Optical excitations in a non-ideal Bose gas

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September 20, 2018

Optical excitations in a Bose gas are demonstrated to be very sensitive to many-body effects. At low temperature the momentum relaxation is provided by momentum exchange collisions, rather than by elastic collisions. A collective excitation mode forms, which in a Boltzmann gas is manifest in a collision shift and dramatic narrowing of spectral lines. In the BEC state, each spectral line splits into two components. The doubling of the optical excitations results from the physics analogous to that of the second sound. We present a theory of the line doubling, and calculate the oscillator strengths and linewidth.

PACS:

Recent experiments on the Bose-Einstein condensation in magnetically trapped gases \(^{12,13,14}\) stimulated studies of many-body phenomena in such systems. Collective excitations of several kinds \(^{13}\) have been investigated, including density waves \(^{14}\) and the second sound \(^{5}\), excited by shaking the trapped BEC samples, or by an abrupt change of the interaction between particles \(^{14}\). All these responses are of hydrodynamical character, with the excitation frequencies being not much greater than the trap frequency, and the wavelengths of order of the sample dimension.

Optical excitations are also sensitive to the nature of quasiparticles and interactions between them. However, quasiparticles in a weakly non-ideal Bose gas, according to Bogoliubov theory, differ from free particles only at very low temperatures \(^{11}\): \(T_B = (4\pi\hbar^2/m)aN \ll T_{\text{BEC}}\), where \(N\) is the gas density, and \(a\) is the \(s\)-wave scattering amplitude. In this letter we describe the many-body phenomena resulting from a change of the particle internal state due to optical transition. We shall see that these many-body effects can be significant even at temperatures as high as \(T \sim T_{\text{BEC}}\), such that the difference of the quasiparticles and particles plays no role.

The reason for the optical excitations being special is that the excited particle spends a long time in the state which is a coherent superposition of the ground state and the excited state. This time, which is of order of the inverse spectral line width, can be very long, so that the excited particle, while being in the superposition state, interacts with many other particles. The collisions of particles in different but non-orthogonal internal states have special properties, first discussed in the context of the problem of spin excitations in gases \(^{13,13,14}\) (see also the work on collision frequency shifts in cesium fountains \(^{14}\)).

Let us consider a gas of identical atoms, all in the ground internal state \(|1\rangle\). Suppose that one of the atoms is transferred to a superposition state \(|1\rangle'\), having finite overlap with the ground state: \(|1\rangle' = \alpha|2\rangle + \beta|1\rangle\). Generally, there are three different kinds of collisions between this atom and other atoms: (i) ordinary elastic collisions, occurring with the frequency \(\tau^{-1}_{\text{el}} = v_T a_{12}^2 N\), where \(v_T = (2T/m)^{1/2}\) is thermal velocity, and \(a_{12}\) is the scattering length; (ii) forward collisions, in which the atoms interact without changing direction and velocity of motion; (iii) momentum exchange collisions, in which interacting atoms switch their trajectories and velocities. The forward and momentum exchange scattering rates are both given by \(\tau^{-1}_{\text{exch}} = 4\pi\hbar a_{12} N/m\), i.e. are temperature independent. Thus, at temperatures \(T \lesssim \hbar^2/m a_{12}^2\) the collisions (ii) and (iii) dominate.

In this regime, named quantum gas by Bashkin \(^{3}\), collective effects appear due to collisions of type (iii). Note that forward collisions (ii) affect the non-interacting particle picture only to the extent that they correct external potential seen by a particle by an amount proportional to the density of other particles. The role of the collisions (iii) is quite different. They provide mechanism of momentum transfer between different particles with the rate \(\tau^{-1}_{\text{exch}}\) much higher than that of energy relaxation. Thus, at times \(\lesssim \tau_{\text{exch}}\) the particles can exchange momenta many times without changing the overall energy distribution. As a result, all excitations in the system with wavelength greater than \(v_T^{-1} \tau_{\text{exch}}\), the path between momentum exchange collisions, become collective modes.

The collective phenomena in optical excitations arising due to momentum exchange collisions differ from those in the spin–wave dynamics \(^{3,13,14}\). The reason is that the interactions between atoms in different orbital states depend on the states, while for the atoms in different spin states all the interactions are the same.

Problem: We consider optical excitations in a Bose gas of uniform density \(N\). Each atom of the gas can be in the ground state or in the excited state (denoted by 1 and 2, respectively). The interaction constants \(\lambda_{ij}\), \(i,j = 1,2\) are related by the factor \(4\pi\hbar^2/m\) with the \(s\)-wave...
scattering lengths $a_{ij}$ ($a_{11} = a$).

The temperature range of interest, $T \leq \hbar^2/ma^2$, includes temperatures both above and below $T_{\text{BEC}}$. For the collective effects to be pronounced, the excitation wavevector $k$ should be $\leq (v_T \tau_{\text{exch}})^{-1}$, which means that $c|k| \ll \omega_0$, the excitation frequency. Thus, optimal situation is that of a two-photon excitation with the photons’ momenta equal and opposite.

For example, this is realized in the recent study of the BEC in spin-polarized hydrogen by using the $1S - 2S$ Doppler free transition [3]. In this experiment $k \approx 2\pi/w$, where $w$ is the width of the laser beam used to excite the $1S - 2S$ transition.

Below we study the excitation above and below $T_{\text{BEC}}$. We calculate the frequency shift and the linewidth of the excitation. In the analysis we ignore spin degrees of freedom of the gas, as well as the finite size of the gas sample confined in the trap. Thus, our results apply to the excitations probed near the central region of a shallow trap, such that the density is nearly uniform. Also, our treatment is restricted to not very low temperatures, $T > \hbar/\tau_{\text{exch}} \sim T_{\text{B}}$, where one can ignore the difference between free particles and Bogoliubov quasiparticles.

Summary of results: We show that the frequency of the excitation is shifted from that of a single atom by an amount different from the mean density shift. The reason for that is that the momentum exchange process couples different states degenerate in energy, and therefore, one has to apply degenerate perturbation theory to the many-body states to determine the correct frequency shift.

For the Boltzmann gas, $T > T_{\text{BEC}}$, by using the many-body version of the degenerate perturbation theory (the random phase approximation), we find the excitation frequency:

$$\omega_{1 \rightarrow 2}(k) = \omega_0 + 2(\lambda_{12} - \lambda_{11})N + \frac{\omega^2 k^2}{3\lambda_{12} N},$$

where the transferred momentum is assumed to be small in the sense discussed above: $|k| < \lambda_{12} N/v_T$. The resonance frequency at $k = 0$ varies linearly with density (see Fig.3). Such a behavior is observed in the experiment [3], and the magnitude of the shift is found to be in agreement with [4].

The linewidth of the excitation [1] due to momentum exchange collisions is found to be

$$\gamma_{\text{exch}} \simeq k v_T \ e^{-(\lambda_{12} N/k v_T)^2}.$$ 

(Elastic collisions contribute $\gamma_{\text{el}} \simeq \tau_{\text{el}}^{-1} \ll \gamma_{\text{exch}}$.) The abrupt narrowing [2] of the spectral line at high densities

$$N > k v_T / \lambda_{12}$$

is similar to the motional (Dicke) narrowing effect (see Fig.1). This is because each momentum exchange collision fully randomizes velocities, and so in the range [2] the collisions path, $v_T / \lambda_{12} N$, becomes smaller than the wavelength $2\pi/k$. Another way to put it is to draw an analogy with Mössbauer effect, i.e., to say that in the regime [3] the recoil momentum is transferred collectively to all of the atoms interacting with the excited atom while it is in phase with the excitation field.

Below $T_{\text{BEC}}$, the main change in the spectrum is that the spectral line splits into two components, both shifted from the single particle frequency $\omega_0$. At $k = 0$ the frequencies are given by

$$\omega_{1,2} = \omega_0 + (\lambda_{12} - 2\lambda_{11})N + X_{1,2},$$

$$(X_{1,2} - \lambda_{11} N)(X_{1,2} - \lambda_{12} N_T) = \lambda_{12}^2 N_c N_T,$$

where $N_c$ is the condensate density, and $N_T = N - N_c$ is the thermal density. The origin of the two frequencies [6] is that in the presence of the condensate the excited atom can be in two distinct states, “correlated” and “uncorrelated”. In the correlated state the kinetic energy of excited atom is $\sim T$, and so it participates in momentum exchange collisions which shift $\omega$ as discussed above. In the uncorrelated state, the velocity of the excited atom is zero, it does not take part in momentum exchange processes, and thus does not acquire the additional energy shift. Besides that, there are momentum exchange collisions which transfer the atom from the correlated to the uncorrelated state and backwards (see discussion below). The difference of the two frequencies [4] gives the frequency of coherent oscillations between the two states.

The behavior of the dispersion and the linewidth due to finite $k$ as a function of temperature and density is qualitatively similar to that above $T_{\text{BEC}}$ (see Figs.2,3).

Calculation The system is described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_{\text{ext}}:$$

$$\mathcal{H}_1 = \sum_p \frac{p^2}{2m} a_p^+ a_p + \sum_{p_1 + p_2 = p_3 + p_4} \frac{1}{2} \lambda_{11} a_{p_1}^+ a_{p_2}^+ a_{p_3} a_{p_4},$$

$$\mathcal{H}_2 = \sum_p \left( \frac{p^2}{2m} + \omega_0 \right) b_p^+ b_p + \sum_{p_1 + p_3 = p_2 + p_4} \lambda_{12} a_{p_1}^+ a_{p_2} b_{p_3}^+ b_{p_4},$$

$$\mathcal{H}_{\text{ext}} = \sum_{p, k} A_k e^{-i \omega t} b_{p+k}^+ a_p + \text{h.c.}$$

where $a_p$ and $b_p$ are canonical Bose operators for two internal states 1 and 2, $\omega$ is the laser frequency, and $A_k$ are Fourier components of the laser field. We ignore the interaction $\lambda_{22}$ of atoms in the excited state, since we are interested in the absorption at small laser power, when the density of excited atoms is negligible with respect to total density $N$.

As discussed above, the interesting regime is that of a (nearly) Doppler free two photon transition, $\vec{k} = \vec{k}_1 + \vec{k}_2$, $\omega = \omega_1 + \omega_2$, where $\omega \simeq \omega_0$ and $|\vec{k}| \simeq \lambda_{12} N/v_T \ll \omega_0/c$.

The absorption spectrum is expressed through the two-particle correlation function by Kubo formula:

$$\mathcal{I}(\omega) = \text{Im} \int_0^\infty e^{i \omega t} \left\langle \hat{C}(t) \hat{C}^+(0) \right\rangle \, dt.$$
\[ \tilde{C} = \sum_{p,k} A_p^* \tilde{n}_{p,k} , \quad \tilde{n}_{p,k} = b_{p+k} a_p^+ \]  

To evaluate the commutator in (8), we consider time evolution of the operators: \[ i\partial_t \tilde{n}_{p,k} = \left[ \tilde{n}_{p,k}, H_1 + H_2 \right] . \] In the situation of interest, when \( \tau_{el} \gg \tau_{exch} \), the commutator can be evaluated by the RPA procedure \[17\]. The resulting equations for \( \tilde{n}_{p,k}(t) \) are linear:  

\[ i\partial_t \tilde{n}_{p,k} = \Omega_{p,k} \tilde{n}_{p,k} + \lambda_{12} n(p) \sum_{p'} \tilde{n}_{p',k} , \]  

where  

\[ \Omega_{p,k} = \omega_0 + \frac{(p+k)^2}{2m} - \frac{p^2}{2m} + (\lambda_{12} - 2\lambda_{11}) N . \]  

To remind the reader how the RPA method works, consider the commutator  

\[ \begin{bmatrix} \tilde{n}_{p,k} , \sum_{p_1 + p_3 = p_2 + p_4} a_{p_1}^+ a_{p_2} b_{p_3}^+ b_{p_4} \end{bmatrix} = \sum_{p_1 + p_2 + k = p_2 + p_4} a_{p_1}^+ a_{p_2} b_{p_3}^+ b_{p_4} - \sum_{p_1 + p_3 = p_2 + p_4} a_{p_1}^+ a_{p_3} b_{p_4}^+ b_{p_2+k} \]  

In the first term, according to the RPA procedure, we keep only two kinds of contributions: with \( p_2 = p_1 \), and with \( p_2 \neq p_1 \). Correspondingly, this gives \( N \tilde{n}_{p,k} + n(p) \sum_{p'} \tilde{n}_{p',k} \), which is the part of (8) proportional to \( \lambda_{12} \). The second term in the commutator (9) is of order of the inverse volume of the system, and so it can be neglected. (The first and second terms in (8) are of different magnitudes because there is only one particle 2 in the systems, while particles 1 have finite density.)  

Solving the system (9), and plugging the result in (8), one gets the spectral power  

\[ \mathcal{I}(\omega) = \text{Im} \sum_k |A_k|^2 \frac{\Pi_0(k,\omega)}{1 - \lambda_{12} \Pi_0(k,\omega)} , \]  

where  

\[ \Pi_0(k,\omega) = \int \frac{n(p)}{\omega - \Omega_{p,k} + i0} \frac{d^3p}{(2\pi\hbar)^3} . \]  

The integrals in (11) over components of \( \vec{p} \) normal to \( \vec{k} \) are evaluated explicitly, and the integral over longitudinal component of \( p \) is evaluated as a Cauchy integral, yielding an infinite (but quickly converging) sum over poles in the complex \( p \) plane \[19\]. The resulting spectrum is shown in Fig. 1 for several increasing densities.  

To get the dispersion relation (11) one expands \( \Pi_0 \) in small \( \Delta \omega \): \( \Delta \omega \ll \omega \). The resulting dispersion (11), which is much stronger than that for a free atom, is a collective mode effect \[8,14\].  

To generalize the above calculation to the BEC situation, we introduce \( \tilde{n}_{0,k} = b_k \psi_0^* \), where \( \psi_0 \) is the condensate amplitude. In the RPA calculation the operator \( \tilde{n}_{0,k} \) is treated separately from other \( \tilde{n} \)'s. Now, the RPA dynamics is the following:  

\[ i\partial_t \tilde{n}_{0,k} = \Omega_{0,k} \tilde{n}_{0,k} + \lambda_{12} n(p) \left( \tilde{n}_{0,k} + \sum_{p'} \tilde{n}_{p',k} \right) , \]  

\[ i\partial_t \tilde{n}_{0,k} = (\Omega_{0,k} + \lambda_{11} N_c) \tilde{n}_{0,k} + \lambda_{12} N_c \sum_{p'} \tilde{n}_{p',k} , \]  

where \( N_c = |\psi_0|^2 \). Solving these equations yields the result of the form (10),  

\[ \mathcal{I}(\omega) = \text{Im} \sum_k |A_k|^2 \frac{\Pi(k,\omega)}{1 - \lambda_{12} \Pi(k,\omega)} , \]  

where  

\[ \Pi(k,\omega) = \frac{N_c}{\omega - \Omega_{0,k} + \lambda_{12} N_c \pi^0} + \Pi_0(k,\omega) \]  

(14)  

The spectrum at \( k = 0 \) consists of two sharp lines, with frequencies given by (11).  

![Fig. 1. Absorption spectrum (10),(11) above BEC at fixed temperature and varying density: \( N = f N_{\text{BEC}}, 0.5 \leq f < 1 \). The frequency shift \( \Delta \omega \) is defined relative to the that of a free atom at rest: \( \Delta \omega = \omega - \omega_0 - k^2/2m \). Spectral power \( \mathcal{I} \) is normalized by particle density \( N \). The excitation wavevector \( k \) is 0.5 in the units of \( \lambda_{12} N_{\text{BEC}}/\sqrt{T} \). The interaction constant \( \lambda_{11} \) is chosen to be 0. Note that the peak position follows the relation (10).](image)  

The physics of the doubling of the excitation below \( T_{\text{BEC}} \) is similar to that of the second sound. The excited particle can be in two different dynamical states, either having energy of order \( T \) and participating in momentum exchange processes, or being at rest. These two states are coupled by the transitions provided by momentum exchange processes (see (12)), in which the excited particle is transferred between the thermal and stationary states by exchanging with a condensate particle. The rate of such (coherent) transitions determines the frequency splitting in (11).
Relative strength of the spectral components given by (13) depends on the condensate fraction $N_c/N$. At $N_c \ll N$ the peak due to the states with thermal energies is much stronger than the other peak, which is due to atoms at rest. Because of that, we call the two peaks “normal” and “condensate”, respectively. At $N_c \rightarrow N$ the strengths of the two peaks become equal, and at $T \ll T_{BEC}$ the peaks approach each other. This behavior is displayed in Figs. 2, 3.

**FIG. 2.** Absorption spectrum (10), (14) in the BEC regime, shown for temperature varying between 0 and $T_{BEC}$; density $N$ fixed. The excitation wavevector $k$ is $2/3$ in the units of $\lambda_{12}N/v_T$. Lines in the base plane indicate the peak positions (4) for $k = 0$. Note narrowing of the spectral line with decreasing $T$, and strengthening of the condensate peak due to increasing condensate fraction. (The frequency shift $\Delta \omega$ is defined in Fig. 1; $\nu_{11} = 0$.)

**FIG. 3.** Absorption spectrum (10), (14) in the BEC regime at fixed temperature and density varying from $N_{BEC}$ and up. Excitation wavevector $k = 2.5$ in the units of $\lambda_{12}N_{BEC}/v_T$. Increasing condensate density leads to narrowing of the peaks and to strengthening of the condensate peak, as in Fig. 1. ($\Delta \omega$ and $I$ are defined in Fig. 1; $\nu_{11} = 0$.)

**Conclusion:** We described phenomena in optical excitations resulting from cold collisions of the excited atom with other atoms of the gas. The main feature that makes the effect of collisions an interesting problem is that, during the optical transition, the excited atom spends a long time in the superposition of the ground and excited state. Because of many collisions that occur during this time, and because of their special coherent momentum–exchange character, the optical excitation represents a collective mode. The collective nature of the excitation is manifest in the frequency shift and in the linewidth narrowing. Below the BEC transition, due to the exchange between the condensate and the normal component, the number of modes doubles, similar to the first and second acoustic modes. By using the RPA method, we calculate the temperature–dependent frequencies of the doublet and the oscillator strengths.

**ACKNOWLEDGMENTS**

We are grateful to Tom Greytak for proposing the problem, and to Dan Kleppner, Tom Killian, and Wolfgang Ketterle for many useful discussions. We acknowledge NSF support under award DMR94-00334.

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