Temperature dependent shifts in collective excitations of a gaseous Bose-Einstein condensate

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The moment method is applied to the quantum theory for a trapped dilute gas, obtaining equations for the evolution of the cloud. These equations proof the existence of undamped oscillations in a two-dimensional harmonic trap with radial symmetry. In all other cases we can, with physically reasonable approximations, solve the equations and find the frequencies of the collective modes for all temperatures, from the pure Bose-Einstein condensate up to the normal gas.

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Ever since the first achievement of a weakly interacting Bose-Einstein condensate in laboratory [1, 2, 3], one of the basic tools for its study were the oscillation modes of the condensed cloud [1, 4]. The measure of the frequencies of these oscillations at very low temperatures, and the comparison with several theoretical predictions [1, 2] were the first important backing to the Gross-Pitaevskii equation, the mean-field model which describes the condensed cloud in the zero temperature limit.

Since those first works, there has been a growing interest on the study of the intermediate regimes, which are far from the zero temperature limit and closer to the critical temperature $T_c$ at which condensation begins. For $T > 0.5 T_c$ the collective modes of the three-dimensional condensate suffer both a frequency shift and a strong damping [3]. These deviations from the mean field theory are due to the uncondensed or normal component of the gas. The role of the thermal cloud has been partially explained using self-consistent solutions of the many-body theory for the condensate [4, 5], theory of relaxation phenomena, linear response theory, etc [See Ref. [6] for a list of references]. Nevertheless the theoretical and experimental studies of these excitations and of their damping are far from complete, and although the sum of all works gives some insight into the behavior of the dilute gas, there is no macroscopic theory which systematically predicts both the finite temperature shifts and the damping of the excitations.

In this work we attempt a different approach to the study of collective modes. Our goal is not to consider the condensed and normal components separately, but to treat the system as a whole. We will start from first principles, studying the quantum Hamiltonian of the dilute gas and deriving equations for a few relevant observables: the widths of the cloud, the kinetic energy on each direction, etc. We will prove that these equations close exactly in the two-dimensional case with radially symmetric trap. This exact closing reveals the existence of undamped radial excitations of the cloud, with a universal frequency $\omega_{2D} = 2 \omega$ which is twice the frequency of the trap. In the last part of this work we will return to the moment equations for arbitrary geometry and we will close them using a reasonable approximation for the interaction energy as a function of the widths. With this hypothesis the dynamical equations can be solved, giving us the temperature dependence of the excitation frequencies in the cloud as a whole. Finally this dependence is compared to other works [3] and to experiments [4].

The model.- The theory for a dilute gas of bosons in a harmonic confinement is developed up from a simple Hamiltonian

$$
\hat{H} = \int \Psi(x)^\dagger \left(-\frac{\hbar}{2m} \Delta + V(x, t)\right) \Psi(x) d^n x \\
+ \int \frac{U}{2} \Psi(x)^\dagger \Psi(x)^\dagger \Psi(x) \Psi(x) d^n x.
$$

(1)

The trapping potential $V(x, t) = \frac{1}{2} \sum \omega_i(t)^2 x_i^2$, may have any symmetry, and it may be even subject to time dependent perturbations. The coupling constant $U = 4 \pi \hbar^2 a / m$ measures the interaction among bosons in terms of the $s$-wave scattering length $a$ and the contact interaction $V_{\text{bosons}}(x, y) = a \delta(x - y)$. Finally, the Hamiltonian has an important hidden parameter which is the dimensionality of the space, $n \in \{1, 2, 3\}$, and that has a crucial role on the behavior of the cloud.

The Hamiltonian $\hat{H}$ must be understood as an operator on a Fock space, where the creation and destruction operators obey the commutation rules

$$
[\Psi(x), \Psi^\dagger(y)] = \delta(x - y), \quad [\Psi(x), \Psi(y)] = 0.
$$

(2)

Below a critical temperature, $T_c$, the dilute gas experiences a phase transition which leads to a macroscopic population of the ground state of $\hat{H}$. By neglecting the number of atoms in the thermal cloud one may approximate $\Psi(x) \simeq \sqrt{N} \phi(x) + \delta \Psi(x)$, where $N$ is the total number of particles of the cloud. The c-number $\phi(x)$ constitutes the order parameter of a mean-field theory, and it obeys the so-called Gross-Pitaevskii equation

$$
i \partial_t \phi(x, t) = \left(-\frac{\hbar}{2m} \Delta + V(x, t) + U N |\phi|^2 \right) \phi(x, t).
$$

(3)
the normal modes, or by performing a numerical study of particles, the trapping strength and of the number of particles in the condensate, has been sometimes explained by changing the effective number of particles. This shift has been referred to as a strong, temperature dependent shift [11].

The word "moment" in this context refers to the expected value of an observable. We will apply an equivalent technique to the study of Bose-Einstein condensates and in the study of nonlinear Schrödinger equations in general [12, 13].

The moment equations.- The word “moment” in this context refers to the expected value of an observable. If we work with the mean-field theory these moments are calculated by averaging over the order parameter. For instance the center of mass of the condensed cloud is

$$\mathbf{X} = \langle \mathbf{x} \rangle = \int \phi(\mathbf{x}) \mathbf{x} \phi(\mathbf{x}) d^nx$$

and it follows an equation which is exact, \( \dot{X}_i = -\omega_i(t)^2 X_i \). These equations and similar ones for other expected values are powerful tools both in the study of Bose-Einstein condensates and in the study of nonlinear Schrödinger equations in general [12, 13].

We will apply an equivalent technique to the study of the quantum Hamiltonian \( \hat{H} \). First of all we adimensionalize \( \hat{H} \), using as fundamental units the transverse frequency of the trap, \( \omega_\perp = \sqrt{\omega_z^2 \omega_y^2} \), and the radial size of this trap, \( a_0 = h/\sqrt{m \omega_\perp^2} \). This way, the Hamiltonian becomes, up to a global factor,

$$\hat{H} = \int \Psi(\mathbf{x})^\dagger \left[ -\frac{i}{2} \Delta + \sum_i \frac{i}{2} \omega_i(t)^2 x_i^2 \right] \Psi(\mathbf{x}) d^n x + \int \frac{g}{2} \Psi(\mathbf{x})^\dagger \Psi(\mathbf{x}) \Psi(\mathbf{x}) d^n x,$$

where \( \omega_i = \omega_i(\omega_\perp) \) and \( g = 4\pi a_0/a_0 \). Next we define a set of one-particle operators

$$\hat{X}_i = \int \Psi(\mathbf{x}) x_i \Psi(\mathbf{x}) d^n x,$$

$$\hat{P}_i = \int \Psi(\mathbf{x}) (-i \nabla_i) \Psi(\mathbf{x}) d^n x,$$

$$\hat{W}_i = \int \Psi(\mathbf{x}) x_i^2 \Psi(\mathbf{x}) d^n x,$$

$$\hat{B}_i = \int \Psi(\mathbf{x}) (-i x_i \partial_t) \Psi(\mathbf{x}) d^n x,$$

$$\hat{K}_i = -\frac{1}{2} \int \Psi(\mathbf{x}) \partial_i^2 \Psi(\mathbf{x}) d^n x,$$

$$\hat{J} = \int \frac{g}{2} \Psi(\mathbf{x}) \Psi(\mathbf{x}) \Psi(\mathbf{x}) \Psi(\mathbf{x}) d^n x,$$

$$\hat{F}_i = \frac{ig}{2} \int \left[ \partial_i \Psi(\mathbf{x}) \right]^2 \Psi^2 - (\Psi)^2 \partial_i \Psi^2 \right] d^n x.$$  

In these equations \( \partial_i \) represents a derivative with respect to \( x_i \). From top to bottom, we have defined the center of mass, its moment, the width of the cloud, the rate of change of the width, the kinetic energy along the \( t \)-th direction, the interaction energy and the rate of change of \( J \) along the \( i \)-th axis.

We use the Heisenberg picture to study the evolution of these operators. In this image the density matrix of the system dictates some initial conditions, \( \rho \), and the time evolution is carried by the observables. Thus, any observable \( \hat{A} \) without explicit time dependence follows the simple equation, \( i\hbar \frac{d}{dt} \hat{A} = [\hat{A}, \hat{H}] \), and its expected value is simply \( \langle \hat{A} \rangle \equiv \text{Tr}(\hat{A}(t) \rho) \).

The first and most important equation is that of the destruction or creation operators,

$$i \partial_t \Psi(x) = \left[ -\frac{i}{2} \Delta + \sum_i \frac{i}{2} \omega_i(t)^2 x_i^2 + U \Psi \right] \Psi.$$  

Combining Eqs. (6) and (7), and using the fact that our operators lack an explicit time dependence, we find the equations for the center of mass

$$\frac{d^2 \mathbf{X}}{dt^2} = -\omega_i(t)^2 \mathbf{X},$$

plus a new set of equations for the widths

$$D_i \dot{W}_i = B_i,$$

$$D_i \dot{B}_i = 4K_i - 2\omega_i(t)^2 W_i + 2J,$$

$$D_i \dot{K}_i = -\frac{i}{2} \omega_i(t)^2 B_i - F_i,$$

$$D_i \dot{J} = \sum_i F_i,$$
where $D_t$ denotes derivative with respect to time.

The first important remark is that Eqs. (3)-(6) are all exact and describe the evolution of one-particle operators. Nevertheless, one may now take expected values around all terms in Eqs. (3), (4) and the same equations will hold for the expected values

$$X = \langle X \rangle = \text{Tr} \{ \hat{X} \rho \},$$

(10)

which is on what we focus from now on. The second remark is that there are less equations than moments, which seems to prevent us from completely determining the behavior of the cloud for arbitrary conditions.

**Undamped oscillations.**—There is an important situation in which the moment equations may be solved, and that is a two-dimensional condensate in a radially symmetric trap, \( n = 2, \omega_1 = \omega_2 = \omega \). In this geometry we define a total width, \( \tau = \sqrt{W_1 + W_2} \), and obtain the following equation

$$\frac{d^2 \tau}{dt^2} = -\omega(t)^2 \tau + \frac{2M}{\tau^3}.$$  

(11)

This equation includes a conserved quantity

$$M = (K_1 + K_2 + J)(W_1 + W_2) - \frac{1}{8}(B_1 + B_2)^2,$$  

(12)

that must be determined up from the initial conditions.

In the case of an static trap, the equation for the width has an equilibrium point given by \( R = 2M/\omega^2 \). The oscillations around this point have a proper frequency, \( \omega_{2D} = 2\omega \), which is independent of the shape of the cloud. Therefore, the cloud may be at any temperature and bear excitations of any multipolarity, but the total width of the cloud will always oscillate with the universal frequency \( \omega_{2D} \) of the monopole mode.

Furthermore, since Eq. (11) is exact and it is conservative, any perturbation of the width of the two-dimensional condensate persist eternally, and the damping of these oscillations can only be explained in terms of higher order contributions to \( H \), such as three- and four-body collisions, interaction with the environment and anharmonicities of the trap.

One may compare Eq. (11) with a similar equation arising from scaling arguments [13]. Those arguments are based on a symmetry of Eq. (7) such that it admits infinite many rescaled solutions

$$\Psi(x, \tau) = \frac{1}{\lambda} \Psi_0(x/\lambda, t) e^{-ix^2 \lambda/(2\lambda)},$$  

(13a)

$$\tilde{\lambda} = -\omega(t)^2 \lambda + \lambda^{-3}, \quad \tilde{\tau} = \lambda^2,$$  

(13b)

for any given solution \( \Psi_0(x, t) \). The parameter \( \lambda \) can thus be related to the width of the cloud, but the problem with scalings is that they implicitly assume a certain type of evolution for the operator, while Eq. (11) makes no such ansatz and it includes further information about final shape of the collective mode, thanks to \( M \).

**Asymmetric traps.**—We now want to study other dimensionalities and other geometries of the trap. An inherent limitation in the study of the moments is that these hierarchies rarely give us closed equations. One must, at some point make a reasonable approximation to estimate some of the unknowns and get a tractable model. Roughly, we will assume that the self-interaction energy is inversely proportional to the effective volume of our \( n \)-dimensional cloud, \( V = (\Pi_i W_i)^{1/2} \), with a constant \( J_0 \) that depends on the initial data:

$$J \approx J_0(\Pi_i W_i)^{-1/2}, \quad F_i \approx -\frac{J}{2}B_i/W_i.$$  

(14)

With Eq. (14) we can close the moments hierarchy, obtaining \( 2n \) differential equations for \( 2n \) moments

$$\begin{align*}
\frac{d^2 x_i}{dt^2} &= -\omega_i(t)^2 x_i + \frac{2M_i}{x_i^3} + \frac{J}{x_i}, \\
\frac{dM_i}{dt} &= J dx_i^2 dt,
\end{align*}$$

(15a)

(15b)

with three new variables \( M_i = K_i W_i - \frac{1}{8}B_i^2 \).

The motivation for the ansatz (14) is multiple. First it arises from scaling considerations. If we assume that \( \{W_1 \ldots W_n\} \) are the only independent variables of our model, and we rescale our model according to \( x_i \rightarrow \lambda_i x_i \), the destruction operator, the widths and the interaction change as \( \Psi \rightarrow \Psi/\Pi_i \lambda_i, \quad W_i \rightarrow \lambda_i^2 W_i \), and \( J \rightarrow J/\Pi_i \lambda_i \), which immediately leads to Eq. (14).

The other motivation for Eq. (14) is that it works in the mean field theory too. Making simulations of Eq. (3) with wave functions of almost any reasonable shape, it is readily seen that \( J_0 \) is conserved up to a 10%, and even in the worst cases the model equations (13a)-(13b) are extremely accurate [12].

**Collective modes.**—Eqs. (15a)-(15b) model the evolution of the widths of a dilute gas at any temperature. They do not make any distinction between condensed and normal components and the role of temperature is to change the equilibrium values of \( M_i \) and \( J \). In order to study the collective modes of the condensate it is easier to go back to Eqs. (4)-(7) and linearize around the equilibrium points \( \{W_i, B_i, K_i, J\} \). To first order in the small variables \( \{w_i, b_i, k_i\} \), with the ansatz (14), we get

$$\begin{align*}
\dot{w}_i &= b_i, \\
\dot{b}_i &= 4k_i - 2\omega_i^2 w_i - \sum_j \frac{J}{W_j} w_j, \\
\dot{k}_i &= -\frac{1}{2\omega_i^2} b_i + \frac{J}{2W_i} b_i.
\end{align*}$$

(16a)

(16b)

(16c)

There are two important limits in these equations. In the ideal gas limit the interaction energy can be neglected, \( J = 0 \). This means that each width decouples from the rest, and that there are three normal modes which oscillate with frequencies \( \nu_i = 2\omega_i \). In the the
Thomas-Fermi limit we rather assume $K_t \ll J$ and just keep the interaction energy and the trap. Then the equilibrium point is given by $J = \omega_i^2 W_i$. For a three-dimensional trap with axial symmetry, $\omega_1 = \omega_2 = 1$, $\omega_3 = \gamma$, the excitation frequencies become
\begin{equation}
\nu_i^2 = 2, \quad \nu_i^2 = 3/2 \gamma + 2 \pm 1/2 \sqrt{9\gamma^2 - 16\gamma + 16},
\end{equation}
in full agreement with \cite{9}. The first frequency corresponds to a $m = 2$ mode in which the $w_x$ and $w_y$ widths oscillate with opposite phases. The second two frequencies correspond to two $m = 0$ modes such that the transverse shape of the condensate is preserved and $w_x = w_y$. There are also three Goldstone modes, $\nu = 0$, which arise from the scaling symmetry of Eq. (8).

**Temperature dependent frequencies.** If we now focus on the temperature, the ideal gas limit and the Thomas-Fermi limit qualitatively describe the $T \geq T_c$ and $T = 0$ limits, respectively. In between these extremes the amount of condensed and normal clouds vary, inducing changes on the values of $\{W_i, J\}$ which cause a continuous evolution of the oscillation frequencies, from $\{2\omega_1\}$ to values which are close to Eq. (17).

In the radially symmetric case, Eq. (16) gives us two different oscillation frequencies
\begin{equation}
\nu_{-2} = \omega \sqrt{4 - 2P}, \quad \nu_{+} = \omega \sqrt{4 + 2P},
\end{equation}
where $P = J/(\omega R^2)$ depends on the actual shape of the cloud. A crude estimate for the interaction energy \cite{10} assigns $P = 1$ and $P = 0$ for the $T = 0$ and $T = T_c$ limits. In between these limits the interaction energy is supposed to scale as $P = (N_0/N)^{2/5} = (1 - t^3)^{2/5}$, where $N_0$ is the number of particles in the condensate, and $t = T/T_c$ is the temperature relative to the phase transition due to the Bose-Einstein condensation \cite{10}. This oversimplified model provides the same frequencies as a condensed cloud with $N_0$ particles and no thermal cloud, and it agrees well with self-consistent calculations in the Popov theory \cite{10}.

As an example, in Figure 1(a) we plot the oscillation frequencies as a function of the relative temperature, $t$, for a spherically symmetric trap. Better estimates of the excitation frequencies require better estimates of the functions $\{J(T), W_i(T)\}$. That task is significantly simpler than full calculations of the excitation spectrum for $N$ particles, but it is yet an open problem.

Finally we have compared our predictions with the experimental results of D. S. Jin et al. \cite{4}. The only difference is on the quadrupolar excitations, $\nu_2(t)$, whose experimental frequency seems to decrease when the temperature increases. This point was already noticed in \cite{7} but now it becomes evident that the deviation could be due to studying the width of the condensate and of the thermal cloud separately. We believe that this apparent contradiction deserves further experimental investigation, preferably by studying the oscillations in clouds with more atoms and various geometries.

**Summary and discussions.** We have studied the collective modes of a trapped dilute gas. By computing the evolution of several operators, we have obtained differential equations for the center of mass and the widths of the cloud. In the two-dimensional case with radially symmetric trap we have predicted the existence of undamped oscillations of the radial width with frequency $\omega_{2D} = 2\omega$ twice the frequency of the trap. This prediction can be confirmed in current experiments \cite{14}.

For other symmetries and dimensionalities we recovered both the Thomas-Fermi limit and the ideal gas limit. We also combined a thermodynamical estimate of the interaction energy with our dynamical equations to obtain the temperature dependence of the collective modes in various traps, with similar results as previous numerical works \cite{13} and experiments \cite{14}.

This work offers new techniques that can be applied to the study of trapped dilute gases in general and to Bose-Einstein condensation in particular. We suggested a new way to perform experiments, by studying the gas cloud as a whole, and we also offered a simple way to relate the normal modes of the cloud to the interaction energy of the gas, without the need to perform difficult self-consistent calculations. Finally, with our analysis it becomes clear why simple models such as scalings \cite{13} have been so useful in analyzing current experiments.

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