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Singular Response of an Ideal Bose Gas.

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Summary. — The concept of singular response is defined and used for the investigation of the Bose-Einstein condensation of an ideal gas. It is shown that, apart from the well-known symmetry that is broken by the transition by the state with $k = 0$, also states with $k \neq 0$ participate in the condensation. The new condensed state is shown to possess off-diagonal long-range order and to be a product of Glauber coherent states with $k = 0$ and $k \neq 0$.

1. – Introduction.

We define singular response of the expectation value of an observable R to an external probe η by

$$\lim_{\eta \to 0} R(\eta) \neq R(0) . \tag{1}$$

In words, we calculate R in the presence of η, then let η go to zero. Next we calculate R with no external probe. If these two results are not the same we say that R responded in a singular way to the probe η. Singular response can be used for the investigation of phase transitions. A simple example for this is the case where eq. (1) holds for all temperatures (T) lower than some critical temperature (T_c), while the response is nonsingular, *i.e.*

$$\lim_{\eta \to 0} R(\eta) = R(0)$$

for $T > T_c$. Note that if the response is singular for all temperatures, it reflects the sensitivity of the system to the probe and the technique can be used to obtain a dispersion relation for internal excitations of the system. The latter case is sometimes used [1] to obtain the plasma-frequency branch of the spectrum for electron-ion system. In general a singular response reflects intrinsic properties of the system on which the probe is applied.

In this paper we wish to study the Bose-Einstein condensation (BEC) from the point of view of singular response (SR). Preliminary results along this spirit were presented elsewhere [2]. In Sect. **2** the early results are rederived in a slightly different way and we show the nonanalytic dependence of the chemical potential μ on the external probe as the latter is set equal to zero at the end of the calculations. The SR for our case of BEC is summarized in Sect. **3**. In this Section one sees the reflection of the singular response in broken symmetry. This latter term means, in the present context, a special case of SR, *viz.* it implies the existence of a quantity K that

$$\lim_{\eta\to 0} K(\eta) \neq 0 ,$$

while $K(0) = 0$. The results of the SR for the BEC are shown to imply the important consequence, which is true also for interacting bosons [3] namely, that for $T < T_c$ the system has a finite fraction of particles in a coherent state as defined by GLAUBER [4]. (Note that everywhere we deal in the limit of particle number $N \to \infty$ while $N/V < \infty$ with V the volume of our system.) The manner of the approach to zero of μ in BEC in our case is dealt with in more detail in Sect. **4** where we show that the SR of the free Bose particle implies that the condensation is of the form of a generalized Bose Einstein condensation (GBEC) as ws introduced by GIRARDEAU [5]. It is shown that at the GBEC the system possesses an off-diagonal long-range order (ODLRO), a concept that was introduced by YANG [6] and discussed extensively since, in particular with its connection to superfluidity [7]. The ODLRO of free bose system for $T > T_c$ was discussed earlier [8]. In Sect. **5** we conclude and make contact between our discussion of the particular phase transition considered and the general discussion of phase transition as was given by EMCH [9].

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2. – Bose-Einstein condensation in the presence of an external source.

In this Section a brief resume of the result obtained in a slightly different way in CR (2) is given. This will fix the notation and will define the problem.

Consider an ideal Bose gas subject to an external field. (It is tempting to associate the helium vapour with the external field when the helium problem is considered; here, of course, the gas is ideal and the physical meaning of the external source is obscure.) The Hamiltonian of the system is

$$H = \sum_k (\varepsilon_k - \mu) a_k^\dagger a_k + \sum_k (\eta a_k^\dagger + \eta^* a_k) . \tag{2}$$

Here $a_k^\dagger$ is the creation operator for a particle in the plane-wave state, ε_k the kinetic energy of the free particle

$$\varepsilon_k = \frac{\hbar k^2}{2m} ,$$

with m the mass of the particle; and η is a fixed, but arbitrary, parameter which, for simplicity, is taken as independent of the wave number k. The operators obey the Bose-Einstein commutation law.

We wish to calculate the Gibbs potential (Ω_η) of this system,

$$\exp[-\beta\Omega_\eta] \equiv \mathrm{Tr}\,[\exp[-\beta H]] \equiv Z_\eta ,$$

where $\beta = (k_B T)^{-1}$ with T the temperature and k_B being Boltzmann's constant; Tr stands for the trace over all states and all particle numbers. Upon diagonalization, the Hamiltonian becomes

$$H = \sum_k (\varepsilon_k - \mu) e^A a_k^\dagger a_k e^{-A} - \frac{|\eta|^2}{\varepsilon_k - \mu} , \tag{3}$$

with

$$A = \sum_k \left\{ \frac{\eta^*}{\varepsilon_k - \mu} a_k + \frac{\eta}{\varepsilon_k - \mu} a_k^\dagger \right\} . \tag{4}$$

Now because of the invariance of the trace with respect to cyclic permutation we obtain the exact result

$$\exp[-\beta\Omega_\eta] = \exp[-\beta\Omega_0] \exp\left[\sum_k \frac{\beta|\eta|^2}{\varepsilon_k - \mu} \right] . \tag{5}$$

Here Ω_0 is the Gibbs potential in the absence of the external source.

The number of particles which are expected to be in the state k is

$$n_k = \langle a_k^\dagger a_k \rangle_\eta \equiv \frac{\mathrm{Tr}\,[a_k^\dagger a_k \exp[-\beta H]]}{Z_\eta}, \tag{6}$$

this quantity must be positive definite. Simple calculation yields

$$n_k = \frac{|\eta|^2}{(\varepsilon_k-\mu)^2} + \frac{1}{\exp[\beta(\varepsilon_k-\mu)]-1}\,. \tag{7}$$

If we assume $\mu > 0$ we arrive at the relation that $\beta|\eta|^2 > \mu$ and since η though fixed is arbitrarily small μ must satisfy $\mu \leqslant 0$ for $T \neq 0$. For $\mu \leqslant 0$, $n_k(\mu)$ is a monotonically increasing function of μ, as is in the usual case [10]. The total number of particles N is

$$N = \sum_k n_k = \sum_k \frac{|\eta|^2}{(\varepsilon_k-\mu)^2} + \sum_k \frac{1}{\exp[\beta(\varepsilon_k-\mu)]-1}\,. \tag{8}$$

Now, as usual [10], we demand that $\varrho_\eta = N/V$ remain finite with both N, $V \to \infty$. This with $\mu \leqslant 0$ and $\varepsilon_k \geqslant 0$, implies that $\mu \to 0$ for large enough ϱ_η. For very large V we can transform the second sum on the right-hand side of eq. (8) into an integral. (If we leave out the first term there (or some terms) we see that for it to contribute μ must go to zero as $1/V$ but then the term $|\eta|^2/\mu^2$ will diverge; thus, this procedure is incorrect here.) We get in the limit $\mu \to 0$

$$N = \sum_k \frac{|\eta|^2}{(\varepsilon_k-\mu)^2} + N_c\,, \tag{9}$$

with

$$N_c = V\int \mathrm{d}^3k\,\frac{1}{\exp[\beta(\hbar k^2/2m)]-1}\,. \tag{10}$$

The apparently (see below) dominant term in the sum that appears in eq. (8) is $|\eta|^2/\mu^2$ and since $N_c/V < \infty$ we have that $|\eta|^2/\mu^2 \sim N/V$, *i.e.* $\mu \sim 1/\sqrt{V}$. This result is true if only one term is kept. However, we see directly that for $\mu \sim 1/\sqrt{V}$ all terms for which $\varepsilon_k \ll 1/\sqrt{V}$ are of the same order of magnitude as the original term for which $k=0$. Hence the correct procedure is the retention of the added term,

$$\sum_k \frac{|\eta|^2}{(\varepsilon_k-\mu)^2}\,,$$

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[10] F. LONDON: *Superfluidity* (New York, 1954).

which when summed must be of the order N. This is dealt with in Sect. **3**. In the next Section we list the results of the naive approach which serves to show the nonanalytic behaviour of the various quantities with respect to a perturbation of the type $\eta a_0^\dagger + \eta^* a_0$.

3. – Singular response of the condensed system.

We refer in this Section to the SR to an external probe $\eta a_0^\dagger + \eta^* a_0$. This is a special case of the general probe eq. (2). Although it is expected that the SR to the general probe reflects the true nature of the condensation, the results of the special case probe serves to show the presence of singular response in the system. The analysis of the previous Section leads to the following results, all valid for temperatures below the transition temperatures, *viz.* with $\mu \to 0$.

1) $$\lim_{\eta\to 0} \Omega_\eta = \Omega_0 ,$$

i.e. the Gibbs potential is continuous in η for $\eta \to 0$. This follows from the result that $|\eta|^2/\mu^2 \neq 0$ in the limit, while Ω has $|\eta|^2/\mu$. Physically this is equivalent to Ω being essentially an energy and although there are many particles in the state $k = 0$, their energy is still zero.

2) $$\langle n_0 \rangle_{\eta=0} \sim \frac{1}{\beta\mu} , \qquad \lim_{\eta\to 0} \langle n_0 \rangle \sim |\eta|^2/\mu^2 .$$

Thus the average number of particles in the $k = 0$ state reacts in a singular manner to the external field η.

3) $$\mu(\eta = 0) \sim 1/V , \qquad \lim_{\eta\to 0} \mu(\eta) \sim 1/\sqrt{V} .$$

μ behaves in a nonanalytic way as a function of η.

4) $$\langle a_0 \rangle_{\eta=0} = 0 , \qquad \langle a_0 \rangle_\eta = \frac{\partial}{\partial \eta^*} \ln Z_\eta = \frac{\eta}{\mu} \to \sqrt{n_0} ,$$

i.e. $\langle a_0 \rangle$ expresses the broken symmetry that occurs at BEC,

$$\langle a_0^\dagger \rangle_\eta = \overline{\langle a_0 \rangle_\eta} = \frac{\eta^*}{\mu} . \tag{11}$$

5) In the limit $\mu \to 0$; N, $V \to \infty$ considered here we get

$$\langle a_0^\dagger a_0 \rangle = \langle a_0^\dagger \rangle \langle a_0 \rangle , \tag{12}$$

i.e. the particles in the $k=0$ state must be in the coherent state of Glauber [4], *viz.*

$$a_0|\alpha_0\rangle = \frac{\eta}{\mu}|\alpha_0\rangle \,. \tag{13}$$

This follows from Schwarz's inequality. Thus we have a more physical meaning to the term broken symmetry: here like a small magnetic field that picks up a direction in the 3-dimensional space, the probe picks up the phase of the Glauber coherent state [2].

In the next Section we discuss the important question of the states with $k \neq 0$.

4. – Condensation of states with $k \neq 0$.

The results of the previous Section are strictly valid only for perturbation

$$H' = \eta a_0^\dagger + \eta^* a_0 \,.$$

This led to $\mu \sim 1/\sqrt{V}$. We now recall that the argument for BEC being a condensation into one state with $k=0$ is based on the result that $\mu \sim 1/V$ and hence negligible when compared with even the lowest single-particle excitation which has a $V^{-\frac{2}{3}}$ volume dependence. Our new result, namely $\mu \sim 1/\sqrt{V}$ drastically alters this, in fact occupation of the states with momentum k, is of the order $|\eta|^2/(\varepsilon_k - \mu)^2$ rather than the usual $\{\exp[\beta(\varepsilon_k - \mu)] - 1\}^{-1}$ for small ε_k, since *now* $V^{-\frac{2}{3}}$ is negligible when compared with $V^{-\frac{1}{2}}$. This is the central result of this paper, so we wish to restate this point; in the thermodynamic limit ($V \to \infty$) and with condensation ($\mu \to 0$) and with a fixed η to be set equal zero at the end we get that, for $\varepsilon_k < \lim_{\eta \to 0} \mu(\eta)$ the result

$$\lim_{\eta \to 0} \langle n_k \rangle_\eta = \frac{|\eta|^2}{(\varepsilon_k - \mu)^2} \,, \tag{14}$$

n_k being the number of particles per unit volume in the state k.

Now by similar argument to the one that led to eq. (10) we conclude that all the states with $\varepsilon_k \lessdot \mu_\eta$ are in the Glauber [4] coherent state. Although there are in the thermodynamic limit many (infinite) such states, they all shrink to $\lim k \to 0$ in the sense that the integral, N_c eq. (10), is now a principle value integral. This type of condensation is the one introduced by GIRARDEAU [5]. We have shown thus that even the condensation of the ideal Bose gas is, from the view adopted here, a «generalized Bose-Einstein condensation» [5]. For convenience we shall replace the sum of these states by an integral with the upper limit $k \to \infty$. This seems reasonable because states with large ε_k will contribute little to the integral (the integral $\sim \varepsilon_k^{-2}$ for large ε_k). If we now consider the high-density limit where the term N_c (eq. (10)) is negligible, we get ($\hbar = 2m = 1$)

$$\frac{N}{V} = |\eta|^2 4\pi \int_0^\infty \frac{k^2 \mathrm{d}k}{(k^2-\mu)^2} = |\eta|^2 \frac{\pi^2}{\sqrt{-\mu}}, \tag{15}$$

which gives the dependence on $|\eta|^2$ of $\sqrt{-\mu}$ for $\mu \to 0^-$.

We can now calculate the spatial off-diagonal matrix elements of the density operator

$$\langle x|\varrho|x'\rangle = V^{-1} \sum_k n_k \exp[ik\cdot(x-x')] \tag{16}$$

The result is $(r = |x-x'|,\ r \neq 0)$

$$\varrho(r) = \frac{N/V}{2\pi} \exp[-\sqrt{-\mu}\, r].$$

In the limit $\mu \to 0^-$ we see that the system possesses an off-diagonal long-range order (ODLRO). Note that the $\mu \to 0$ must be taken before the $r \to \infty$ limit since the limit $\mu \to 0$ is associated with the thermodynamic ($V \to \infty$) limit.

The fact that the calculations were carried out in the high-density limit ($N \gg N_c$) does not affect the result that ODLRO exists in our system even at lower densities (but with BEC, of course). This is so because retention of the term N_c will not affect the calculations apart from replacing N/V in eq. (15) by $(N-N_c)/V$. It is perhaps satisfying that the result for the general probe (all k) leads to an intensive μ, as it should.

5. – Concluding remarks.

The theory of singular response has not as yet been formulated in its full generality in the literature. Nonetheless as a calculational technique the method has been used extensively. In this paper we investigated the well-known Bose-Einstein condensation of an ideal gas from the point of view of the SR. We obtained in agreement with a previous result (2) that the phase transition that occurs here breaks a symmetry in the phase of the wave functions, whose mode, k, participates in the condensate. It was shown that the onset of the condensation leads to the coherent state of Glauber (4). The result for the simple Bose-Einstein condensation was generalized to systems of interacting bosons (3). The results are basically the same. It is believed that also the generalized BEC could be formulated for the case of interacting bosons.

Central to the discussion was the manner of approach to zero of the chemical potential. In fact upon reflecting on the mathematics used, one sees that μ played a role as a part of the Hamiltonian of the system. Thus the phase transition here fits the general discussion of phase transition that is given by EMCH (9) in that the elements of the diagonalized Hamiltonian are temperature-dependent. Here this was so even for $T > T_c$ but the temperature-dependence at $T > T_c$ of μ is not important.

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RIASSUNTO (*)

Si definisce il concetto di risposta singolare e lo si usa per lo studio della condensazione di Bose-Einstein di un gas ideale. Si dimostra che, oltre alla ben nota simmetria infranta dalla transizione dello stato con $k = 0$, anche stati con $k \neq 0$ partecipano alla condensazione. Si dimostra che il nuovo stato condensato possiede fuori della diagonale un ordine di lungo raggio che è il prodotto di stati coerenti di Glauber con $k = 0$ e $k \neq 0$.

(*) *Traduzione a cura della Redazione.*

Сингулярное поведение идеального Бозе-газа.

Резюме (*). — Определяется концепция сингулярного поведения, которая используется для исследования конденсации Бозе-Эйнштейна в случае идеального газа. Показывается, что кроме хорошо известной симметрии, которая нарушается переходом в состояние с $k=0$, также состояния с $k \neq 0$ участвуют в конденсации. Отмечается, что новое конденсированное состояние имеет диагональный порядок в в большой области и является произведением когерентных состояний Глаубера с $k=0$ и $k \neq 0$.

(*) *Переведено редакцией.*