Finite temperature dynamic structure function of the free Bose gas

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Abstract

A detailed calculation of the finite temperature dynamic structure function of the free Bose gas is presented and discussed. After a short derivation of the expressions describing the exact response $S(q, \omega; T)$ and the impulse approximation (IA) $S_{IA}(q, \omega; T)$, their main properties and their evolution with $q$ and $T$ are analyzed. The lowest order energy weighted sum rules of both $S(q, \omega; T)$ and $S_{IA}(q, \omega; T)$ are also derived and commented. Finally, the $q \to \infty$ asymptotic behavior is analyzed and discussed in terms of scaling laws.

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Neutron scattering on systems like pure $^4$He has proved to be among the most fruitful methods to gather relevant information about the fundamental properties of Bose condensed systems [1]. Although high momentum transfer neutron scattering is known to provide much information about the structure of the Bose condensate, no particular formalism has been able to accurately describe how temperature influences the dynamic structure function $S(q, \omega)$ and how the temperature dependence of the condensation fraction value affects $S(q, \omega)$ at high and low momentum transfers. More recently, the experimental discovery of Bose condensation in clouds of alkali atoms has revived the interest in the analysis of free Bose systems and the way in which Bose–Einstein condensation sets in [2,3]. In previous works we presented detailed calculations of the $T = 0$ and $T > 0$ dynamic structure function of the free Fermi gas, their coherent and incoherent parts and the way in which they evolve with momentum transfer [4,5]. In this work we extend this analysis to free Bose systems, focussing on the evolution of $S(q, \omega)$ and its coherent and incoherent parts with $q$ and $T$, the role of the Bose–Einstein condensate in the response and finally on scaling laws.

The dynamic structure function $S(q, \omega; T)$ describes the way in which a system of $N$ particles responds to a probe which produces a density fluctuation modelized through the operator $ho_q = \sum_{j=1}^{N} e^{i q r_j}$. At finite temperature this is given by [6–8]

\begin{equation}
S(q, \omega; T) = \sum_{\{n,m\}} \frac{1}{Z} e^{-\beta(E_n - \mu N)} \frac{1}{N} |\langle m | \rho_q | n \rangle|^2 \times \delta(E_m - E_n - \omega),
\end{equation}
where $q$ and $\omega$ are the momentum and energy transferred by the probe to the system. $Z = \sum_{\{n\}} e^{-\beta(E_n - \mu N)}$ stands for the grand canonical partition function, while $\beta = 1/k_BT$ is the inverse of the temperature and $\mu$ is the chemical potential.

The dynamic structure function is related by Fourier transformation to the density–density response function $S(q,t)$ which may in turn be separated in its coherent and incoherent parts

$$S_{\text{inc}}(q,t;T) = \frac{1}{Z} \sum_{\{n\}} e^{-\beta(E_n - \mu N)}$$

$$\times \frac{1}{N} \sum_{j=1}^{N} \left( e^{-i q r_j} e^{i \beta \tilde{H} t} e^{i q r_j} e^{-i \beta \tilde{H} t} \right) |n\rangle,$$

$$S_{\text{coh}}(q,t;T) = \frac{1}{Z} \sum_{\{n\}} e^{-\beta(E_n - \mu N)}$$

$$\times \frac{1}{N} \sum_{i \neq j=1}^{N} \left( e^{-i q r_i} e^{i \beta \tilde{H} t} \right) |n\rangle.$$ (2)

$H$ and $r_j$ being the Hamiltonian of the system and the position operator of particle $j$, respectively. With these definitions the incoherent response takes into account only the diagonal terms of the density–density response function, while the coherent response incorporates the contribution coming from all the other terms in $S(q,t)$. Notice that these definitions are not unique as in fact frequently $S_{\text{coh}}(q,t)$ is identified with $S(q,t)$ while the last function in Eq. (3) becomes simply the difference between the new $S_{\text{coh}}(q,t)$ and $S_{\text{inc}}(q,t)$.

The dynamic structure function is also related to the imaginary part of the dynamic susceptibility $\chi(q,\omega;T)$. Taking into account that $\Re \chi(q,\omega;T) = -\pi (1 - e^{-\beta \omega})S(q,\omega;T)$, one finds

$$\tilde{S}(q,\omega;T) = e_0 S(q,\omega;T)$$

$$\left( 1 - e^{-\beta \omega} \right) \delta(\omega - q^2) - \delta(\omega + q^2) \right]$$

$$\frac{1}{16\pi^2 \tilde{q}^2} \left( 1 - e^{-\beta \omega} \right)$$

$$\times \ln \left[ \frac{1 - z e^{-\beta(\tilde{q}^2-q^2)/4T}}{1 - z e^{-\beta(\tilde{q}^2+q^2)/4T}} \right].$$ (4)

that is written in terms of the dimensionless variables $\tilde{q} = q/k_0$, $\tilde{\omega} = \omega/\epsilon_0$ and $\tilde{T} = T/\epsilon_0$, where $k_0 = \rho^{1/3}$ and $\epsilon_0 = k_0^2/2m$ define the momentum and energy scales. Finally, in Eq. (4) $z$ stands for the fugacity that is related to the dimensionless chemical potential through $z = e^{\tilde{\mu}/T}$, where $\tilde{\mu} = \mu/\epsilon_0$. This last quantity can be derived recalling that at equilibrium particle number conservation imposes

$$\int_0^\infty \frac{e^{1/2} d\epsilon}{z^{-1} e^\epsilon - 1} = \frac{4\pi^2}{T^{3/2}} \left[ 1 - n_0(\tilde{T}) \right].$$ (5)

where $n_0(\tilde{T})$ is the condensate fraction value at temperature $\tilde{T}$. For the free Bose gas, at $T \leq T_c$,

$$n_0(\tilde{T}) \approx 1 - \left( \frac{T}{T_c} \right)^{3/2},$$ (6)

where $T_c \approx 6.63$ is the value of the dimensionless Bose–Einstein transition temperature which in the current dimensionless scheme becomes density and mass independent.

Notice that the first term in Eq. (4) is proportional to the condensate fraction value $n_0(\tilde{T})$ and thus characteristic of Bose liquids: when the system is given a net momentum transfer $\tilde{q}$, all particles in the condensate respond equally to the perturbation and the response peaks at the two frequencies $\tilde{\omega} = \tilde{q}^2$. On the other hand, the second term is the contribution of all the other particles not laying in the condensate and is similar to the particle–hole contribution to the total response of Fermi systems.

In the free case and due to the absence of an interatomic potential, the incoherent response coincides with the impulse approximation,

$$\tilde{S}_{\text{inc}}(\tilde{q},\tilde{\omega};\tilde{T})$$

$$= \tilde{S}_{\text{inc}}(\tilde{q},\tilde{\omega};\tilde{T})$$

$$= \frac{1}{(2\pi)^3} \int d\mathbf{k} n(\mathbf{k}) \delta(\mathbf{k} + \tilde{q})^2 - k^2 - \tilde{\omega}.$$ (7)

Using the momentum distribution of the free Bose gas one gets the following result:

$$\tilde{S}_{\text{inc}}(\tilde{q},\tilde{\omega};\tilde{T}) = n_0(\tilde{T}) \delta(\tilde{\omega} - \tilde{q}^2)$$

$$- \frac{\tilde{T}}{16\pi^2 \tilde{q}^2} \ln \left[ 1 - z e^{-\beta(\tilde{q}^2-q^2)/4T} \right].$$ (8)
while $\tilde{S}_{\text{coh}}(\tilde{q}, \tilde{\omega}; \tilde{T})$ is the difference between (4) and (8).

Below the Bose–Einstein transition temperature, where $\zeta = 1$, one can introduce a new set of variables $Q = \tilde{q}/\tilde{T}^{1/2}$ and $v = \tilde{\omega}/\tilde{T}$, such that the ratio of the non-condensate contributions and $\tilde{T}^{1/2}$ becomes temperature independent for all three responses when $Q$ and $v$ are taken as new independent variables. Therefore, it is useful to introduce three new structure functions that take this fact into account,

$$\hat{S}(Q, v) = \frac{1}{\sqrt{T}} \tilde{S}_{\text{nc}}(\tilde{q}, \tilde{\omega}; \tilde{T})$$

$$\equiv -\frac{1}{16\pi^{2}Q} \frac{1}{(1 - e^{-v})} \left[ 1 - ze^{-(v/Q - Q)^{2}/4} \right],$$

$$\hat{S}_{\text{inc}}(Q, v) = \frac{1}{\sqrt{T}} \tilde{S}_{\text{nc, inc}}(\tilde{q}, \tilde{\omega}; \tilde{T})$$

$$\equiv -\frac{1}{16\pi^{2}Q} \ln \left[ 1 - ze^{-(v/Q - Q)^{2}/4} \right],$$

and the fugacity becomes smaller than 1, thus moving the poles from the real axis into the complex plane and hence removing the previous singular behavior from all three responses. In this sense, the presence of these singularities in the non-condensate part of the response may be considered as an indirect signature of the existence of a Bose condensate.

At fixed $\tilde{T}$, the low $\tilde{q}$ response presents nonvanishing contributions coming from both the coherent and the incoherent parts of the response. Notice that, in contrast to what happens in the free Fermi gas case [5], the low $\tilde{q}$’s coherent response may actually overcome the incoherent one. As $\tilde{q}$ is risen, the coherent response decays rapidly to zero and thus the total response becomes mainly incoherent. As the temperature is risen, coherent contributions become more relevant and eventually, depending on the value of $\tilde{q}$, at $\tilde{T} \approx \tilde{q}^{2}$ both $\tilde{S}_{\text{inc}}$ and $\tilde{S}_{\text{coh}}$ carry similar contributions to the total response. Therefore the evolution with $\tilde{T}$ at fixed $\tilde{q}$ can be understood as follows: at very low $\tilde{T}$, $Q$ is large and so the response behaves as if it were in the high momentum transfer limit, where $\tilde{S}(Q, v) \approx S_{\text{inc}}(Q, v)$ and $S_{\text{coh}}(Q, v) \rightarrow 0$. As the temperature rises, $Q$ shrinks and takes its lowest
value at $\bar{T} = \bar{T}_c$ before the Bose condensate disappears. When $q^2 \gg \bar{T}_c$, the response still remains in the high momentum transfer limit, otherwise it enters into the low momentum regime.

The behaviour of the three responses changes when the temperature rises above the Bose–Einstein transition temperature. In fact, at $\bar{T} > \bar{T}_c$ the chemical potential is strictly negative and thus the fugacity $z$ is smaller than 1. Under such circumstances, the poles of the responses that at $\bar{T} < \bar{T}_c$ were at $v = \pm Q^2$ now move to $v = \pm Q^2 \pm i2Q\sqrt{-\ln z}$, and thus the singular points are removed from the real $v$ axis, splitting each real pole into two complex ones. When either $q$ or $\bar{T}$ increases, the distance from the poles to the real $v$ axis grows and the shape of the response is smoothened.

This behaviour is shown in Figs. 2, 3 and 4, where the total, coherent and incoherent responses are depicted for several values of $Q$ in comparison with the classical response $\hat{S}_c(Q, v; \bar{T})$ computed from a

Fig. 2. Temperature dependence above $\bar{Q}_T$ of the total ($\hat{S}(Q, v; \bar{T})$, solid line), coherent ($\hat{S}_\text{coh}(Q, v; \bar{T})$, dashed lines) and incoherent ($\hat{S}_\text{inc}(Q, v; \bar{T})$, dotted line), in all cases at $Q = 0.7$. The classical limit $\hat{S}_c(Q, v; \bar{T})$ is also shown at each temperature (dot-dot-dashed lines).

Fig. 3. Same plots as in Fig. 2 at $Q = 1.5$.

Fig. 4. Same plots in Fig. 2 at $Q = 2$. 
Maxwellian momentum distribution
\[ \hat{S}_{cl}(Q, v; T) = \frac{1}{2Q^{3/2}\sqrt{\pi}} e^{-\frac{1}{2}(Q^2 - Q_v^2)^2}, \] (12)
which corresponds to the limiting case to which \( \hat{S}(Q, v; \bar{T}) \) should approximate when the temperature increases.

As it can be seen from the figures, the way in which \( \hat{S}(Q, v; \bar{T}) \) approaches \( \hat{S}_{inc}(Q, v; \bar{T}) \) (incoherent limit) and \( \hat{S}_{cl}(Q, v; \bar{T}) \) (classical limit) depends on the momentum transfer and on the temperature. At low \( \bar{T} \) greater than \( \bar{T}_c \), the total response approaches the incoherent one when \( \bar{q} \) grows. However, both \( \hat{S}(Q, v; \bar{T}) \) and \( \hat{S}_{inc}(Q, v; \bar{T}) \) differ from \( \hat{S}_{cl}(Q, v; \bar{T}) \) because the momentum distribution at those temperatures noticeably depart from the gaussian shape of the classical \( n(k) \). When the temperature is risen, the difference between the momentum distribution in the classical and quantum cases is reduced and so the high \( \bar{q} \) response of the free Bose gas approaches the classical limit. Notice, however, that the difference between \( \hat{S}(Q, v; \bar{T}) \) and \( \hat{S}_{inc}(Q, v; \bar{T}) \) is rather high temperatures.

The evolution with \( \bar{T} \) of the different responses can also be analyzed from the sum rules they satisfy. Sum rules are defined as the different energy-weighted moments of the responses
\[ \hat{m}^{(0)}_{inc}(\bar{q}; \bar{T}) = n_0(\bar{T}) [2n(\bar{q}) + 1] + \frac{\hat{m}^{(0)}_{inc}(\bar{q}; \bar{T})}{\bar{T}} = \frac{\hat{S}(\bar{q}; \bar{T})}{\bar{T}}, \] (14)
\[ \hat{m}^{(0)}_{coh}(\bar{q}; \bar{T}) = n_0(\bar{T}) + \frac{\hat{m}^{(0)}_{coh}(\bar{q}; \bar{T})}{\bar{T}} = 1, \] (15)
\[ \hat{m}^{(0)}_{coh,nc}(\bar{q}; \bar{T}) = 2n_0(\bar{T}) n(\bar{q}) + \frac{\hat{m}^{(0)}_{coh,nc}(\bar{q}; \bar{T})}{\bar{T}} = \frac{\hat{S}(\bar{q}; \bar{T})}{\bar{T}} - 1, \] (16)
\[ \hat{m}^{(1)}_{inc}(\bar{q}; \bar{T}) = n_0(\bar{T}) \bar{q}^2 + \frac{\hat{m}^{(1)}_{inc}(\bar{q}; \bar{T})}{\bar{T}} = \bar{q}^2, \] (17)
where \( \hat{m}^{(0)}_{inc}(\bar{q}; \bar{T}) \) and \( \hat{m}^{(0)}_{inc,nc}(\bar{q}; \bar{T}) \) refer to the contribution to the sum rules coming from the integral of the non-condensate parts of the different responses.

Eq. (14) yields the values of the static structure factor \( S(\bar{q}; \bar{T}) \) as obtained from the direct integration of Eq. (4). Two different contributions appear at temperatures below \( \bar{T}_c \). The first one results from the condensate term in \( S(\bar{q}, \omega; \bar{T}) \) and so is proportional to \( n_0(\bar{T}) \). The contribution of this term to the \( \hat{m}^{(0)}_{inc}(\bar{q}; \bar{T}) \) sum rule grows as \( n_0(\bar{T})/\bar{T}^2 + 1/\bar{T} \) at low momentum transfer because at \( \bar{T} < \bar{T}_c \) the low \( \bar{q} \) states close to the condensate are populated according to a \( \bar{T}/\bar{q}^2 \) law. Notice that this is an entirely coherent effect as can be seen from Eqs. (15) and (16). This behaviour can be smeared out when particle interactions are allowed to take place as happens in liquid \( ^4 \)He at low temperatures. Also, as \( \bar{T}^{-1/2} \hat{S}_{inc}(\bar{q}, \omega; \bar{T}) = \hat{S}_{inc}(Q, v; \bar{T}) \) is a \( T \)-independent function of \( Q \) and \( v \) at \( \bar{T} \leq \bar{T}_c \), the zero order \( v \)-weighted moment of \( \hat{S}_{inc}(Q, v) \) yields an universal curve from where both the evolution with \( \bar{q} \) and the evolution with \( \bar{T} \) of \( \hat{S}_{inc}(\bar{q}; \bar{T}) \leq \bar{T}_c \) can be extracted. According to the previous definitions \( M^{(n)}_{inc}(Q) = \int v^n \hat{S}(Q, v; \bar{T}) d\bar{T} = \bar{T}^{n/2+1/2} \hat{m}^{(n)}_{inc}(\bar{q}; \bar{T}) \).

Eq. (15) is depicted in the upper plot of Fig. 5. At low \( Q \), that is, at low momenta compared to \( \bar{T}^{1/2} \), the divergences appearing in \( \hat{S}(Q, v) \) at \( v = \pm Q^2 \) take most of the strength and as a result \( M^{(0)}_{inc}(Q) \) increases. However, the singularities in \( \hat{S}(Q, v) \) at \( v = \pm Q^2 \) are of the logarithmic type and thus their \( v \)-weighted integrals of the response give always finite results consistent with Eqs. (17)–(19). On the other hand, in the large \( Q \) limit \( M^{(0)}_{inc}(\bar{q}) \) approaches the constant value \( \bar{T}_c^{-3/2} \approx 0.058 \), a result that is consistent with \( m^{(0)}(\bar{q}, \bar{T}) \) going to 1 and \( n_0(\bar{T}) \) and the temperature dependence of the condensate fraction value reported in Eq. (6). When this value is reached the total \( \hat{S}(\bar{q}, \bar{T}) \) equals 1. The high \( Q \) limit can be reached either rising \( \bar{q} \) at fixed \( \bar{T} \) or lowering \( \bar{T} \) at fixed \( \bar{q} \). Therefore, no matter what the value of \( \bar{q} \) is, at \( \bar{T} \rightarrow 0 \) the static structure factor goes to 1, a fact that is consistent with \( \hat{S}(\bar{q}, \omega; \bar{T} = 0) \) being completely incoherent and equal to \( \delta(\omega - \bar{q}^2) \). When the temperature is risen, the total response receives contributions from the non-condensate terms and thus
As the logarithmic singularities in the dynamic structure function are smeared out at $\bar{T} > \bar{T}_c$, the limiting value $\tilde{S}(\tilde{q} \to 0; \bar{T})$ now becomes finite. When $\tilde{q}$ increases, $\tilde{S}(\tilde{q}; \bar{T})$ decreases and asymptotically approaches 1 from above, thus indicating that the total response is reaching the incoherent limit in which $\tilde{S}(\tilde{q}, \tilde{q}; \bar{T}) \approx \tilde{S}_{inc}(\tilde{q}, \tilde{q}; \bar{T})$ and $\tilde{S}_{coh}(\tilde{q}, \tilde{q}; \bar{T}) \approx 0$. In the high $\bar{T}$ limit $\tilde{S}(\tilde{q}; \bar{T}) \approx 1$ at all $\tilde{q}$’s and this reveals that the classical limit has almost been reached, as $\tilde{S}_{cl}(\tilde{q}; \bar{T})$ is known to be equal to 1 for all $\tilde{q}$.

Moreover, this limit is consistently reached when $\bar{T} \to \infty$, as in fact it is straightforwardly seen from the very definition of $\bar{T}$ that this can be achieved either increasing the temperature at fixed density or reducing the density at fixed temperature.

Another interesting feature of the high momentum transfer behaviour of the response is the scaling property, as it is well known that when $\tilde{q} \to \infty$ the dynamic structure function does not depend anymore on $\tilde{q}$ and $\tilde{q}$ separately but only through the West scaling variable $\bar{y} = (\tilde{q}/\sqrt{\bar{T}} - \tilde{q})/2$[10].

In the free Bose gas case scaling may be reached in two different ways depending on the temperature. At $\bar{T} \leq \bar{T}_c$, this can be done introducing a Compton profile $\tilde{S}_{inc}(\tilde{q}, \bar{y}; \bar{T})$ as follows:

$$\tilde{S}_{inc}(\tilde{q}, \bar{y}; \bar{T}) = 2Q \tilde{S}(Q, \bar{v}; \bar{T}),$$

(20)

where $\bar{y} = (\bar{v}/Q - \bar{q})/2$. With this definition, the non-condensate contribution to the incoherent response becomes temperature and momentum indepen-
and so becomes an universal function valid for all values of $Y$ as long as $\bar{T} \leq \bar{T}_c$. The non-condensate contribution to the total response reaches the incoherent limit at high momentum transfers, so $\hat{J}_{\text{nc}}(Q, Y; \bar{T})$ approaches $\hat{J}_{\text{nc, inc}}(Y)$ when $Q \to \infty$. This is indeed the case as shown in Fig. 6. As can be seen, already at $Q = 2$ the incoherent limit seems to be almost reached, which means that at any temperature below $\bar{T}_c$ scaling is well recovered when the transferred momentum is larger than $\bar{q} = 2\sqrt{\bar{T}_c} \approx 5$.

Scaling can also be recovered at temperatures above the Bose–Einstein transition temperature. However, in that case the following alternative definition of the Compton profile may be used:

$$\hat{J}^+(Q, Y; \bar{T}) = 2Q \bar{T}^{3/2}\hat{S}(Q, v; \bar{T}).$$

With this definition, the classical response becomes $Q$- and $\bar{T}$-independent according to the expression

$$\hat{J}^+_\text{cl}(Y) = \frac{1}{\sqrt{\pi}} e^{-Y^2},$$

and therefore this is the limiting case to which the response of the free Bose gas tends when the temperature is risen. The response $\hat{J}^+(Q, Y; \bar{T})$ and the incoherent response $\hat{J}^+_{\text{nc}}(Q, Y; \bar{T})$ at $Q = 1$ are compared at different $\bar{T}$’s with $\hat{J}^+_{\text{cl}}(Y)$ in Fig. 7. Both functions approach the classical behaviour when the temperature is risen, even though it is remarkable how far should the temperature go in order to reach that limit. In any case and as expected, the incoherent response approaches faster $\hat{J}^+_{\text{cl}}(Y)$, a fact that can be understood recalling that the total response contains also coherent contributions that do not scale in the same variables. In this way, the different velocity at which both functions approach $\hat{J}^+_{\text{cl}}(Y)$ gives a measure of how fast the coherent response goes to zero. Finally the main reason why the scaling in Eq. (22) is proportional to $\bar{T}^{3/2}$ may be understood recalling that in the classical regime $z$ is proportional to $\bar{T}^{3/2}$, so that in the end both dependencies cancel and $\hat{J}^+_\text{cl}(Y)$ becomes $\bar{T}$-independent. This explains why the scaling law at $\bar{T} > \bar{T}_c$ and $\bar{T} \leq \bar{T}_c$ should be different, as in the latter case the fugacity vanishes and therefore it cannot introduce any explicit dependence on $\bar{T}$ as happens at high temperatures.

In summary, the dynamic structure function of the free Bose gas at finite temperatures is shown to contain both coherent and incoherent contributions. At low temperatures compared to the Bose–Einstein transition temperature $\bar{T}_c$, the total response is mainly incoherent and tends to the limiting incoherent value $\delta(\omega - q^2/2m)$. When the temperature is risen, coherent contributions presenting logarithmic singularities at $\omega = \pm q^2/2m$ appear, and they actually over-
come the contribution of the incoherent response when $T \approx T_c$. When $T$ is increased above $T_c$, the logarithmic divergences disappear but a visible signature of their presence below $T_c$ still remain in both $S_{\text{inc}}$ and $S_{\text{coh}}$. When $T \gg T_c$ the coherent response cancels while the incoherent and total responses approach the classical limit.

The incoherent limit is always recovered when the transferred momentum is high, while the classical limit is only reached at high $T$. Below $T_c$, the presence of singularities in the response is also reflected in their lowest order energy-weighted sum rules. Finally, in the high $q$ limit the total response can be written in the form of a Compton profile that scales in the West scaling variable $Y$. The temperature dependence can also be removed from the response by using an appropriate redefinition of $Y$, even though the transformation is different at $T < T_c$ and at $T > T_c$ due to the different temperature dependence of the chemical potential. Despite the simplicity of the system analyzed and the fact that the excitation spectrum of an interacting Bose system will be different the results described in this work are expected to enlight some aspects of the finite temperature response of both weakly and strong interacting Bose systems.

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