Signature of Quantum Depletion in the Dynamic Structure Factor of Atomic Gases

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We study the linear response and the dynamic structure factor of weakly interacting Bose gases at low temperatures. Going beyond lowest order in the weak coupling expansion allows us to determine the contribution of the thermal and quantum depletion of the condensate to the dynamic structure factor. We find that the quantum depletion produces a pronounced peak in the dynamic structure factor, which allows for its detection via a spectroscopic analysis.

The main characteristic of bosonic quantum gases is the formation of a condensate at low temperatures as observed in $^3$He and atomic gases \cite{1,2}. In superfluid $^4$He, strong interactions produce a large depletion of the zero-momentum state and the condensate involves only a small fraction of the particle density; the condensate was observed experimentally by measuring the dynamic structure factor with neutron scattering \cite{3,4}. In turn, interactions are weak in atomic gases and the condensate involves nearly the full particle density, while the quantum depletion is small. However, recent progress in tuning atomic gases allows to increase the interaction strength via Feshbach resonances \cite{5,6} or optical lattices \cite{7,8}. It is this strongly correlated regime with large quantum depletion which is currently attracting a lot of experimental and theoretical interest. In this letter, we study the contribution of the quantum depletion to the dynamic structure factor, and propose that, in analogy to superfluid $^4$He, spectroscopic studies provide a powerful tool for characterizing the structure of atomic gases and allow for the detection of the quantum depletion.

The dynamic structure factor of an ideal bosonic gas exhibits a delta function peak $S(\omega,k) = n \delta(\omega - \epsilon_k)$, thus probing excitations from the condensate with the energy $\epsilon_k = \hbar^2k^2/2m$, see Fig. 1(a). Previous studies of the dynamic structure factor in atomic Bose gases accounted for the modification of such single-particle excitations via interaction and finite trapping: while the interaction modifies the quasi-particle excitation spectrum and the weight of the delta function peak \cite{9,10}, the finite size of the trap induces a broadening of this peak \cite{11,12}. In this letter, we determine the linear response function and the dynamic structure factor of weakly interacting Bose gases within a microscopic analysis going to first order in the interaction parameter $\sqrt{n a^3}$ (here, $n$ is the particle density and $a$ denotes the scattering length). We find, that the structure factor contains two contributions: The first accounts for excitations of quasi-particles from the condensate, see Fig. 1(a), and involves the condensate density $n_0$. The second term is due to excitations of two quasi-particles and accounts for the quantum depletion $n_0 = 1 - n_0$ of the condensate, see Fig. 1(b); particle-hole excitations [see Fig. 1(c)] only contribute to the structure factor at finite temperatures.

The quantum depletion $n_0$ is well understood within the weak coupling Bogoliubov theory and accounts for the interaction-induced expulsion of particles from the zero momentum state. Although the extension of this theory to finite traps is successful in explaining many phenomena observed in cold atomic gases, the detection of the quantum depletion $n_0$ itself has not been achieved so far. We show below that the quantum depletion produces a pronounced peak in the dynamic structure factor allowing for its observation via a spectroscopic analysis.

![FIG. 1: Diagrams representing the excitations created by the external drive $\delta V$ (wiggly line). (a) Creation of a quasiparticle (straight line) from the condensate $n_0$ (zigzag line). (b) Creation of two quasi-particles probing the quantum depletion. (c) Creation of a particle-hole pair probing the thermal depletion.](image)

The microscopic Hamiltonian of interacting bosons takes the form

$$H = \int dx \psi^+(x) \left( \frac{-\hbar^2 \Delta}{2m} \right) \psi(x)$$

$$+ \int dxdy U(x-y)\psi^+(x)\psi^+(y)\psi^+(y)\psi(x)$$

with $\psi^+(x)$ and $\psi(y)$ the bosonic field operators and the interaction potential $U(x)$. In the low-density limit, the microscopic interaction potential $U(x)$ is replaced by the $s$-wave scattering potential $U(x) = g\delta(x)$ with $g = 4\pi\hbar^2a/m$ \cite{12,13,14}. The expansion parameter in this weakly interacting Bose gas is $\sqrt{n a^3}$.

The response $\delta \rho(t,x)$ of the bosonic density relates to a small external potential $\delta V(t,x)$ via the integral relation

$$\delta \rho(t,x) = \int dt' dx' \chi(t-t',x-x')\delta V(t',x')$$

with the linear response function \cite{15} \cite{16} \cite{17} (\( \rho = \psi^+\psi \))

$$\chi(t,x) = -i\Theta(t)\langle[\rho(t,x),\rho(0,0)]\rangle.$$
Here, $\langle \ldots \rangle$ denotes the quantum statistical average at fixed temperature $T$ and chemical potential $\mu$. The response function $\chi(t, x)$ is conveniently calculated via its relation to the density-density correlation function in imaginary time $D(\tau, x)$ \cite{12, 13, 14},

$$D(\tau, x) = -\left[\langle T \rho(\tau, x) \rho(0, 0) \rangle - \langle \rho \rangle \langle \rho \rangle \right]$$

(4)

with $T$ the time ordering operator. Then, the response $\chi(\omega, x)$ is the proper analytic continuation of the density-density correlation function $D(\Omega_s, x)$, which respects the retarded character of $\chi(t, x)$. Here, $\Omega_s = 2\pi T s$ denote the Matsubara frequencies with $s \in \mathbb{Z}$.

$$D_0 = \begin{bmatrix} G(-\tau, x) & G'(-\tau, x) \end{bmatrix} + \begin{bmatrix} F^+(\tau, x) & \end{bmatrix}$$

$$D' = \begin{bmatrix} D_0' & \end{bmatrix} + \begin{bmatrix} F_0' & \end{bmatrix}$$

FIG. 2: Diagrams contributing to the response function $D$ to first order in $\sqrt{n a^3}$. $D_0$ collects diagrams involving the condensate density $n_0$, while the diagrams in $D'$ probe the depletion of the condensate. The thick solid line denotes the normal and anomalous Green’s functions $G$, $F^+$, and $F$ within Bogoliubov approximation. Zigzag lines account for the creation $\xi^+$ and annihilation $\xi$ of particles from the condensate.

In the following, we apply standard quantum field theory methods for interacting bosons at low temperatures \cite{12, 13, 14}. We separate the bosonic operators $\xi^+$ and $\xi$ accounting for creation and annihilation of the zero momentum state from the field operator,

$$\psi^+(\tau, x) = \xi^+ + \psi^+(\tau, x), \quad \psi(\tau, x) = \xi + \psi(\tau, x).$$

(5)

Within each diagrammatic expression the operators $\xi$ and $\xi^+$ are considered as $c$-numbers contributing a factor $\sqrt{n_0}$; $n_0$ denotes the condensate fraction and has to be determined self-consistently. The difference $n_D = n - n_0$ between the averaged particle density $n = \langle \rho \rangle$ and the condensate fraction $n_0$ is due to the thermal and quantum depletion of the condensate. Here, we focus on the low density limit and expand the density-density correlation function $D$ in the small parameter $\sqrt{n a^3}$; the relevant diagrams are shown in Fig. 2. All additional diagrams involve a vertex operator $\Gamma$ and contribute to higher order terms in the expansion parameter $\sqrt{n a^3}$; they will be dropped in the following.

The diagrammatic representation of the leading contribution $D_0$ to the density-density correlation function $D$ is shown in Fig. 2 and takes the form

$$D_0(\Omega_s, k) = -n_0 \left[ G'(\Omega_s, k) + G'(-\Omega_s, -k) \right]$$

(6)

+ $F^+(\Omega_s, k) + F(\Omega_s, k)$.

The normal Green’s function $G'$ and the anomalous Green’s functions $F^+$ and $F$ are defined as

$$G'(\tau, x) = -\langle T \psi'(\tau, x) \psi'(0, 0) \rangle,$$

$$F^+(\tau, x) = -\frac{1}{n_0} \langle T \xi^+ \psi'(\tau, x) \psi'(0, 0) \rangle,$$

$$F(\tau, x) = -\frac{1}{n_0} \langle T \xi \psi'(\tau, x) \psi'(0, 0) \rangle.$$

Note, that $G'$ is related to the depletion of the condensate, $n_0 = G'(\tau \rightarrow 0^+)$. Within first order in the expansion parameter $\sqrt{n a^3}$, the Green’s functions take the Bogoliubov form \cite{12, 13}

$$G'(\Omega_s, k) = \frac{i \Omega_s + \xi_k + \mu}{(i \Omega_s)^2 - E_k^2},$$

$$F^+(\Omega_s, k) = \frac{F(\Omega_s, k)}{-E_k^2}$$

(9)

with the excitation spectrum $E_k = \sqrt{\xi_k^2 + 2\xi_k \mu}$ and the chemical potential $\mu = g n$. The analytic continuation of $D_0(\Omega_s, k)$ provides the contribution

$$\chi_0(\omega, k) = -\frac{2 \xi_k n_0}{(\hbar \omega + i \delta)^2 - E_k^2}$$

(10)

to the response. The structure factor $S(\omega, \mathbf{k})$ is related to the imaginary part of the response function, $\text{Im} \chi = -\pi[1 - \exp(-\beta \hbar \omega)] S$, and using (10) we find $(\beta = 1/T)$

$$S_0(\omega, \mathbf{k}) = \frac{n_0 e^{\beta \hbar \omega}}{e^{\beta \hbar \omega} - 1} \frac{\delta (\hbar \omega - E_k) + \delta (\hbar \omega + E_k)}{\hbar \omega - E_k}$$

(11)

accounting for the excitation of single quasi-particles from the condensate, the process illustrated in Fig. 1(a). Furthermore, $S_0(\omega, \mathbf{k})$ nearly exhausts the f-sum rule

$$\int_{-\infty}^{\infty} d\omega \omega S_0(\omega, \mathbf{q}) = \frac{n_0 \hbar^2 Q^2}{2m}$$

(12)

the missing part $n_0 \hbar^2 Q^2/2m$ derives from the structure of the thermal and quantum depletion of the condensate. With $n_0 \propto n \sqrt{n a^3}$, its effect is usually ignored to lowest order in the expansion $\sqrt{n a^3}$ \cite{12, 13, 14}, but with increasing interaction its contribution plays a substantial role.

The first diagram in the correction $D' = D'_1 + D'_2$, see Fig. 2, takes the form

$$D'_1(\Omega_s, k) = -T \sum_{\mathbf{q} \in \mathbf{Z}} \int d\Omega \frac{\Omega_s + \epsilon_q + \mu}{(i \Omega)^2 - E_q^2} + \frac{\Omega_{s+q} + \epsilon_{k+q} + \mu}{(i \Omega_{s+q})^2 - E_{k+q}^2}.$$
The poles account for the creation of two particles out of the condensate with energy \( \hbar \omega = E_k + E_{k+q} \) [see Fig. 1(b)] and the scattering of thermally excited quasi-particles \( \hbar \omega = E_k - E_{k+q} \) [see Fig. 1(c)]. This creation of particle-hole-pairs dominates in the high temperature limit \( T \gg \mu \). Then, the response derives from Eq. (13) taking the limit \( \mu \to 0 \) and reduces to the bosonic Lindhard function

\[
\chi'(\omega, k) = \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{2E_{\mathbf{q}}} \left\{ \frac{E_{\mathbf{q}} + \epsilon_{\mathbf{q}} + \mu}{e^{\beta E_{\mathbf{q}}} - 1} \left[ \frac{\hbar \omega + E_{\mathbf{q}} + \epsilon_{\mathbf{q}+\mathbf{k}} + \mu}{\hbar \omega + \delta + E_{\mathbf{q}}^2 - E_{\mathbf{q}+\mathbf{k}}^2} + \frac{-\hbar \omega + E_{\mathbf{q}} + \epsilon_{\mathbf{q}-\mathbf{k}} + \mu}{\hbar \omega + \delta - E_{\mathbf{q}}^2 - E_{\mathbf{q}-\mathbf{k}}^2} \right] \right. \\
+ \left. \frac{E_{\mathbf{q}} + \epsilon_{\mathbf{q}} + \mu}{1 - e^{-\beta E_{\mathbf{q}}}} \left[ \frac{\hbar \omega - E_{\mathbf{q}} + \epsilon_{\mathbf{q}+\mathbf{k}} + \mu}{\hbar \omega + \delta - E_{\mathbf{q}}^2 - E_{\mathbf{q}+\mathbf{k}}^2} + \frac{-\hbar \omega - E_{\mathbf{q}} + \epsilon_{\mathbf{q}-\mathbf{k}} + \mu}{\hbar \omega + \delta + E_{\mathbf{q}}^2 - E_{\mathbf{q}-\mathbf{k}}^2} \right] \right\}.
\]

(13)

with \( f = 1/(\exp(\beta \varepsilon) - 1) \) the bosonic distribution function.

Here, we are interested in the low temperature limit \( T \ll \mu \) of the response, where thermally excited quasi-particles are quenched and the response function (13) accounts for the quantum depletion alone. We set \( T = 0 \), and obtain the correction to the dynamic structure factor

\[
S'(\omega, k) = n_0 \frac{\hbar^2 k^2}{2m} \frac{1}{4\mu^2} \tilde{S}' \left( \frac{\varepsilon_k}{4\mu}, \frac{\hbar \omega}{2\mu} \right)
\]

with \( n_0 = (8/3\sqrt{\pi}) n \sqrt{\mu a^3} \) the quantum depletion within Bogoliubov theory (13). The dimensionless function \( S'(\alpha, x) \) vanishes below the two-particle excitation threshold \( x^2 < \alpha^2 + 2\alpha \), while for \( x^2 > \alpha^2 + 2\alpha \) we obtain

\[
\tilde{S}'(\alpha, x) = \frac{3}{8\sqrt{2} \alpha^3/2} \int \varepsilon^- \left[ 1 - \frac{1}{(\alpha + 1 + \varepsilon)^2 - x^2} \right]^{1/2},
\]

where \( \varepsilon^- = -1 + \alpha + \sqrt{1 + x^2} \). The upper integration limit \( \varepsilon^- \) is determined by \( \varepsilon_1 < \varepsilon^- < \varepsilon_2 < \varepsilon_3 \) with \( \varepsilon_1, \varepsilon_2, \varepsilon_3 \) the solutions of the cubic equation

\[
x^3 - \left( (\alpha + \varepsilon + 1)^2 - 1 + 4\alpha \varepsilon \right) x^2 + 4\alpha \varepsilon (\alpha + \varepsilon + 1)^2 = 0.
\]

Combining the results (11) and (15) provides the dynamic structure factor \( S(\omega, k) = S_0(\omega, k) + S'(\omega, k) \) within first order in the expansion parameter \( \sqrt{na}^{-1} \). Using the relation \( \int_0^\infty dx xS'(\alpha, x) = 1 \), the f-sum rule is satisfied as required in a consistent calculation to order \( \sqrt{na}^{-1} \). The dimensionless function \( \hbar \omega \tilde{S}'/2\mu \) is shown in Fig. 3. At low momenta \( |k| < 2\sqrt{m\beta h} \), the peak in the structure factor appears at \( \hbar \omega \approx 2\mu \), while at high momenta \( |k| > 2\sqrt{m\beta h} \) this peak follows the Bogoliubov energy \( \hbar \omega = E_k \).

Subjecting the Bose gas to an optical lattice, we have to replace the free dispersion relation \( \varepsilon_k \) by the band structure of a particle in a periodic potential (in the tight binding limit, \( \varepsilon_k = 2J [3 - \cos(k_x b) - \cos(k_y b) - \cos(k_z b)] \) with the hopping energy \( J \) and the lattice constant \( b \)). In addition, Umklapp processes transferring momentum to the optical lattice have to be considered. Restricting the analysis to the lowest Bloch band and small momenta \( k \to 0 \), the expressions for the response function (10) and (13) remain valid and the contribution \( S'_c(\omega, k) \) to the

FIG. 3: Density plot of the dimensionless structure factor \( \hbar \omega \tilde{S}'/2\mu \) for an interacting gas at zero temperature; the momentum \( k_\mu \) is measured in units \( \sqrt{m\beta h} \). The white line denotes the energy threshold for the two-particle creation. At low momenta \( |k| < 2\sqrt{m\beta h} \), the peak in the structure factor appears at \( \hbar \omega \approx 2\mu \), while at high momenta \( |k| > 2\sqrt{m\beta h} \) this peak follows the Bogoliubov energy \( \hbar \omega = E_k \).

FIG. 4: Structure factor \( \hbar \omega \tilde{S}'/2\mu \) (a) and \( \hbar \omega \tilde{S}' / 2\mu \) (b) in the limit of small momenta \( k \to 0 \). The structure factor exhibits a peak at \( \omega \approx 2\mu \), and is quenched above twice the bandwidth \( \approx 24J \) in the presence of an optical lattice (b).
structure factor takes the form
\[ S'_c(\omega, \mathbf{k}) = \frac{2\mu^2}{(\hbar^2\omega)^2} \int_K \frac{d\mathbf{q}}{(2\pi)^3} (\mathbf{k} \cdot \nabla \epsilon_{\mathbf{q}})^2 \delta(\hbar\omega - 2E_{\mathbf{q}}) \] (16)
with \( K \) the first Brillouin zone. Furthermore, the structure factor turns quasi-periodic, \( S'_c(\omega, \mathbf{k} + \mathbf{K}) = |c_\mathbf{k}|^2 S'_c(\omega, \mathbf{k}) \) for \( \mathbf{k} \to 0 \) with \( \mathbf{K} \) a reciprocal lattice vector and \( c_\mathbf{k} \) a numerical prefactor accounting for the shape of the wave function within a potential well (c.f., Ref. 17 for a similar discussion of the quasi-periodicity). In Fig. 2(b) we show the structure factor \( S'_c(\omega, \mathbf{K}) \) at these frequencies [17]; in the following we attempt an explanation involving the quantum depletion of the Bose gas enhanced by the quantum depletion of the condensate. A measurement of the structure factor not only allows for the detection of the quantum depletion in atomic gases but provides additional non-trivial information on the ground state of strongly interacting Bose gases, thus opening up new possibilities in studying complex quantum phases in atomic gases.

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\[ \text{The main energy transfer observed in [18] resides at large energies and is incompatible with the vanishing spectral weight in } S_0 \text{ at these frequencies [18]; in the following we attempt an explanation involving the quantum depletion. The structure factor } \hat{S}(\omega, \mathbf{K}) \text{ has to account for the finite trapping potential: the wave functions describing the Bogoliubov excitations involve momenta with a spread } \Delta \mathbf{k}. \text{ The structure factor in a finite trap derives from its counterpart in the homogeneous system via the average } \hat{S}(\omega, \mathbf{K}) \approx \langle S'(\omega, \mathbf{K} + \mathbf{q}) \rangle_{|\mathbf{q}|<|\Delta \mathbf{k}|}. \text{ In the interesting regime } \hbar \omega \approx \mu, \text{ the structure factor } S' \text{ involves two-particle excitations with large momenta and the finite level spacing in the trap plays a minor role. In estimating the relevant spread } \Delta \mathbf{k} \text{ we have to account for the trap size } R \text{ (Thomas Fermi radius) and the condensate healing length } \xi \text{ describing the rapid decay of the wave function at the trap boundary; making use of the excitations derived in Ref. 21}, \text{ we obtain a spread of order } |\Delta \mathbf{k}| \approx 1/(R\xi)^{1/2}. \text{ Combining the quasi-periodicity of the structure factor in an optical lattice and the spread induced by the trapping potential, we find the estimate}
\[ \hat{S}(\omega, \mathbf{K}) \approx |c_\mathbf{k}|^2 \langle S'_c(\omega, \mathbf{q}) \rangle_{|\mathbf{q}|<|\Delta \mathbf{k}|} \] (18)
with \( S'_c(\omega, \mathbf{k}) \) shown in Fig. 3(b). In their experiments, Stöferle et al. [18] report (among other) on the energy transfer to a trapped Bose gas subject to a 3D optical lattice residing in the superfluid phase. They find a pronounced peak in the excitation spectrum centered at a frequency \( \hbar \omega \approx 2\mu \) and with a width of order of the band width, in rough agreement with our result for \( S'_c \). Accounting for the smearing in the structure factor due to the finite trap as discussed above, the transferred energy [17] assumes the correct order of magnitude. We then are tempted to associate the observations made in [18] with the quantum depletion of the Bose gas enhanced by the presence of the optical lattice. We note that the optical lattice applied in the experiments is already appreciable. Hence, we expect the weak coupling analysis above to reproduce correctly the qualitative features in the experiment, while a quantitative discussion requires to include higher order corrections in the parameter \( \sqrt{n a^3} \).

In conclusion, the structure factor of a weakly interacting Bose gas exhibits a characteristic behavior associated with the structure of the quantum depletion of the condensate. A measurement of the structure factor not only allows for the detection of the quantum depletion in atomic gases but provides additional non-trivial information on the ground state of strongly interacting Bose gases, thus opening up new possibilities in studying complex quantum phases in atomic gases.

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\[ \text{References}
[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornel, Science 269, 198 (1995).
[2] A. Griffin, Excitations in a Bose-Condensed liquid (Cambridge University Press, 1993).
[3] D. G. Henshaw and A. B. Woods, Phys. Rev. 121, 1266 (1961).
[4] S. L. Cornish et al., Phys. Rev. Lett. 85, 1795 (2000).
[5] D. Jaksch, C. Bruder, J. I. Cicci, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
[6] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[7] D. M. Stamper-Kurn et al., Phys. Rev. Lett. 83, 2876 (1999).
[8] J. Steinhauer, R. Ozeri, N. Katz, and N. Davidson, Phys. Rev. Lett. 88, 120407 (2002).
[9] S. Stenger et al., Phys. Rev. Lett. 82, 4569 (1999).
[10] W.-C. Wu and A. Griffin, Phys. Rev. A 54, 4204 (1996).
[11] F. Zambelli, L. Pitaevskii, D. M. Stamper-Kurn, and S. Stringari, Phys. Rev. A 61, 063608 (2000).
[12] N. M. Hugenholtz and D. Pines, Phys. Rev. 116, 489 (1959).
[13] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, Methods of Quantum Field Theory in Statistical Physics (Dover Publications, 1963).
[14] P. Nozières and D. Pines, Theory of Quantum Liquids: Superfluid Bose Liquids (Addison-Wesley, 1990).
[15] J. W. Negele and H. Orland, Quantum Many-Particle Systems (Perseus Books, Massachusetts, 1998).
[16] C. Castellani, C. D. Castro, F. Pistolesi, and G. C. Strinati, Phys. Rev. Lett. 78, 1612 (1997).
[17] C. Menotti, M. Kraemer, L. Pitaevskii, and S. Stringari, Phys. Rev. A 67, 053609 (2002).
[18] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, cond-mat/0312440 (2003).
[19] P. M. Chaikin and T. C. Lubensky, Principles of condensed matter physics (Cambridge, 1995).
[20] S. Stringari, Phys. Rev. Lett. 77, 2360 (1996).}