

\[c_s^2(T) = \frac{5h^2}{3mV^{2/3}} + \frac{10h^2}{3mV^{2/3}} \left[ \left( \frac{T}{T_c} \right)^3 - \frac{68}{15} \sqrt{\frac{a^3N}{V\pi}} + \frac{4\pi a h^2}{mV} N \right]. \tag{18}\]

**IV. DISCUSSION AND CONCLUSIONS**

Our last expression allows us to predict the speed of sound, as a function of the temperature, of course, this happens only in the regime \(T \leq T_c\). Notice that our prediction does not include a dependence upon the amplitude of the disturbance, a fact that matches with the experimental output \[7, 13\].

It has already been recognized that many theoretical studies, in the realm of BEC, ignore the role that the thermally excited atoms play in the definition of the characteristics of the gas \[6\]. The assumption of vanishing temperature is not correct, as a matter of fact thermodynamics tells us that in a practical sense the achievement of this temperature is impossible \[10\]. Therefore, the deduction of the speed of sound under the assumption of \(T = 0\) is an approximation, the one should be improved. A point that has to be underlined in the present manuscript concerns this issue. Indeed, a fleeting glimpse at \[12\] tells us that the second term on the right-hand side takes into account the contribution to the kinetic energy of the thermal cloud of the system as a function of the temperature, i.e., we do not assume \(T = 0\).

In the context of the assumptions here accepted, of course, we have, as mentioned before, discarded the possibility of having, in this kinetic term, transitions between excited states and the ground state. In order to have this case we must consider that not only the first excited state is populated, but also higher states. From this last comment we expect a very small contribution to the speed of sound stemming from this neglected possibility. An additional simplification has been introduced, but now in relation with \[13\]. If we consider \[14\], we, immediately, notice that we have only considered interactions between particles in the ground state with particles in the same state. Of course, more possibilities are present, for example, a particle in the ground state might interact with a particle in the first excited state. Since the number of particles in the ground state is much larger than those in excited states we expect that the probability of having a ground state–ground state interaction is larger than having a ground state–first excited state interaction, and this last one is larger than the first state–first state interaction. In this sense has to be understood the assumption.

Let us now confront our theoretical prediction against the extant experimental results. We will consider the case of a BEC comprised by sodium atoms. This choice is done since we have already experimental results in this direction; \(N = 5 \times 10^6\), \(n = 10^{12} m^{-3}\), \(T_c = 2 \times 10^{-6} K\), \(m = 2.02 \times 10^{-27} Kg\), \(l \sim 10^{-2} m\) \[15\]. Finaly, the scattering length, for sodium, has already been measured \[16\], namely, \(a = 0.75 \times 10^{-2} m\). We need also an assumption for our temperature, here we assume \(T = 0.9T_c\). These values imply

\[c_s = 2.2 \times 10^{-3} m/s. \tag{19}\]

A careful look at the present measurement outputs entails that our result is not a bad one \[13\], i.e., it provides the correct order of magnitude. The shortcomings of the present manuscript, at least in the realm of its compatibility with the experimental results, are also shared by other approaches \[15, 18\]. The most intriguing interrogant in this sense is related to the fact that in the region of the thermodynamical space in which the assumption of MFT is strongly satisfied the theoretical prediction has its worst behavior \[18\]. Several conjectures could be put forward, in order to solve this puzzle. The inclusion of additional terms, for instance, in connection with the discussion about the number of significant terms related to \(E\) would, surely, modify the result. In this direction an alternative way is related to the deduction of the speed of sound resorting to the generalized Gross–Pitaevski equation (usually known as Zaremba–Nikuni–Griffin equation (ZNG) \[6\]) the one takes into account a coupling between the condensate and non–condensate components of the corresponding system. A physical motivation behind this statement can be found in the fact that sound can be understood as density waves. Clearly, changes in the density, which involve changes in the separation among particles, are determined by the interactions among the constituents of the gas. This explains in a very simple way why the idea of interaction plays a relevant role in the determination of the speed of sound. The ZNG equation \[6\] includes in the dynamics of a BEC a coupling between the condensate and the noncondensate part of
the gas. We may rephrase this last conjecture asserting that one of our assumptions, namely, \textit{no interaction between condensate and noncondensate components} could define a wrong premise in this context. In other words, the present approaches render the correct order of magnitude for this speed, but finer details involved in the correct deduction of it could stem from the use of the ZNG equation.

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