Planck, Photon Statistics, and Bose-Einstein Condensation

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Abstract

The interplay between optical and statistical physics is a rich and exciting field of study. Black body radiation was the first application of photon statistics, although it was initially treated as a problem of the cavity oscillators in equilibrium with the photon field. However Planck surprisingly resisted the idea that anything physical would be quantized for a long time after he had solved the problem. We trace this development.

Then, after the invention of the laser itself, it proved difficult to develop a theory of laser action that could account for photon statistics, i.e. fluctuations near threshold. This was accomplished in 1965. After Bose-Einstein condensation was successfully achieved, the same problem arose in this case. The fluctuation problem had not been treated adequately even for the ideal Bose gas. However this problem has now been solved using the same techniques as in the theory of laser action.

1 Introduction

Optics was the original handle by which classical physicists learned to pry their way into the mysteries of quantum physics. This was appropriate because optics possesses a dual character, in one limit the purely classical wave theory, and in the other the purely quantum mechanical particle limit. In 1900, when the spectrum of black body radiation was being studied in detail, only the classical side was known. This was used to connect it with Thermodynamics, from which many of its properties could be derived. But the Wien spectral law, which characterized the general, but not specific form of the spectral law, was as far as thermodynamics could take one.
In order to get a specific law, Planck had to also draw on the probabilistic considerations of Boltzmann, a real departure for Planck, and he inadvertently drew into focus the particle aspect of the problem, without at that time understanding just how radical his innovation was. But this added statistics and fluctuations into the mix. A main point in this paper will be to show the role that fluctuations played in Planck’s and Einstein’s thinking in the early days of quantum theory, the important role it played in the development of the quantum theory of the laser, and finally, how the laser theory allows one to treat the fluctuations in a Bose-Einstein gas, both above and below the critical temperature.

A second major theme in the paper will be to pursue the historical thread running through Planck’s work. In their desire to present a coherent story, leading from classical physics to quantum physics, most textbooks leave out or distort the history of the subject, which is consequently not well known. But in this case, the courage of Planck in abandoning his lifelong distrust of probability, coupled with his total reluctance to abandon the principles of classical physics, led to a series of fascinating ironies that strongly affected the history of the subject, and they deserve to be better known.

A further hidden element guiding the development of the early quantum theory, the laser, and Bose-Einstein condensation, was the connection between advancing technology and experimental technique. The effects of technology are apparent in the laser and Bose-Einstein condensation, although they are usually not appreciated as an input into early quantum theory, but the accurate measurements of the black body spectra were made possible by the invention of the bolometer by Langley, who became the first director of the Smithsonian Institution in America. But also, the funding for the improvements of the bolometer so that measurements could be extended into the infrared, which became the most relevant measurements, leading to the breakdown of Wien’s specific radiation law, was provided by the power company of Berlin, which city had recently been electrified. Black body radiation is the least efficient means of illumination (one wants to be far from equilibrium) and it set a standard against which to measure efficiencies. So it turns out that the interest in funding such an abstruse subject as black body radiation was actually driven by the technology of the day.

The interconnections between all these threads forms an interesting subject in itself, but here we shall only go so far as to follow a few of them. We shall emphasize some of the interesting historical details that surround Planck’s work, which seem to be almost unknown to physicists. We have drawn heavily on Planck’s original papers, [Planck (1900 a,b)], reproduced with comments in [Ter Haar (1967)], and Planck’s book on heat radiation [Planck (1913)]. We have also extensively used [Kuhn (1978)], [Hermann (1971)], [Jammer (1966)], and [Heilbron (1996)]. Some other good references are [Klein (1975)],
We go on to describe in some detail exactly what Planck did, and did not do, and the importance of fluctuations in his work. Their true meaning and importance was established by Einstein [Einstein (1909)]. We then describe how fluctuations enter into the theory of the laser, and how this theory has been used to treat fluctuations in Bose-Einstein Condensation.

2 Planck’s Black Body Radiation Law

2.1 Some Ironical Historical Details Concerning Planck

It is rather universally assumed that when Planck introduced the quantum in 1900, [Planck (1900a), Planck (1900b)] he quantized the energy levels of an oscillator. But in fact, what he did was very ambiguous [Kuhn (1978)], and we shall produce some strong evidence that at that time he was thinking more along the lines of quantizing the size of cells in phase space. Furthermore, he fought the idea of quantizing both radiation and the oscillator. In fact, as late as 1913, when he published the second edition of his book on heat radiation [Planck (1913)], he did not believe that the energy levels of either the oscillator or the radiation were quantized, even though Einstein had quantized both of them, the photon in 1905, [Einstein (1905)] and the oscillator in 1907 [Einstein 1907]. We shall introduce a number of quotes from Planck’s original theoretical paper on quantum theory [Planck (1900b)] which is usually taken as the birth of quantum theory, and from his heat radiation book, to prove his aversion to quantizing anything physical. It was not until Bohr had quantized the levels of the hydrogen atom [Bohr (1913)], and the discussions that followed this, that Planck and most of his colleagues accepted quantization as a fact of nature.

It is well known that Planck rejected the idea of photons until quite late, but here is a quote from the introduction of his 1913 book that not only proves that, but that also outlines his philosophy on the subject, which we think not only explains his opinions, but also made it possible for him to discover the law of black body radiation long before either he or anyone else understood its consequences. He says, “While many physicists, through conservatism, reject the ideas developed by me, or at any rate maintain an expectant attitude, a few authors have attacked them for the opposite reason, namely, as being inadequate, and have felt compelled to supplement them by assumptions of a still more radical nature, for example, by the assumption that any radiant energy whatever, even though it travel freely in a vacuum, consists of indi-
visible quanta, or cells. Since nothing probably is a greater drawback to the successful development of a new hypothesis than overstepping its boundaries, I have always stood for making as close a connection between the hypothesis of quanta and the classical dynamics as possible, and for not stepping outside of the boundaries of the latter until the experimental facts leave no other course open. I have attempted to keep to this standpoint in the revision of this treatise necessary for a new edition.” Obviously he is referring disapprovingly to Einstein’s photons in the quote. However we shall see that the last part of the quote is also very relevant in deciding what he actually did.

What then led to the radically new form of the radiation law? It was the breaking up of the energy cells into finite units, so that statistics could be applied, which as he said he took directly from Boltzmann [Boltzmann (1877)] (who ultimately let the cell size go to zero), and his introduction of a new way of counting microstates. We point out that the introduction of the quantum alone was not enough to produce his formula. This is because when one uses Boltzmann statistics, if one changes the cell size, one merely changes the thermodynamic probability by an exponential multiplicative factor, which in turn leads to an additive constant in the entropy. Since in classical entropy, an additive constant has no physical significance, this is why the cell size doesn’t matter in classical physics. Planck’s argument, which led to a counting scheme that looks very like Bose statistics, introduced a cell size that is unique, and in fact is a fundamental constant of nature, and this was caused by his taking the entities that occupied these quantized units as indistinguishable. He was silent on this matter, and it took a long time for people to realize it.

The first inkling of what was happening came from two papers in 1911, one by Natanson [Natanson (1911)], and the other by Ehrenfest (1911)]. They both singled out Einstein’s derivation of the localized photon-like properties of electromagnetic waves [Einstein (1905)] in the limit where Wien’s radiation formula worked (Einstein took Wien’s formula as his starting point). They pointed out that his argument would not work with Planck’s formula instead of Wien’s and that Einstein’s argument presumes Boltzmann statistics. They then point out that Planck’s argument assumes that the energy units are indistinguishable, which they each find very puzzling. (Of course with hindsight, we realize that Wien’s formula holds in the particle-like domain where Einstein was operating, while the Rayleigh-Jeans formula holds in the wave-like regime. Einstein’s later 1909 paper on fluctuations [Einstein (1909)] sets out the particle-wave dichotomy for photons for the first time.)

Before we begin, we would like to point out that there were many historical ironies in Planck’s development. His thesis advisor (1879), Phillip von Jolly, told him that the development of the first and second laws of thermodynamics had completed the structure of theoretical physics and that a bright young man should think twice about entering the field [quoted by Heilbron (1996)].
(This in spite of the fact that Maxwell’s equations had been developed only ten years earlier. But it is known that Einstein in 1900 couldn’t find a course on electrodynamics at Zurich, and had to teach himself. New advances percolated at a slow rate in those days.)

Planck nonetheless thought that there was a lot left to do regarding entropy, and spent most of his early career developing the consequences of the second law, namely in chemical thermodynamics. This led to a call to Berlin in 1889 for him to replace Kirchoff, who had retired (but Planck was not initially appointed as a full professor). He soon complained in a letter that “nobody in Berlin is interested in entropy” [Heilbron (1996)]. But when he started working on black body radiation, he immediately looked for the connection between entropy and energy, while he said everyone else was looking for the connection between frequency and temperature.

Although he was initially under the influence of Ostwald and Mach (the great disbelievers in atomic theory, since atoms were then considered unobservable), Planck had slowly come to believe in atoms, as he thought it was the only way to treat certain problems, such as heat conduction and osmotic pressure, but he was sure that they were to be treated by mechanics. He was bitterly against the probability arguments of Boltzmann, whom he otherwise respected, because he thought the second law had to be exact. In fact he set an assistant, Zermelo (later of axiomatic set theory fame), to develop one of the two main arguments against Boltzmann, the “ergodic” argument [Zermelo (1896a,b), Boltzmann (1896a,b)], that a system in phase space will ultimately return to a point arbitrarily close to where it is now, even if far from equilibrium. (The other argument, due to Loschmidt, was the “time reversal” argument [Boltzmann (1877b)], that for every state heading toward equilibrium, there is another time-reversed state heading away from it).

He started to work on the black body radiation problem in 1896, and he thought [Planck (1900c)] he had proven Wien’s empirical radiation law (an exponential form, which actually holds only at relatively low temperatures, or high $\nu/T$). By 1900, experiments were being carried out at higher temperatures and lower, infra-red frequencies, and the experimentalists, Lummer and Pringsheim, and Planck’s colleagues, Rubens and Kurlbaum, were finding out that Wien’s law did not work. The energy at a given frequency at higher temperatures was becoming linear in the temperature (in accord with the not-yet-stated Rayleigh-Jeans law).

Planck developed his radiation law in a somewhat ad-hoc manner, which law worked very well, and he then set about to develop a theoretical explanation. At that time, there were a number of proposed hypothetical laws to deal with the discrepancy being discovered in Wien’s law. Planck’s worked almost perfectly, and was quickly accepted by the experimentalists. But it was clear that
for any law to be taken seriously, it had to be theoretically motivated. Planck
had become convinced that one could never discover the universal energy func-
tion by purely thermodynamic means, and he reluctantly decided to switch to
Boltzmann’s methods. In a later famous letter that Planck wrote about the
success of that effort, [letter to R. W. Wood, quoted in Hermann (1971)], he
said that switching to probability arguments was “an act of desperation”, but
that breaking the cell into units of $h\nu$ was “purely a formal assumption and
I really did not give it much thought” (since the dependence on $\nu$ is actually
required by Wien’s spectral law, a direct consequence of the second law).

In order to apply the probability theory, Planck wrote $S = k_B \ln W$, to con-
nect the thermodynamic probability $W$ with the entropy $S$. In doing so, he
wrote this equation for the first time, as Boltzmann, on whose tombstone
the equation appears, never actually wrote it. Boltzmann always used the $H$-
theorem, or something equivalent. Another related irony is that Boltzmann
never wrote $k_B$ as a separate constant, but always used $(R/N_0)$, the gas-
constant per molecule. Planck’s radiation law allowed one to calculate $h$, $k_B$
and $N_0$ accurately for the first time, as well as the electrical charge e, from the
Faraday constant. As a result, Planck thought it only simple justice that $k_B$
should be called Planck’s constant, or at least the Planck-Boltzmann constant,
but it never happened. The poor fellow was stuck with $h$!

In 1908, Arrhenius (who wielded tremendous influence) tried to convince the
Swedish Academy [quoted in Heilbron (1996)] to give Planck the Nobel Prize
because “it has been made extremely plausible that the view that matter con-
sists of molecules and atoms is essentially correct... No doubt this is the most
important offspring of Planck’s magnificent work.” No mention of the quantum
of action. But Planck had to wait another 10 years, because Lorentz [Lorentz
(1908)] had come up with an argument that the Rayleigh-Jeans law had to be
the correct classical law, and that the reason it failed at high temperature
was that the system could not come to equilibrium at high temperatures.
He withdrew this opinion after the experimentalists convinced him that if
the Rayleigh-Jeans law were correct, with its ultraviolet catastrophe, many
substances would glow in the dark at room temperature. But the Academy
decided that the jury was still out on Planck’s work.

An even further irony is that Planck was ultimately convinced of the truth of
the new quantum theory by Nernst’s Heat Theorem, that $C_V \to 0$ as $T \to 0$.
This implies that $W \to 1$, and $S' \to 0$, with no additive constant, so that
there is an absolute minimum entropy reached at absolute zero. This is a
purely probabilistic argument, so far had Planck gone in changing his view.
The ultimate irony is that when Boltzmann committed suicide, from sickness
and frustration with all his critics, the University of Vienna offered Planck his
chair. (Planck, who loved Vienna and was a professional quality pianist, was
tempted. But his colleagues at Berlin managed to make it worthwhile for him
Planck [Planck (1913)] praises Einstein’s derivation of $C_V$, but he never mentions his quantization of the energy levels of the oscillator to $E_n = n\hbar \nu$, or uses it. He merely says it is beyond the scope of his book, but it strikes us as rather strange that he chose not to further comment on it, as it seems to disagree with Planck’s interpretation.

### 2.2 Thermodynamic Background Leading to the Radiation Law

The concept of a black body was introduced by Kirchoff in 1860 [Kirchoff (1860)]. In what follows, including Planck’s Law, we are going to give a rather self-contained argument that will not always be historically complete, although we will indicate certain occasions where historic remarks are relevant, because they determine motivations, and provide a context for what people did. We note that the history is often fairly complicated, controversies arose and sometimes took many years to get resolved. Sometimes it is even true that no one knew precisely what had been accomplished until much later. (As an example, we note that the “ultraviolet catastrophe” was not even named as such [Ehrenfest 1911] until 11 years after Planck had solved the problem!) We are not professional historians, but at least in the case of Planck, there are many “smoking guns” within his work to justify what we say.

Kirchoff knew from looking at spectral lines from the sun that there was heat energy in empty space, and postulated equilibrium radiation. But the knowledge of what it consisted of was primitive. Maxwell’s equations had not yet been postulated, and the identity of heat rays and light rays had not yet been established. Nor had the existence of atoms in the walls of a cavity, nor that an oscillator radiates and absorbs electromagnetic energy, or that such energy carries momentum. Thus it is rather amazing that Kirchoff should have established on the basis of relatively simple arguments that within a cavity at equilibrium, this radiation should be independent of the substance of the walls of the cavity, and that at a fixed temperature a good emitter of radiation should be a good absorber. A perfect absorber should then radiate an energy equivalent to everything that falls upon it within the cavity at equilibrium, independently at each frequency. The radiation emitted by such a perfect absorber he called black radiation, and there should then be a universal function $u(\nu, T)$ that describes the radiation density in equilibrium with the walls, that on average gets both absorbed and reemitted, at any particular frequency and temperature.

Because of the unknown nature of what happened within the cavity, Kirchoff was attacked for each of the assumptions he made leading to this conclusion,
and the existence of this universal function was dismissed by many. Meanwhile
others tried to change the assumptions and re-derive the results. Even after
the turn of the century this argument went on (well after Planck’s work).
Although Planck does not explicitly mention these controversies in the 1913
edition of his book on heat radiation, he was nonetheless clearly affected by
them, as he takes over 20 pages to discuss and justify Kirchhoff’s law.

However, after Maxwell, Boltzmann tried to find a thermodynamic “equation
of state” for the radiation in 1884 (similar to $PV = NRT$ for particles) [Boltz-
mann (1884)], and after Hertz had produced electromagnetic waves in 1888,
Wien tried in 1893 [Wien (1893)] to find the spectral function of Kirchhoff. He
succeeded to the extent of reducing the problem to a single function of $\nu/T$,
which is as far as one can go thermodynamically, and for which he ultimately
won the Nobel Prize.

Since the radiation hitting an area $A$ of the wall of a cavity carries both mo-
mentum density and energy density, Boltzmann was able to treat it similarly
to a particle flux hitting the wall, and showed that

$$P(T) = \frac{1}{3} u(T)$$  \hspace{1cm} (2.1)

where $P_\nu$ and $u_\nu$ refer to the pressure and energy density between frequencies
$\nu$ and $(\nu + d\nu)$. The difference between this formula and the non-relativistic
one is the factor $1/3$, rather than the $2/3$ for particles, which comes from
the non-relativistic form for the energy ($E = mv^2/2 = pv/2$) rather than
the extreme relativistic form for light ($E = pc$). Boltzmann then used this in
connection with the second law of thermodynamics

$$dU = TdS - PdV, \quad \left(\frac{\partial U}{\partial V}\right)_T = T \left(\frac{\partial S}{\partial V}\right)_T - P = T \left(\frac{\partial P}{\partial T}\right)_V - P,$$  \hspace{1cm} (2.2)

together with $U = Vu$, to get

$$u = T \left(\frac{1}{3} \frac{du}{dT}\right) - \frac{1}{3} u,$$

$$4u = T \frac{du}{dT},$$

$$\ln u = 4 \ln T + \text{const}, \quad u = \sigma T^4,$$  \hspace{1cm} (2.3)

the Stefan-Boltzmann law. Before Boltzmann derived it theoretically, Stefan
had correctly guessed its form by examining some data that was not only
inadequate, but that we now know was inaccurate as well.
For the entropy, we again use the equation (2.2). If we define the entropy density $s$ as $S = Vs$, then

$$u = Ts - \frac{1}{3}u,$$

$$s = \frac{4}{3} \frac{u}{T}, \quad S = Vs = \frac{4}{3} \sigma T^3 V.$$  \hspace{1cm} (2.4)

Eq. (2.4) implies that during an adiabatic expansion of the cavity, so that the entropy is constant, we will have $VT^3 = \text{const.}$

### 2.2.1 Wien’s Spectral Law

In 1888 Hertz showed the reality of Maxwell waves. In 1893 Wien applied the laws of thermodynamics and electromagnetism to the problem of black body radiation [Wien (1893)] and succeeded in reducing Kirchhoff’s universal function to a function of one variable. That is as far as one can go in classical physics. Wien tackled the problem of including the frequency in the black body law by considering an adiabatic motion of a wall of the cavity. This induced a Doppler shift on the radiation, while at the same time the wall did work on the radiation. Born’s Atomic Physics book [Born (1929)] has a simplified treatment in an appendix. But we will consider a much simpler technique based on adiabatic invariance, that was not available to Wien, but was first introduced by Ehrenfest in 1913 [Ehrenfest (1913)]. Ehrenfest was looking for some quantity that would not change while the external parameters of the system undergo a slow adiabatic change. He reasoned that such a quantity would be a good candidate for quantization, since it would not undergo a gradual change during the process, but could only change abruptly. This became the theoretical underpinning for the Bohr-Sommerfeld-Wilson quantization rule.

First we have to find the normal modes of the radiation. We assume the cavity is a cube, of side $L$, since for all but the lowest normal modes the shape does not matter. We also assume that the walls are fully reflecting and use standing wave boundary conditions. Then the modes for a Fourier expansion of the field satisfy

$$k_x L = n_x \pi, \quad k_y L = n_y \pi, \quad k_z L = n_z \pi, \quad k^2 = \omega^2 / c^2.$$  \hspace{1cm} (2.5)

The last of these equations comes from the wave equation for the fields. Here the $n$’s are positive integers. The number of modes in a region is given by

$$\Delta n_x \Delta n_y \Delta n_z = \Sigma_n = \frac{L^3}{\pi^3} \Delta k_x \Delta k_y \Delta k_z \rightarrow \frac{L^3}{8\pi^3} 4\pi k^2 dk = \frac{L^3}{8\pi^3} 4\pi \frac{8\pi^3}{c^3} \nu^2 d\nu.$$  \hspace{1cm} (2.6)
The 8 in the denominator of the first line is due to the fact that the \( n \)'s are positive, so only the first octant is important, but we are integrating the \( k \)'s over all of \( k \) space. Finally we must introduce another factor of 2 because there are two degrees of polarization for each direction in \( k \) space. So

\[
\Sigma_n = V \frac{8\pi}{c^3} \nu^2 d\nu. \tag{2.7}
\]

Rayleigh introduced the counting of modes of the field [Rayleigh (1900)] in 1900. He did it only qualitatively, following an earlier procedure he had used for sound waves. He then said the total energy density should be

\[
u_\nu d\nu = dU/V = \Sigma n \bar{\epsilon}_n = \frac{8\pi}{c^3} \nu^2 k_B T d\nu. \tag{2.8}
\]

Here represents the average energy of a mode, which by the equipartition theorem should be \( k_B T \). In 1905 he added the numerical factors in the above equation [Rayleigh (1905)], but made a minor mistake which was corrected by Jeans [Jeans (1905)], who emphasized how important and inescapable the above formula is. It has since been known as the Rayleigh-Jeans Law. Later Lorentz also gave a very general derivation [Lorentz (1908)], and for a while he and Jeans believed that the reason the equation did not work experimentally was because it was difficult to establish equilibrium at high frequencies, and the experiments were therefore not correct. But the equation blows up at high frequencies and so cannot be correct, a problem labeled by Ehrenfest as the “ultraviolet catastrophe” in 1911 [Ehrenfest (1911)].

To establish Wien’s law, one need only note that in Eq. (2.5), if one slowly changes \( L \), then \( k_i \) will slowly change, but \( n_i \) cannot and will stay fixed [Ter Haar (1967)]. This leads to

\[
k_i L = \text{const}, \quad \nu L = \text{const}, \quad \nu^3 V = \text{const},
\]

\[
T^3 V = \text{const}, \quad (\text{adiabatic change})
\]

\[
\nu/T = \text{const}.
\tag{2.9}
\]

The second line above is just Eq. (2.4), and so since the entropy of each node, \( s_n \), remains constant during an adiabatic change, one must have

\[
S/V = \Sigma_n s_n = \frac{8\pi}{c^3} \int \nu^2 s_n(\nu)(\nu/T)d\nu \equiv \int s_\nu d\nu, \tag{2.10}
\]

and therefore

\[
u_\nu = \frac{3}{4} T s_\nu = \frac{3}{4} \nu^3 (T/\nu) \frac{8\pi}{c^3} s_n(\nu/T) = \nu^3 f(\nu/T). \tag{2.11}
\]
The Rayleigh-Jeans law obviously takes this form, and so does an empirical radiation law proposed by Wien, [Wien (1996)]

\[ u_\nu = a\nu^3 e^{-b\nu/T}. \] (2.12)

(We call this Wien’s radiation law, to differentiate it from Eq. (2.11), Wien’s spectral law, firmly embedded in the laws of thermodynamics. Eq. (2.11) is sometimes called Wien’s displacement law, but we reserve this for the statement concerning the frequency where the energy distribution \( u_\nu \) is a maximum, \( \nu_{\max}/T = \text{const}, \) a consequence of Eq. (2.11).) Prior to 1900, all measurements were taken in the relatively high frequency domain, and Wien’s empirical law held pretty well. In fact, Planck had convinced himself that it must be the universal law. But the situation started changing after improvements were made to the experimental equipment. Then Rubens reported to Planck that at higher temperature for a given frequency the results were becoming linear in \( T \), and Planck realized he had to rethink his ideas.

2.3 Planck’s Introduction of the Quantum of Action

In his first theoretical paper in 1900, Planck [Planck (1900b)] makes two very confusing statements about the quantization of energy. He gives two successive sentences that are totally contradictory. After telling us that he will use Boltzmann’s method, he says, “If \( E \) [the energy of the \( N \) resonators of energy \( \nu \)] is considered to be a continuously divisible quantity, this distribution is possible in infinitely many ways. We consider, however - this is the most essential point of the whole calculation - \( E \) to be composed of a very definite number of equal parts and use thereto the constant of nature \( h = 6.55 \times 10^{-27} \text{erg} \cdot \text{sec}. \) This constant multiplied by the common frequency \( \nu \) of the resonators gives us the energy element \( \varepsilon \) in erg, and dividing \( E \) by \( \varepsilon \) we get the number \( P \) of energy elements which must be divided over the \( N \) resonators.” This statement is often quoted in history of quantum theory books and articles, and it certainly looks like Planck is talking about quantized energy levels.

However the very next sentence reads, “If the ratio is not an integer, we take for \( P \) an integer in the neighborhood.” Now if he really meant for the energy units to be quantized, \( P \) would naturally be an integer. Instead, we believe that he meant that the resonators could have any energy between \( n\varepsilon \) and \( (n+1)\varepsilon \), and one just lumped them all together as \( n\varepsilon \). In other words, he was quantizing in phase space, as Boltzmann had done, because as he said, one could not count states otherwise. He went on to count and characterize the energy elements, \( \varepsilon \), but he never said that an oscillator’s total energy must be \( n\varepsilon \), as Einstein later did. This is because, as we shall show below, he never believed it to be so.
In 1906-7, Planck gave a series of lectures in Berlin, which were published as a rather comprehensive book on “heat radiation”. He put out a second edition in 1913, [Planck (1913)] So the statements in the book should be indicative of how Planck thought about the subject as late as 1913.

There is no doubt that he introduced a quantum of action. He says as much in opening the preface to the second edition, “Recent advances in physical research have, on the whole been favorable to the special theory outlined in this book, in particular to the hypothesis of an elementary quantity of action.” But exactly what was quantized? He says on p. 125, “By the preceding developments the calculation of the entropy of a system of N molecules in a given thermodynamic state is, in general, reduced to the single problem of finding the magnitude $G$ of the region elements in the state space. That such a definite finite quantity really exists is a characteristic feature of the theory we are developing, as contrasted with that due to Boltzmann, and forms the content of the so-called hypothesis of quanta.”

It would seem fairly certain from this statement that his interest was in quantizing phase space. Shortly thereafter, in Part III, chapter III, p. 135, he introduces a model of the linear harmonic oscillator, specifically in phase space. He talks about the energy as an ellipse, and makes the transition from the coordinates $p$ and $x$ to $E$ and $\varphi$. He introduces the unit of action and takes the ellipses to have the average energy $(n + 1/2)\varepsilon$. He then makes an argument defending the appearance of what we now call “zero-point energy” (although his interpretation of it is totally different, having nothing to do with the uncertainty principle). It is hard to see why he would do that unless he thought the actual energies were distributed throughout the ellipse.

In part IV, chapter III, he shows in more detail his ideas about the emission of radiation. To modern eyes, this new theory of Planck’s looks very strange, as it makes absorption and emission totally different processes. But it was used by a number of people for a while, and it could explain the photoelectric effect, and a few other things, but it was forgotten relatively soon after Bohr quantized the Hydrogen atom later that year. (Bohr’s theory itself took some time to become accepted.) But it shows how Planck’s thinking was totally in flux, and how even then he was unwilling to believe in the quantization of energy levels. On p. 161, he says, “Whereas the absorption of radiation by an oscillator takes place in a perfectly continuous way, so that the energy of the oscillator increases continuously and at a constant rate, for the emission we have, in accordance with sec. 147, the following law: The oscillator emits in irregular intervals, subject to the laws of chance; it emits, however only at a moment when its energy of vibration is just equal to an integral multiple $n$ of the elementary quantum $\varepsilon = h\nu$, and then it always emits its whole energy of vibration $n\varepsilon$.”
He then describes how the oscillator absorbs energy at a constant rate, so that its energy increases linearly in time, and as it passes a given energy $n\varepsilon$, it may or may not radiate. If not, it continues on toward $(n + 1)\varepsilon$. So the oscillator energy is not quantized, but it emits in quantized units, of multiples of the quanta. On the basis of this model, he then goes on to calculate, p. 166, “Hence in the state of stationary equilibrium the number of oscillators whose energy lies between $n\hbar\nu$ and $(n + 1)\hbar\nu$ is...” and proceeds to give a complicated formula. But it is clear that the energy levels of the oscillator are not quantized, nor is the absorption of radiation. Only the emission of radiation is. Presumably after emission, the radiation got thermalized. So by this time in his thinking, something was quantized, but it did not stay quantized. He even draws a diagram giving the saw-toothed form described above for the energy of a single oscillator as a function of time.

We would like to say something about Planck’s intellectual attitude, which was summarized in the quote we gave at the beginning. He was an insider, an intellectual leader of the German community, and a man of total integrity. He had not the slightest desire to overthrow, or to see the overthrow, of the hard-won victories of classical science. And yet in times of crisis, he had the moral courage both to introduce a notion that he knew was radical, and whose implications no one could comprehend at the time, and also to suddenly abandon a strong belief that had sustained him throughout his career until then, namely that statistical considerations could not play a fundamental role in the understanding of physics at a profound level. The quote shows clearly that he would willingly go as far as he thought he had to go, but absolutely no further, and he lived up to this conviction.

For this reason, we believe that nobody but Planck could have made the advance that he made, when he did. His first paper was a purely phenomenological gimmick, which he made by performing his analysis in terms of entropy. As he said, he had devoted his life to examining entropy, which few people at the time took seriously. In his second paper he realized that the gimmick of the first paper had to correspond to a fundamental finite unit of action. But what that meant, nobody was prepared to say at that time. His own explanations were fuzzy, arbitrary, and had many loopholes. We think his revelation took the subject as far as it could have gone without a deeper analysis, which after all would consume many years of work by many people. In the total state of ignorance at that time, we think he did exactly what he was mentally inclined to do. He took the subject as far as it could go at that time, and no further. He introduced the quantum of action, and it worked, but its significance was very obscure. However it is important to realize that quantized energy levels, for both radiation and matter, are features of nature. Quantized cells in phase space are artifacts of theory. It is interesting that he was willing to accept the latter, which he could hope to fix, but was not willing for a long time to accept the former, which would invalidate most of classical physics.
His conservatism led him for many years to try to find a close-to-classical explanation for what he had done, and he was strongly inclined against the radical advances of others, which is why it was left for Einstein to quantize both the oscillator levels and the electromagnetic field. On the other hand, in subjects where radical ideas could immediately lead to clear conceptual advances, he was quick to approve, and he was one of the earliest supporters of relativity theory, and in fact spent most of his research time between 1905 and 1908 trying to advance the theory, and convince his peers of its validity.

Planck’s position in the German Physical Society made his voice the primary one in deciding what should be published in *Annalen der Physik*, the leading physics journal of the time, and his openness to radical new ideas, such as Einstein’s, is almost without parallel (one wonders whether a paper such as Einstein’s special relativity paper would get published in *Physical Review* today?) He even allowed Einstein to publish his photon paper, with which he strongly disagreed.

### 2.4 Planck’s Derivation of the Black Body Radiation Law

When Planck attacked the problem of black body radiation, he realized that since the results were independent of the nature of the material in the cavity, one could use a simple model for the cavity. So he chose to consider a damped harmonic oscillator as a model for the material in the walls. His results are arrived at simply in Born’s book [Born(1949)]. For absorption of radiation, if one has an oscillator of natural frequency $\omega_0$, and weak damping, $\gamma$, which is being driven at frequency $\omega$, the equation of motion will be the real part of

$$m\ddot{x} + m\gamma \dot{x} + m\omega_0^2 x = E_0 x e^{i\omega t}. \quad (2.13)$$

Then when one compensates for the 3-dimensionality of the problem, and assumes that $E_0$ represents the equilibrium radiation present at temperature $T$, one finds that the power absorbed is

$$\frac{dE_{\text{abs}}}{dt} = \frac{\pi \kappa e^2}{3m} u(\nu_0), \quad (2.14)$$

where $\kappa = 1/4\pi \epsilon_0$ in mks units, while the power radiated is given by

$$\frac{dE_{\text{rad}}}{dt} = \frac{2\kappa e^2 a^2}{3mc^3} = \frac{2\kappa e^2 \omega_0^2}{3mc^3} \bar{\varepsilon}, \quad (2.15)$$

where the term with $a$ is the average of the acceleration-squared, and $\bar{\varepsilon}$ represents the average energy of the oscillator. Combining Eqs. (2.14) and (2.15)
gives
\[ u_\nu = \frac{8\pi\nu^2}{c^3}\bar{\varepsilon}. \] (2.16)

Planck had this result well before Rayleigh had published his node-counting argument. All Planck had to do was insert the equipartition result \( k_B T \) for \( \bar{\varepsilon} \), and he would have had the Rayleigh-Jeans formula considerably before Rayleigh.

But he never did, and there has been considerable debate as to why. Could he have not known about equipartition, since at this time he was an avid attacker of the entire statistical mechanics enterprise? This would seem very unlikely, as he was interested in specific heats, and would have known about the Dulong-Petit law controversy [Dulong, Petit (1819)] (some solids did and some did not have \( U = 3RTV \)). Or was he aware of it but already had no confidence in it, as Wien’s empirical law, eq. (2.12), seemed to be holding up nicely. We are unlikely to ever know.

At any rate in 1900 Planck found out that Wien’s law was not holding up, and he had to make a report to the Berlin physical society. From his long experience in thermodynamics, he later said that he immediately started searching for the solution in the relation between entropy and energy, while everyone else was worried about the relation between \( \nu \) and \( T \). Planck had derived a formula for the approach to equilibrium by an oscillator in a black body cavity that had a small excess energy \( \Delta U \) over its equilibrium value [Planck (1900d)]. Then if its energy changed by \( dU \), the change in entropy of the entire system (oscillator plus field) would be
\[ dS_{\text{tot}} = \frac{3}{5} \frac{d^2S}{dU^2} dU \Delta U. \] (2.17)

So the function \( \frac{d^2S}{dU^2} \) is clearly connected to fluctuations about equilibrium, although at the time Planck was not thinking statistically. It was Einstein in 1909 [Einstein (1909)] who clearly brought out the direct meaning of this function as a statistical measure of fluctuations. He inverted the formula \( S = k_B \ln W \) to the form \( W = e^{S/k_B} \). Then one can connect the entropy of an arbitrary state to its probability. If \( W \) is a maximum for \( S = S_0 = S(E_0) \), the maximum entropy and minimum energy state, then very close to equilibrium we can write
\[ S = S_0 - \alpha(E - E_0)^2, \quad -\alpha = \frac{1}{2} \left( \frac{\partial^2 S}{\partial E^2} \right)_0, \]
\[ W = e^{S_0/k_B} e^{-\alpha(E - E_0)^2/k_B}. \] (2.18)
There is no linear term since $S_0$ is a maximum. If we then ask for the energy fluctuations about equilibrium, we get

$$< \Delta E^2 > = < (E - E_0)^2 > = \frac{\int (E - E_0)^2 W(E) dE}{\int W(E) dE} = \frac{k_B}{2\alpha},$$  \hspace{1cm} (2.19)$$

So $1/\alpha = -2/\left( \frac{\partial^2 S}{\partial E^2} \right)_0$ is a measure of the energy fluctuation.

Planck’s first derivation of his radiation formula was a purely numerical manipulation. Nonetheless, it is very interesting because it is profoundly and directly connected to fluctuations, in a way that Planck could not have foreseen. He knew that entropy was the key to the problem, and he thought the answer was directly related to the quantity $1/\alpha$ of Eqs. (2.18) and (2.19), which governed the return to equilibrium, via Eq. (2.17). Until a few days earlier, when Rubens had come to him, he thought that Wien’s empirical law, Eq. (2.12), was the correct solution to the problem. Using his own Eq. (2.16), together with Eq. (2.12), he wrote

$$\bar{\epsilon} = \frac{c^3}{8\pi \nu^2} u_\nu = \frac{ca\nu}{8\pi} e^{-b\nu/k_BT},$$  \hspace{1cm} (2.20)$$

One could use this to express $S$ directly in terms of $E$ by eliminating $T$, since at constant $V$, $1/T = \left( \frac{\partial S}{\partial \bar{\epsilon}} \right)_V = \frac{\partial s}{\partial \bar{\epsilon}}$, where $s$ is the entropy per oscillator. Therefore from Eq. (2.20),

$$1 \over T = -\frac{1}{b\nu} \ln \frac{8\pi \bar{\epsilon}}{c^3 a\nu} = \frac{\partial s}{\partial \bar{\epsilon}}$$

$$\frac{\partial^2 s}{\partial \bar{\epsilon}^2} = -\frac{1}{b\nu \bar{\epsilon}}.$$  \hspace{1cm} (2.21)$$

This is the expression Planck had previously thought exact, and even that he could derive it with some plausible assumptions.

The new knowledge given to him by Rubens, that at low frequencies in the newly accessible infra-red region, $u_\nu \approx \nu^2 T$, as had just been predicted by Rayleigh, he wrote as (using $u_\nu = A\nu^2 T$)

$$\bar{\epsilon} = \frac{c^3}{8\pi \nu^2} u_\nu = \frac{c^3}{8\pi} AT = k_BT,$$

$$1 \over T = \frac{\partial s}{\partial \bar{\epsilon}} = \frac{k_B}{\bar{\epsilon}}, \hspace{1cm} \frac{\partial^2 s}{\partial \bar{\epsilon}^2} = -\frac{k_B}{\bar{\epsilon}^2}.$$  \hspace{1cm} (2.22)$$

(The last equation of the first line is just the equipartition theorem, which was used by Rayleigh, although not by Planck, to give the value of $A$.) Planck
says he spent the next few days looking for an extrapolation between these two extremes, that gave plausible behavior, and finally came up with

$$\frac{\partial^2 s}{\partial \bar{\varepsilon}^2} = -\frac{k_B}{\bar{\varepsilon}(\Delta + \bar{\varepsilon})},$$

(2.23)

where $\Delta$ is independent of the temperature. In the limit $\bar{\varepsilon} \ll \Delta$,

$$\frac{\partial^2 s}{\partial \bar{\varepsilon}^2} \rightarrow -\frac{k_B}{\bar{\varepsilon}\Delta}, \quad \Delta = bk_B\nu \equiv h\nu,$$

(2.24)

where $h$ is a new physical constant. The fact that $\Delta$ must depend linearly on $\nu$ comes from Wien’s spectral theorem, a thermodynamic necessity. In the other limit, $\bar{\varepsilon} \gg \Delta$, we have Eq. (2.22), the Rayleigh-Jeans law. We can of course integrate Eq. (2.23), to get Planck’s formula, which is still valid today,

$$\frac{\partial^2 s}{\partial \bar{\varepsilon}^2} = -\frac{k_B}{\bar{\varepsilon}(\Delta + \bar{\varepsilon})} = -\frac{k_B}{\Delta} \left(1\frac{1}{\bar{\varepsilon}} - 1\frac{1}{\Delta + \bar{\varepsilon}}\right),$$

$$\frac{\partial s}{\partial \bar{\varepsilon}} = \frac{1}{T} = -\frac{k_B}{\Delta} \ln \frac{\bar{\varepsilon}}{\Delta + \bar{\varepsilon}}, \quad \frac{\Delta + \bar{\varepsilon}}{\bar{\varepsilon}} = e^{\Delta/k_B T} = e^{h\nu/k_B T},$$

$$\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/k_B T} - 1},$$

(2.25)

2.4.1 Planck’s Theoretical Derivation

As we have said, Planck imagined that there were a series of oscillators in the walls, in equilibrium with the radiation. Since each oscillator reaches equilibrium with the same frequency of radiation as the oscillator itself, and those of different frequencies all behave independently, we can consider each frequency independently. This had previously given rise to much controversy, the problem being how independently behaving oscillators could ever come to equilibrium, especially if one considered the walls of the cavity to be perfectly reflecting. The prevailing opinion was that this was an abstraction, and if one thought of a small lump of coal (that absorbed all frequencies) as also being inside the cavity, it would force all frequencies to come to equilibrium together.

Next he considered that for each frequency, if there were $N$ oscillators, the total energy was divided into $P$ discrete units of size $\varepsilon = h\nu$. As we have said, it doesn’t matter whether one considers this to be because the energy is quantized, or because one considers all the energy $E$ between frequencies $\nu$ and $\nu + d\nu$ to be lumped together and considered as $E/\varepsilon = P$ discrete units. Planck in any case was psychologically not disposed to seeing the energy as quantized, and as we have emphasized, long resisted it.
If Planck were to continue following Boltzmann, he could further divide this into \( n_k \) oscillators with energy \( k\varepsilon \) so that
\[
\sum n_k = N, \quad \sum k\varepsilon n_k = E,
\] (2.26)

and then find the distribution of \( n_k \)'s which has maximum probability. But Planck stated that one didn’t even have to go this far. He merely said that most of the time the system will be very close to equilibrium, and the rest constitute rare events that will hardly contribute, so he just took the total number of possible ways to distribute the \( P \) units of energy over the \( N \) oscillators. How many such ways are there?

A simple way to see this (due to Ehrenfest) is just to draw two vertical bars, and randomly distribute \( P \) circles, and \( N-1 \) other bars between them. For example, the arrangement
\[
|oo||o|ooo||oo|......|oo|o|
\]
would represent 2 units of energy in the first box (oscillator), none in the second, 1 in the third, 3 in the fourth, etc., altogether taking up \( N \) boxes. How many possible such arrangements are there? There are \( N-1+P \) objects, which we can distribute in \((N-1+P)!\) ways, and since the order of the circles and bars do not matter, the total becomes
\[
W = \frac{(N-1+P)!}{(N-1)!P!}
\] (2.27)

This is the total number of ways of distributing the energy amongst the oscillators, and the overwhelming majority of such arrangements lie close to equilibrium.

Planck next assumed that \( N \gg 1, P \gg 1, \) and \( \ln N! \approx N \ln N - N. \) Thus
\[
S = k_B \ln W \approx k_B[\ln(N + P)! - \ln N! - \ln P!] =
\]
\[
k_B[(N + P) \ln(N + P) - (N + P) -
\]
\[
(N \ln N - N) - (P \ln P - P)] + k_BN\left[\left(1 + \frac{P}{N}\right) \ln \left(1 + \frac{P}{N}\right) - \frac{P}{N} \ln \frac{P}{N}\right].
\] (2.28)

So the entropy only depends on the average number of energy units per oscillator, \( P/N. \) Then since
\[
\bar{\varepsilon} = E/N = P\varepsilon/N, \quad P/N = \bar{\varepsilon}/\varepsilon.
\] (2.29)
We have been using $\bar{\varepsilon}$ to represent the average energy per oscillator, while $\varepsilon$ is just $h\nu$, the energy unit.) So finally,

$$s = S/N = k_B \left[ \left(1 + \frac{\bar{\varepsilon}}{\varepsilon}\right) \ln \left(1 + \frac{\bar{\varepsilon}}{\varepsilon}\right) - \frac{\bar{\varepsilon}}{\varepsilon} \ln \left(\frac{\bar{\varepsilon}}{\varepsilon}\right) \right]. \quad (2.30)$$

Then, as before

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{\partial s}{\partial \bar{\varepsilon}} = \frac{k_B}{\varepsilon} \ln \frac{\bar{\varepsilon} + \varepsilon}{\bar{\varepsilon}},$$

$$\bar{\varepsilon} = \frac{\varepsilon}{e^{\varepsilon/k_B T} - 1},$$

$$u_\nu = \frac{8\pi\nu^2}{c^3} \bar{\varepsilon} = \frac{8\pi\nu^2}{c^3} \frac{\varepsilon}{e^{\varepsilon/k_B T} - 1} \quad (2.31)$$

This is Planck’s derivation of his formula. If we take an extra derivative of the first line of Eq. (2.31), we get

$$\frac{\partial^2 s}{\partial \bar{\varepsilon}^2} = -\frac{k_B}{\bar{\varepsilon}(\bar{\varepsilon} + \varepsilon)}. \quad (2.32)$$

This reduces to Planck’s previous numerical formula, where we see that $\varepsilon$ plays the role of his constant $\Delta$, which was necessary to make the formula work. If $\varepsilon \to 0$, we lose the behavior of Wien’s empirical formula at high energies, which is the limit in which Einstein introduced the particle behavior of photons. Rosenfeld, in writing a history of early quantum theory [Rosenfeld (1936)] claimed that Planck probably worked backward from Eq. (2.31) to get the entropy Eq. (2.30), from which he could guess the right combinatorial law for $W$, Eq. (2.27), which appears in Boltzmann’s original article, [Boltzmann (1877a)].

2.5 Some Comments on the Planck Derivation

There are a number of things to notice about Planck’s derivation, some of which we have noted earlier. First, what does it mean to keep $\varepsilon$ finite, since for the case of particles using classical statistics, cell size doesn’t matter? We pointed out earlier that it was noticed independently by Natanson and Ehrenfest in 1911 that the Planck derivation treats all the energy elements as equivalent, so that it is clearly different from Boltzmann’s statistics, and in fact makes them indistinguishable. Ehrenfest also showed in 1906 [Ehrenfest (1906)] that the Planck derivation puts an extra constraint on the system that he said could be satisfied in several ways, but that the most natural was to
strictly quantize the energy levels of the oscillators. Einstein actually did this [Einstein (1907)] in 1907, in his famous specific heat paper.

A number of people noticed that since $\varepsilon = h\nu$, one of the basic assumptions of the theory cannot work. Eqs. (2.29) and (2.31) assume that $N$ and $P >> 1$. But for high enough frequencies at a given temperature, $\varepsilon$ becomes quite large, and most of the oscillators will be in their ground state. This is why equipartition breaks down, since classical physics scales the frequency so that all frequencies are equally important, and they all have the same average energy, $k_B T$. The Planck formula correctly identifies the parameter $\varepsilon/k_B T$ as the important dividing line, but the assumptions of the derivation also break down at high frequency. The Einstein derivation of 1907 (where the energy levels are quantized, and the probability that a state $E_n = n\varepsilon$ is occupied is $P_n = A \exp(-n\varepsilon/k_B T)$), does not suffer from this defect.

Once he had shown that the energy levels of the oscillator are quantized, Einstein also realized that Eq. (2.16), connecting $u_\nu$ with the average energy of an oscillator, $\bar{\varepsilon}$, is inconsistent, since it was derived using a classical oscillator that absorbs and emits energy continuously. But he thought the equation must be true on the average. So it is clear why Planck’s derivation left the situation in a state of great confusion for a long time.

### 2.6 Einstein’s Fluctuation Argument

In 1909, Einstein looked at the fluctuations in the Planck formula [Einstein (1909)] and noticed a simple, but very deep relation. It was in this paper that Einstein introduced Eq. (2.19) for the fluctuations. We can see the result already from Planck’s early ad-hoc derivation of his result, Eq. (2.23). and if we insert Eq. (2.23) into Eq. (2.19), we get

$$<\Delta E^2> = \frac{k_B}{2\alpha} = -\frac{k_B}{\partial^2 s/\partial \bar{\varepsilon}^2} = \bar{\varepsilon} \Delta + \bar{\varepsilon}^2,$$

(2.33)

If one believes that the energy levels of the oscillator are quantized, so that $E_n = n\Delta = n\hbar \nu$, as Einstein did, and $\bar{\varepsilon} = \bar{n}\Delta$, where $\bar{n}$ represents the average level of the oscillator, one can also put this into the form,

$$\frac{<\Delta E^2>}{\Delta^2} = <(\Delta n)^2> = \bar{n} + \bar{n}^2.$$

(2.34)

This also holds true for the field excitations if one considers the field modes to be oscillators. He then pointed out that in his paper on photons in 1905 (they were not explicitly called “photons” until 1926 [Lewis (1926)]), he had used
the Wien radiation formula when he discussed the radiation as resembling individualized excitations, and had shown how it resembled the independent particles of a perfect gas. He then identified the first term with the fluctuations of a group of independent particles, while the second term must correspond to the fluctuations in a cavity of classical waves. (This result was expressed in terms of the energy density of a small finite volume of the cavity, via Eq. (2.16), but the justification was essentially a dimensional argument, which said that in the classical limit where $\Delta$ doesn’t contribute, and one has nothing else with the dimensions of energy, one needs $<\Delta E^2>: \bar{\varepsilon}^2$. An explicit later calculation by Lorentz [Lorentz (1912)] proved the result.) But the Eqs. (2.33) and (2.34) are exact and hold even when one is not in either of the two classical limits represented by particles or waves. And so this paper is generally taken as the birth of the wave-particle duality that has perplexed physicists up to the present time.

2.7 Einstein’s A and B Coefficients

In 1917, Einstein [Einstein (1917)] published his famous $A$ and $B$ coefficients paper. The paper was in two parts, the first of which discussed energy transformations and rates of absorption and emission for the various processes that go on in an atom or molecule in equilibrium with the radiation in a cavity. The second part discusses momentum transfer during these processes. This paper was very seminal in that it taught us how to think about radiation. It is not only the starting point for laser physics, but it also pretty much made the existence of energy levels essential, showing how they lead naturally to Planck’s radiation law. Einstein assumed that the molecule could occupy only a discrete set of allowed states $\{Z_n\}$ which had energies $\{\varepsilon_n\}$, and whose relative probability of occupation at temperature $T$ is

$$W_n = p_n e^{-\varepsilon_n/k_B T}, \quad (2.35)$$

where the $p_n$ represent statistical weights. He then assumes that a molecule can decay spontaneously from a state $Z_m$ to $Z_n$, (such that $\varepsilon_m > \varepsilon_n$), and emit energy $\varepsilon_m - \varepsilon_n$. The probability per molecule for this to occur in time $dt$ he takes as

$$dW = A^m_n dt. \quad (2.36)$$

As analogies, he quotes radioactive $\gamma$ decay and Hertzian oscillators.

He then assumes that there are induced (stimulated) emission and absorption processes, which he calls a quantum theoretical hypothesis, that he assumes
take place with a probability

\[ dW = B^n_m u_\nu dt, \quad (2.37) \]

for absorption from the lower level to the higher level, and

\[ dW = B^m_n u_\nu dt, \quad (2.38) \]

for emission from the higher level to the lower level. These are for transitions induced by the external field. Even without introducing the quantized states, in the classical picture for absorption and emission used by Planck, Eqs. (2.14) and (2.15), the rates were proportional to the density of the surrounding radiation.

If we then equate emission and absorption at equilibrium (detailed balance), we get

\[ p_n e^{-\varepsilon_n/k_B T} B^n_m u_\nu = p_m e^{-\varepsilon_m/k_B T} (B^m_n u_\nu + A^n_m). \quad (2.39) \]

Then if we take the limit \( T \to \infty \), for which also \( u_\nu(T) \to \infty \), then \( p_n B^n_m = p_m B^m_n \), and

\[ u_\nu = \frac{A^n_m/B^m_n}{e^{(\varepsilon_m-\varepsilon_n)/k_B T} - 1}. \quad (2.40) \]

This formula immediately leads to the Bohr rule \( \varepsilon_m - \varepsilon_n = h\nu \), and in the high temperature limit, where the Rayleigh-Jeans law holds, we can evaluate \( A/B \), which leads to the Planck radiation law. Even after the development of non-relativistic quantum mechanics, until the advent of field theory, Einstein’s derivation was needed to calculate the spontaneous emission of radiation.

Like in much of the rest of this story, there is an irony in Einstein’s introduction of his \( A \) and \( B \) coefficients. To Einstein himself, the most important part of the paper was the second part. The derivation in this part is more difficult, and is usually ignored today, but the point of the calculation was the consideration of momentum conservation in the radiation process, rather than merely energy conservation. By methods reminiscent of his derivation of Brownian motion, he proved that to preserve thermal equilibrium in a gas of atoms, or molecules, during the decay process one must consider that in the individual decays, the atom recoils, acquiring the appropriate momentum. In his words, “If the molecule undergoes a loss of energy of magnitude \( h\nu \) without external influence, by emitting this energy in the form of radiation (spontaneous emission), this process is also a directed one. There is no emission in spherical waves. The molecule suffers in the spontaneous elementary process
a recoil of magnitude $h\nu/c$ in a direction which is in the present state of the theory determined only by 'chance'."

The irony implicit in this derivation is brought out in his subsequent statement, “These properties of the elementary processes required by Eq. (12) [an equilibrium equation of the momentum fluctuations] make it seem practically unavoidable that one must construct an essentially quantum theoretical theory of radiation. The weakness of the theory lies, on the one hand, in the fact that it does not bring any nearer the connection with the wave theory and, on the other hand, in the fact that it leaves moment and direction of the elementary processes to 'chance'; all the same, I have complete confidence in the reliability of the method used here.”

This is the paper that introduced chance into the radiation process in an essential way. After this, it was an inevitable and inescapable part of the quantum landscape. He had to introduce it in order to make it clear that the photons were emitted in individual quantum processes, and carried both energy and momentum. This was very important to him, because even at this late date, which was already 1917, the existence of the photon was not yet generally accepted. But even as he introduced the element of chance in an essential way, he lamented it.

There is a strong parallel here between Einstein and Planck, who both introduced revolutionary thoughts brought about by necessity after a long intellectual odyssey. Yet no sooner had Planck let the genie of the quantum out of the bottle, than he devoted many years effort to unsuccessfully trying to force it back in, without destroying the revolution it had brought about. And Einstein had the same experience. Once he had let the genie of chance out of the bottle, he unsuccessfully spent the rest of his life trying to stuff it back in. Not that this diminishes by one iota the accomplishments of these two great men, but it does point up the ironies that life has in store for the best of us.

3 Bose-Einstein Condensation

In 1924, Bose made the seminal observation that it is possible to derive Planck’s radiation law from purely corpuscular arguments without invoking at all the wave properties of light resulting from Maxwell’s field equations. The main ingredient in Bose’s argument was the indistinguishability of the particles in question and a new way of counting them — now universally known as “Bose-Einstein statistics” — which pays careful attention to what is implied by their being indistinguishable. In the case of light quanta, an additional feature is that their number is not conserved, because light is easily emitted and absorbed. Massive particles (atoms, molecules, . . . ), by contrast, are conserved
and therefore, as Einstein emphasized [Einstein (1924), Einstein (1925)], their indistinguishability has further consequences, of which the phenomenon of Bose-Einstein condensation (BEC) is the most striking one.

Bose-Einstein condensation has long been a fascinating subject and has attracted renewed interest in light of successful experimental demonstrations of BEC in dilute $\text{He}^4$ [Crooker et al. (1983), Chan et al. (1988), Crowell et al. (1995)] and ultracold atomic gases [Anderson et al. (1995), Bradley et al. (1995), Davis et al. (1995), Fried et al. (1998), Miesner et al. (1998)]. Furthermore the production of “coherent atomic beams”, the so called atom laser [Mewes et al. (1997), Andrews et al. (1997), Anderson and Kasevich (1998), Bloch et al. (1999)], and its relation to the conventional laser is intriguing; as is the relation between the BEC phase transition and the quantum theory of the laser [Scully and Lamb (1966), Scully and Zubairy (1997)].

The physics of BEC is subtle with many pitfalls and surprises. For example, Uhlenbeck criticized Einstein’s arguments concerning the implied singularity in the equation of state at the critical temperature $T_c$. Einstein’s results require that the thermodynamic limit be taken, i.e., the number of particles $N$ and the volume $V$ are taken to be infinite with the density $N/V$ being finite. This however leaves the question of how best to think about and define $T_c$ for finite mesoscopic systems.

A canonical ensemble, in which $N$ particles inside a trap can interact and exchange energy with a thermal reservoir at temperature $T$, provides a natural approach to BEC. This canonical ensemble approach is a useful tool in studying BEC properties in the current experiments on cold dilute gases [Anderson et al. (1995), Bradley et al. (1995), Davis et al. (1995), Han et al. (1998), Ernst et al. (1998), Hau et al. (1998), Esslinger et al. (1998), Anderson and Kasevich (1999), Miesner et al. (1998), Fried et al. (1998), Mewes et al. (1997), Andrews et al. (1997), Anderson and Kasevich (1998), Bloch et al. (1999)]. It is also directly relevant to the He-in-vycor BEC experiments [Crooker et al. (1983), Chan et al. (1988), Crowell et al. (1995)]. The dynamics and statistics of the condensate is then obtained from the canonical partition function. However the $N$-particle constraint associated with the canonical ensemble is rather cumbersome and no simple analytic expressions for the canonical partition function are known to exist for three-dimensional traps. Even numerical calculations for large $N$ may become impractical. A way out is to calculate the grand canonical properties for the ideal Bose gas where the constraint of fixed particle number is relaxed. This was how Einstein derived the characteristics of the condensate and obtained the expression for the critical temperature. In general, we would expect that the macroscopic properties of the condensate for both canonical and grand canonical ensembles should be equivalent. However, as we discuss below, only properties related to mean number of condensed particles are almost identical in the two ensembles and the mean-square...
fluctuations are remarkably different. Even as the temperature $T$ approaches zero when all $N$ particles condense in the ground state, the fluctuations in the grand canonical ensemble becomes huge, of the order of $N^2$, as discussed below. This is clearly unacceptable.

Recently, realizing the inherent similarity in the phase transition behavior between laser and the Bose-Einstein condensation, a new approach is developed to study the nonequilibrium approach to BEC in the canonical ensemble using the methods employed in the quantum theory of laser [Scully (1999), Kocharovsky et al. (2000a)]. The advantage of this approach is that analytic, though approximate, expressions are obtained for the canonical partition function for the Bose-Einstein condensate for arbitrary traps. The various moments for the condensate based on these analytic expressions and the exact numerical results are in most cases negligible. This approach also allows us to extend the critical temperature concept to the mesoscopic systems, involving say $10^3$ atoms, in a natural fashion.

However, before proceeding to give the details of the laser theory based analysis of BEC, we recall Einstein’s arguments based on grand canonical ensemble and see whether we can extend these arguments in a natural way to describe a mesoscopic system. We also present the salient features of the quantum theory of laser that become relevant in seeing the close connection between the nonequilibrium approach to the dynamics and statistics of the condensate of $N$-atom Bose gas and the photons inside a laser.

### 3.1 Average condensate particle number

Here we present a derivation of the average condensate particle number following the original derivation of Einstein. We recall that Einstein considered particles inside a box in the thermodynamic limit. We consider particles in a harmonic trap and first discuss the thermodynamic limit. The difference between a box and the harmonic trap is in the density of states. We then go on to consider the mesoscopic number of particles.

Following Einstein we work with the grand canonical ensemble in which the average condensate particle number $\bar{n}_0$ is determined as follows [Ketterle and Druten (1996)]. The total number of atoms $N$ in the trap is given by

$$N = \sum_{k=0}^{\infty} \bar{n}_k = \sum_{k=0}^{\infty} \frac{1}{\exp[\beta(\varepsilon_k - \mu)] - 1},$$  \hspace{1cm} (3.1)

where for the three dimensional (3D) isotropic harmonic trap we have $\varepsilon_k = \hbar \Omega (k_x + k_y + k_z)$, $\Omega$ is the trap frequency, $\beta = 1/k_B T$ and $\mu$ is the chemical
potential.

In the following we demonstrate how to calculate the mean number of condensed particles $\bar{n}_0$ for a 3D isotropic harmonic trap. Using $\bar{n}_0 = 1/(\exp(-\beta \mu) - 1)$, we can relate the chemical potential $\mu$ to $\bar{n}_0$ as $1 + 1/\bar{n}_0 = \exp(-\beta \mu)$ and rewrite Eq. (3.1) as

$$N = \sum_{k=0}^{\infty} \langle n_k \rangle = \sum_{k=0}^{\infty} \frac{1}{(1 + 1/\bar{n}_0) \exp(\beta \varepsilon_k) - 1}. \quad (3.2)$$

For large $\bar{n}_0$ we neglect $1/\bar{n}_0$ in comparison with 1. Following Einstein, we proceed to separate off the ground state so that Eq. (3.2) can be written as

$$N - \bar{n}_0 = \mathcal{H}, \quad (3.3)$$

where

$$\mathcal{H} = \sum_{k>0} \frac{1}{e^{\beta \varepsilon_k} - 1}. \quad (3.4)$$

For an isotropic harmonic trap with frequency $\Omega$ the degeneracy of the $n$th energy level is $(n+2)(n+1)/2$, and we obtain

$$\mathcal{H} = \frac{1}{2} \sum_{n=1}^{\infty} \frac{(n+2)(n+1)}{\exp(\beta n \hbar \Omega) - 1} \approx \frac{1}{2} \int_1^{\infty} \frac{(x+2)(x+1)}{\exp(x \beta \hbar \Omega) - 1} dx. \quad (3.5)$$

In the limit $k_B T \gg \hbar \Omega$ we find

$$\mathcal{H} \approx \frac{1}{2} \int_0^{\infty} \frac{x^2}{\exp(x \beta \hbar \Omega) - 1} dx = \left(\frac{k_B T}{\hbar \Omega}\right)^3 \zeta(3), \quad (3.6)$$

where $\zeta(x)$ is the Riemann zeta-function. We define the critical temperature $T_c$ such that when $T = T_c$ we have $\bar{n}_0 = 0$. This yields

$$T_c = \frac{\hbar \Omega}{k_B} \left(\frac{N}{\zeta(3)}\right)^{1/3} \quad (3.7)$$

as the temperature of BEC transition in the thermodynamic limit. The resulting expression for the mean number of particles in the condensate is

$$\bar{n}_0(T) = N \left[1 - \left(\frac{T}{T_c}\right)^3\right] \quad (3.8)$$
which shows a cusp at $T = T_c$. For mesoscopic number of particles (e.g., a few hundred) Eq. (3.8) becomes inaccurate as the thermodynamic limit is not reached. To improve the accuracy we first rewrite Eq. (3.2) in the following way [Kocharovsky et al. (2006), Jordan et al. (2006)]

$$N - \bar{n}_0 = \frac{1}{\bar{n}_0} \sum_{k>0} \frac{1}{e^{\beta \varepsilon_k} - \frac{n_0}{\bar{n}_0 + 1}}. \quad (3.9)$$

For $\bar{n}_0 \gg 1$, the term $\bar{n}_0 / (\bar{n}_0 + 1)$ inside the summation may be approximated by 1. Then we obtain a quadratic equation for the mean number of particles in the ground state

$$N - \bar{n}_0 = \frac{\mathcal{H}}{\bar{n}_0 + 1} \implies \bar{n}_0^2 + \bar{n}_0(1 + \mathcal{H} - N) - N = 0 \quad (3.10)$$

whose solution is

$$\bar{n}_0 = \frac{1}{2} \left( N - \mathcal{H} - 1 + \sqrt{(N - \mathcal{H} - 1)^2 + 4N} \right). \quad (3.11)$$

Analytical expression (3.11) shows a smooth crossover near $T_c$ for a mesoscopic number of particles $N$ as shown in Fig. 1. Here we compare the mean condensate number as given by Eq. (3.11) obtained in the grand canonical ensemble (solid line) for $N = 200$ and the solution (3.8) (dashed line) that is valid only for a large number of particles $N$ with the numerical calculation of $\bar{n}_0(T)$ from the exact recursion relations in the canonical ensemble (dots) [Wilkens and Weiss (1997)]. In the canonical ensemble the total number of particles $N$ is fixed, rather then the chemical potential. We see that, for the average particle number, both ensembles (grand canonical and canonical) yield very close answers. The interesting observation is that the approximate expression (3.8) obtained in a suitable limit within the grand canonical ensemble yields results that are indistinguishable from the exact results from the canonical ensemble. However, as we discuss below, this is not the case for the BEC fluctuations.

### 3.2 Fluctuations in the number of particles in the condensate

Condensate fluctuations are characterized by the central moments $\mu_m = \langle (n_0 - \bar{n}_0)^m \rangle$. The first of them is the squared variance

$$\langle (n_0 - \bar{n}_0)^2 \rangle = \langle n_0^2 \rangle - \langle n_0 \rangle^2, \quad (3.12)$$

When the temperature $T$ approaches zero, all $N$ particles are forced into the system’s ground state, so that the mean square $\langle (\Delta n_0)^2 \rangle$ of the fluctuation of
The average condensate particle number versus temperature for $N = 200$ particles in an isotropic harmonic trap. Solid line is Eq. (3.11), while the dash line shows the thermodynamic limit formula (3.8). “Exact” dots are obtained numerically in the canonical ensemble [Wilkens and Weiss (1997)].

the ground-state occupation number has to vanish for $T \to 0$. However the grand canonical description gives $\langle (\Delta n_0)^2 \rangle \to N(N+1)$, clearly indicating that with respect to these fluctuations the different statistical ensembles are no longer equivalent. What, then, would be the correct expression for the fluctuation of the ground-state occupation number within the canonical ensemble, which excludes any exchange of particles with the environment, but still allows for the exchange of energy? Various aspects of this riddle have appeared in the literature over the years [Ziff et al. (1977), ter Haar (1970), Fierz (1956)], mainly inspired by academic curiosity, before it resurfaced in 1996 [Grossmann and Holthaus (1996), Politzer (1996), Gajda and Rzążewski (1977), Wilkens and Weiss (1997), Weiss and Wilkens (1997)], this time triggered by the experimental realization of mesoscopic Bose–Einstein condensates in isolated micro traps. Condensate fluctuations can be measured by means of a scattering of series of short laser pulses [Idziaszek (2000)] (see also [Chuu et al. (2005)]. Since then, much insight into this surprisingly rich problem has been gained. Much of this insight follows directly from the quantum theory of the laser, to which we now turn.

4 The Quantum Theory of the Laser

The quantum (photon) picture of maser/laser operation is a difficult problem in the interaction of radiation with matter. Even several years after the development of the maser and the laser there was not a fully quantized theory of laser action. The difficulties inherent in this problem were most succinctly
stated by Roy Glauber in his 1964 Les Houches lectures in this way [Glauber (1964)]:

“The only reliable method we have of constructing density operators, in general, is to devise theoretical models of the system under study and to integrate [the] corresponding Schrödinger equation, or equivalently to solve the equation of motion for the density operator. These assignments are formidable ones for the case of the laser oscillator and have not been carried out to date in quantum mechanical terms. The greatest part of the difficulty lies in the mathematical complications associated with the nonlinearity of the device. The nonlinearity physics plays an essential role in stabilizing the field generated by the laser. It seems unlikely, therefore, that we shall have a quantum mechanically consistent picture of the frequency bandwidth of the laser or of the fluctuations of its output until further progress is made with these problems.”

Following the Les Houches meeting, Marlan Scully and Willis Lamb took up the challenge and developed a fully quantum mechanical theory of laser that yielded the photon statistics above, at, and below threshold (diagonal elements of the laser field density matrix), showed that the laser linewidth was contained in the time decay of the off-diagonal elements of the density matrix, and made the physics clearer by comparing the laser threshold to a ferromagnetic phase transition [Scully and Lamb (1966)]. They presented their theory of “optical maser” at the famous Puerto Rico Conference on the “Physics of Quantum Electronics” in the summer of 1965.

The treatment of the laser near threshold must include nonlinear active medium consisting of atoms that are pumped in their excited states and a damping mechanism to account for the loss of photons from the cavity through end mirrors. To obtain laser pumping action we introduce atoms in their upper level $|a>$ at random times $t_i$, decaying to a far-removed ground state $|b>$. Cavity field damping is included by coupling the field to an ensemble of atoms in their ground state ($\gamma$ subsystem in Fig. 2).

Here we concentrate on the study of the photon distribution function for the laser field which is given by the diagonal matrix elements of the reduced density operator of the field. The photon statistical distribution for the laser is of interest for several reasons. Historically, it was initially thought by some that the statistical photon distribution should be a Bose-Einstein distribution. A little reflection shows that this can not be, since the laser is operating far from thermodynamic equilibrium. However, a different paradigm recognizes many atoms oscillating in phase produce what is essentially a classical current, and this would generate a coherent state; the statistics of which is Poissionian. But, for example, the photon statistics of a typical Helium-Neon laser is substantially different from a Poissonian distribution. Of course, well above threshold, the steady-state laser photon statistical distribution is Poisson which is the
characteristic of a coherent state. In order to see these interesting features we consider the master equation of the laser in various regimes of operation.

\[
\dot{\rho}(n) = -\left[\frac{(n+1)A}{1+(n+1)B/A}\right]\rho(n) + \left(\frac{nA}{1+nB/A}\right)\rho(n-1) - Cnp(n) + C(n+1)p(n+1).
\]

(4.1)

Here we omit details of the full theory and point out that the diagonal elements \(\rho_{nn} \equiv p(n)\), which represent the probability of \(n\) photons in the field, satisfy the equation of motion

\[
\dot{p}(n) = -\left[\frac{(n+1)A}{1+(n+1)B/A}\right]p(n) + \left(\frac{nA}{1+nB/A}\right)p(n-1) - Cnp(n) + C(n+1)p(n+1).
\]

where \(A\) is the linear gain coefficient, \(B\) is the self-saturation coefficient and \(C\) is the decay rate. The first two terms in the right hand side of Eq. (4.1) describe pumping and the last two terms come from damping (decay). It is interesting to note that the diagonal elements are coupled only to diagonal elements. More generally, only off-diagonal elements \(\rho_{nn'}\) with the same difference \((n - n')\) are coupled.

Before we begin the solution of the above equation we want to give a simple intuitive physical picture of the processes it describes in terms of a probability flow diagram, Fig. 3.

The left-hand-side is the rate of change of the probability of finding \(n\) pho-
tons in the cavity. The right-hand-side contains the physical processes that contribute to the change. Each process is represented by an arrow in the diagram. The processes are proportional to the probability of the state they are starting from and this will be the starting point of the arrow. The tip of the arrow points to the state the process is leading to.

![Diagram](image)

Fig. 3. Detailed balance and the corresponding probability flow diagram.

A simple physical meaning can be given to Eq. (4.1) for the photon distribution function in terms of a probability flow diagram (Fig. 3) by expanding the terms in the denominator of Eq. (4.1). There we see the ‘flow’ of probability in and out of the |n⟩ state from and to the neighboring |n + 1⟩ and |n − 1⟩ states. For example, the A(n + 1)p(n) term represents the flow of probability from the |n⟩ state to the |n + 1⟩ state due to the emission of photons by lasing atoms initially in the upper states. Here An is the rate of stimulated emission, A is the spontaneous emission rate and these rates are multiplied by p(n) to yield the total probability flow rate. Since the probability flows out of p(n), this term is negative. The first term in the expansion of the square-bracketed term in (4.1), namely B(n + 1)2p(n) = A(n + 1)(B/A)(n + 1)p(n), corresponds to the process in which photons are emitted and then reabsorbed, the reabsorption rate being (B/A)(n + 1). Similar explanations exist for the other terms including the loss terms.

After this brief discussion of the meaning of the individual terms we now turn our attention to the solution of the laser master equation (4.1). Although it is possible to obtain a rather general time-dependent solution to Eq. (4.1), our main interest here is in the steady-state properties of the field. To obtain the steady-state photon statistics, we replace the time derivative with zero. Notice that the right-hand-side of the equation is of the form $F(n + 1) - F(n)$, where

$$F(n) = Cnp(n) - \frac{nA}{1 + nB/A}p(n - 1),$$  \hspace{1cm} (4.2)

simply meaning that in steady-state $F(n + 1) = F(n)$. In other words $F(n)$ is independent of $n$ and is, therefore, a constant $c$. Furthermore, the equation $F(n) = c$ has normalizable solution only for $c = 0$. From Eq. (4.2) we then immediately obtain

$$p(n) = \frac{A/C}{1 + nB/A}p(n - 1),$$  \hspace{1cm} (4.3)

which is a very simple two-term recurrence relation to determine the photon-
number distribution. Before we present the solution a remark is called for here. The fact that $F(n) = 0$ and $F(n + 1) = 0$ hold separately is called the condition of detailed balance. As a consequence we do not need to deal with all four processes affecting $p(n)$. It is sufficient to balance the processes connecting a pair of adjacent levels in Fig. 3 and instead of solving the general three-term recurrence relation, resulting from the steady state version of Eq. (4.1), it is enough to solve the much simpler two-term recursion, Eq. (4.3).

It is instructive to investigate the photon statistics in some limiting cases before discussing the general solution. Below threshold the linear approximation holds. Since only very small $n$ states are populated appreciably, the denominator on the right-hand-side of (4.3) can be replaced by unity in view of $nB/A \ll 1$. Then

$$p(n) = p(0) \left( \frac{A}{C} \right)^n.$$ (4.4)

The normalization condition, $\sum_{n=0}^{\infty} p(n) = 1$, determines the constant $p(0)$, yielding $p(0) = (1 - A/C)$. Finally

$$p(n) = (1 - A/C) \left( \frac{A}{C} \right)^n.$$ (4.5)

Clearly, the condition of existence for this type of solution is $A < C$. Therefore, $A = C$ is the threshold condition for the laser. At threshold, the photon statistics changes qualitatively and very rapidly in a narrow region of the pumping parameter. It should also be noted that below threshold the distribution function (4.5) is essentially of thermal character. If we introduce an effective temperature $T$ defined by

$$e^{-\hbar \omega_0/kT} = A/C,$$ (4.6)

we can cast (4.5) to the form

$$p(n) = (1 - e^{-\hbar \omega_0/kT})e^{-n\hbar \omega_0/kT}.$$ (4.7)

This is just the photon number distribution of a single mode in thermal equilibrium with a thermal reservoir at temperature $T$. The inclusion of a finite temperature loss reservoir to represent cavity losses will not alter this conclusion about the region below threshold.

There is no real good analytical approximation for the region around threshold although the lowest order expansion of the denominator in (4.3) yields some
insight. The solution with this condition is given by

\[ p(n) = p(0) \left( \frac{A}{C} \right)^n \prod_{k=0}^{n} (1 - kB/A). \]  

(4.8)

This equation clearly breaks down for \( n > \frac{A}{B} = n_{\text{max}} \), where \( p(n) \) becomes negative. The resulting distribution is quite broad exhibiting a long plateau and a rapid cut-off at \( n_{\text{max}} \). The broad plateau means that many values of \( n \) are approximately equally likely and, therefore, the intensity fluctuations are large around threshold. The most likely value of \( n = n_{\text{opt}} \) can be obtained from the condition \( p(n_{\text{opt}} - 1) = p(n_{\text{opt}}) \) since \( p(n) \) is increasing before \( n = n_{\text{opt}} \) and decreasing afterward. This condition yields \( n_{\text{opt}} = (A - C)/B \) which is smaller by the factor \( C/A \) than the value obtained from the full nonlinear equation.

The third region of special interest is the one far above threshold. In this region \( \frac{A}{C} \gg 1 \) and the \( n \) values contributing the most to the distribution function are the ones for which \( n \gg \frac{A}{B} \). We can then neglect 1 in the denominator of (4.3), yielding

\[ p(n) = e^{-\bar{n}} \frac{\bar{n}^n}{n!}, \]  

(4.9)

with \( \bar{n} = \frac{A^2}{(CB)} \). Thus the photon statistics far above threshold are Poissonian, the same as for a coherent state. This, however, does not mean that far above threshold the laser is in a coherent state. As we shall see later, the off-diagonal elements of the density matrix remain different from those of a coherent state for all regimes of operation.

Figure 4 shows photon number distribution in different limits.

5 Bose-Einstein Condensation: Laser Phase-Transition Analogy

Bose-Einstein condensation in a trap has intriguing similarities with the threshold behavior of a laser which also can be viewed as a kind of a phase transition [DeGiorgio and Scully (1970), Graham and Haken (1970), Kocharovsky et. al. (2006)]. In both cases stimulated processes are responsible for the appearance of the macroscopic order parameter. The main difference is that for the Bose gas in a trap there is also interaction between the atoms which, in particular, yields stimulated effects in BEC. On the other hand there are two subsystems for the laser, namely the laser field and the active atomic medium. The crucial point for lasing is the interaction between the field and the atomic medium. Thus, the effects of different interactions in the laser are easy to trace and
As we discussed in the previous section, the laser light is conveniently described by a master equation obtained by treating the atomic (gain) media and cavity dissipation (loss) as reservoirs which when “traced over” yield the coarse grained equation of motion for the reduced density matrix for laser radiation. We thus arrive at the equation of motion for the probability of having \( n \) photons in the cavity given by Eq. (4.1). From Eq. (4.8) we have that partially coherent laser light has a sharp photon distribution (with width several times Poissonian for a typical He-Ne laser) due to the presence of the saturation nonlinearity, \( B \), in the laser master equation. Thus, we see that the saturation nonlinearity in the radiation-matter interaction is essential for laser coherence.

Next we turn to an ideal Bose gas and derive a master equation for the particles in the condensate. The steady-state description of the condensate arises from the inherent nonlinearities in the system. One naturally asks: Is the corresponding nonlinearity in BEC due to atom-atom scattering? or Is there a nonlinearity present even in an ideal Bose gas? In the following we show that the latter is the case.
5.1 Condensate master equation

Here we consider a model of a dilute Bose gas of atoms wherein interatomic scattering is neglected. This ideal Bose gas of \( N \) atoms is confined inside a trap and the atoms exchange energy with a reservoir at a fixed temperature \( T \) [Scully (1999), Kocharovsky et al. (2000a), Kapale and Zubairy (2001)]. The “ideal gas + reservoir” model corresponds to a canonical ensemble and it allows us to demonstrate most clearly the master equation approach to the analysis of dynamics and statistics of BEC. It provides the simplest description of many qualitative and, in some cases, quantitative characteristics of the experimental BEC. In particular, it explains many features of the condensate dynamics and fluctuations and allows us to obtain the particle number statistics of the BEC. An extension of the present approach to the case of an interacting gas which includes usual many-body effects due to interatomic scattering will be discussed in the next section.

For many problems a concrete realization of the reservoir system is not very important if its energy spectrum is dense and flat enough. For example, one expects (and we find) that the equilibrium (steady state) properties of the BEC are largely independent of the details of the reservoir. For the sake of simplicity, we assume that the reservoir is an ensemble of simple harmonic oscillators whose spectrum is dense and smooth, see Fig. 5. The interaction between the gas and the reservoir is described by the interaction picture Hamiltonian

\[
V = \sum_j \sum_{k \neq l} g_{j,k,l} b_j^\dagger a_k a_l^\dagger e^{-i(\omega_j - \nu_k + \nu_l)t} + H.c.,
\]

(5.1)

where \( b_j^\dagger \) is the creation operator for the reservoir \( j \) oscillator (“phonon”), and \( a_k^\dagger \) and \( a_k \) \( (k \neq 0) \) are the creation and annihilation operators for the Bose gas atoms in the \( k \)th level. Here \( \hbar \nu_k \) is the energy of the \( k \)th level of the trap, and \( g_{j,k,l} \) is the coupling strength.

Following along the lines of the quantum theory of the laser we can derive an equation of motion for the distribution function of the condensed bosons
\( \dot{p}_{n_0} = -\kappa \{ K_{n_0}(n_0 + 1)p_{n_0} - K_{n_0-1}n_0p_{n_0-1} + H_{n_0}n_0p_{n_0} - H_{n_0+1}(n_0 + 1)p_{n_0+1} \} \),

(5.2)

where \( \kappa \) embody the spectral density of the bath and the coupling strength of the bath oscillators to the gas particles and

\[
K_{n_0} = \sum_{k>0} (\eta_k + 1)\langle n_k \rangle_{n_0}, \quad H_{n_0} = \sum_{k>0} \eta_k (\langle n_k \rangle_{n_0} + 1),
\]

(5.3)

with

\[
\eta_k = \frac{1}{e^{\nu_k/T} - 1}.
\]

(5.4)

The particle number constraint comes in since \( \sum_{k>0} \langle n_k \rangle_{n_0} = N - \bar{n}_0 \).

The steady state distribution of the number of atoms condensed in the ground level of the trap can be determined from Eq. (5.2) and the various moments, including the mean value and the variance, can then be determined. It is clear that there are two processes: cooling and heating. The cooling process is represented by the first two terms with the cooling coefficient \( K_{n_0} \), and the heating by the third and fourth terms with heating coefficient \( H_{n_0} \). In the cooling process the atoms in the excited atomic levels in the trap jump to the condensate level and transfer energy to the thermal reservoir whereas, in the heating process, the atoms in the condensate absorb energy from the reservoir and get excited. The cooling and heating coefficients have the analogy with the saturated gain and cavity loss in the laser master equation (4.1). According to Eq. (5.3), these coefficients depend upon trap parameters such as the shape of the trap, the total number of bosons in the trap, \( N \), and the temperature \( T \).

In general, the cooling and the heating coefficients are complicated and depend upon the condensate probability distribution \( p_{n_0} \). In this sense, Eq. (5.2) is a transcendental equation for \( p_{n_0} \). This equation can however be simplified in certain approximations and we obtain analytic results for the condensate distribution that are close to the exact numerical results.

\subsection*{5.2 Low temperature approximation}

At low enough temperatures, the average occupations in the reservoir are small and \( \eta_k + 1 \simeq 1 \) in Eq. (5.3). This suggests the simplest approximation for the
cooling coefficient
\[ K_{n_0} \simeq \sum_{k>0} \langle n_k \rangle_{n_0} = N - \bar{n}_0. \] (5.5)

In addition, at very low temperatures the number of non-condensed atoms is also very small. We can therefore approximate \( \langle n_k \rangle_{n_0} + 1 \) by 1 in Eq. (5.3). Then the heating coefficient is a constant equal to the total average number of thermal excitations in the reservoir at all energies corresponding to the energy levels of the trap,
\[ H_{n_0} \simeq \mathcal{H}, \quad \mathcal{H} \equiv \sum_{k>0} \eta_k = \sum_{k>0} \frac{1}{(e^{\hbar \nu_k/T} - 1)}. \] (5.6)

Under these approximations, the condensate master equation (5.2) simplifies considerably and contains only one non-trivial parameter \( \mathcal{H} \). We obtain
\[ \dot{p}_{n_0} = -\kappa \{(N - n_0)(n_0 + 1)p_{n_0} - (N - n_0 + 1)n_0p_{n_0-1} \]
\[ + \mathcal{H}[n_0p_{n_0} - (n_0 + 1)p_{n_0+1}]\}. \] (5.7)

It may be noted that Eq. (5.7) has the same form as the equation of motion for the photon distribution function in a laser operating not too far above threshold \( (\mathcal{B}\langle n \rangle/\mathcal{A} << 1) \). The identification is complete if we define the gain, saturation, and loss parameters in laser master equation by \( \mathcal{A} = \kappa(N + 1) \), \( \mathcal{B} = \kappa \), and \( \mathcal{C} = \kappa \mathcal{H} \), respectively. The mechanism for gain, saturation, and loss are however different in the present case.

The resulting steady state distribution for the number of condensed atoms is given by
\[ p_{n_0} = \frac{1}{Z_N} \frac{\mathcal{H}^{N-n_0}}{(N-n_0)!}, \] (5.8)

where \( Z_N = 1/p_N \) is the partition function. It follows from the normalization condition \( \sum_{n_0} p_{n_0} = 1 \) that
\[ Z_N = e^{\mathcal{H} \Gamma(N + 1, \mathcal{H})/N!}, \] (5.9)

where \( \Gamma(\alpha, x) = \int_x^\infty t^{\alpha-1}e^{-t}dt \) is an incomplete gamma-function.

The mean value and the variance can be calculated from the distribution (5.8) for an arbitrary finite number of atoms in the Bose gas,
\[ \langle n_0 \rangle = N - \mathcal{H} + \mathcal{H}^{N+1}/Z_NN!, \] (5.10)
\[
\Delta n_0^2 \equiv \langle n_0^2 \rangle - \langle n_0 \rangle^2 = \mathcal{H} \left( 1 - (\langle n_0 \rangle + 1)\mathcal{H}^N / Z_N N! \right).
\] (5.11)

As we shall see from the extended treatment in the next section, the approximations (5.5), (5.6) and, therefore, the results (5.10), (5.11) are clearly valid at low temperatures, i.e., in the weak trap limit, \( T \ll \varepsilon_1 \), where \( \varepsilon_1 \) is an energy gap between the first excited and the ground levels of a single-particle spectrum in the trap. However, in the case of a harmonic trap the results (5.10), (5.11) show qualitatively correct behavior for all temperatures, including \( T \gg \varepsilon_1 \) and \( T \sim T_c \) [Scully (1999)].

In particular, for a harmonic trap we have from Eq. (5.6) that the heating rate is
\[
\mathcal{H} = \sum_{l,m,n} \frac{1}{\exp[\beta \hbar \Omega (l + m + n) - 1]} \approx \left( \frac{k_B T}{\hbar \Omega} \right)^3 \zeta(3) = N \left( \frac{T}{T_c} \right)^3. \] (5.12)

Thus, in the low temperature region, the master equation (5.7) for the condensate in the harmonic trap becomes [Scully (1999)]
\[
\frac{1}{\kappa} \dot{p}_{n_0} = - \left[ (N + 1)\langle n_0 + 1 \rangle - \langle n_0 + 1 \rangle^2 \right] p_{n_0} + \left[ (N + 1)n_0 - n_0^2 \right] p_{n_0-1} \] 
\[
- N \left( \frac{T}{T_c} \right)^3 \left[ n_0 p_{n_0} - (n_0 + 1) p_{n_0+1} \right]. \] (5.13)

The resulting plots for \( \bar{n}_0 \), the variance and the third and fourth central moments are given in Fig. 6 (dash line). These analytical results give qualitatively correct description of the ideal Bose gas when compared with the exact solution for the moments as derived in the canonical ensemble. These quantitative agreement with the exact numerical results can be considerably improved in the quasithermal approximation to which we turn next.

5.3 Quasithermal approximation for non-condensate occupations

At arbitrary temperatures, a very reasonable approximation for the average non-condensate occupation numbers in the cooling and heating coefficients in Eq. (5.3) is given by
\[
\langle n_k \rangle_{n_0} = \eta_k \sum_{k>0} \langle n_k \rangle_{n_0} / \sum_{k'>0} \eta_{k'} = \frac{(N - \bar{n}_0)}{(e^{\varepsilon_k/T} - 1) \mathcal{H}}, \] (5.14)
Equation (5.14) satisfies the canonical-ensemble constraint, \( N = n_0 + \sum_{k>0} n_k \), independently of the resulting distribution \( p_{n_0} \). This important property is based on the fact that a quasithermal distribution (5.14) provides the same relative average occupations in excited levels of the trap as in the thermal reservoir.

The cooling and heating coefficients (5.3) in the quasithermal approximation of Eq. (5.14) are

\[
K_{n_0} = (N - n_0)(1 + \eta), \quad H_{n_0} = \mathcal{H} + (N - n_0)\eta. \tag{5.15}
\]

Compared with the low temperature approximation (5.5) and (5.6), these coefficients acquire an additional contribution \( (N - n_0)\eta \) due to the cross-excitation parameter, i.e.,

\[
\eta = \frac{1}{N - n_0} \sum_{k>0} \langle \eta_k \rangle \langle n_k \rangle_{n_0} = \frac{1}{\mathcal{H}} \sum_{k>0} \frac{1}{(e^{\varepsilon_k/T} - 1)^2}. \tag{5.16}
\]

At arbitrary temperatures, the condensate master equation (5.2) contains two non-trivial parameters, \( \mathcal{H} \) and \( \eta \),

\[
\dot{p}_{n_0} = -\kappa \{(1 + \eta)[(N - n_0)(n_0 + 1)p_{n_0} - (N - n_0 + 1)n_0p_{n_0-1}] + \left[\mathcal{H} + (N - n_0)\eta\right]n_0p_{n_0} - \left[\mathcal{H} + (N - n_0 - 1)\eta\right](n_0 + 1)p_{n_0+1}\}. \tag{5.17}
\]

The steady-state solution of Eq. (5.17) is given by

\[
p_{n_0} = \frac{1}{Z_N} \frac{(N - n_0 + \mathcal{H}/\eta - 1)!}{(\mathcal{H}/\eta - 1)!(N - n_0)!} \left(\frac{\eta}{1 + \eta}\right)^{N-n_0}, \tag{5.18}
\]

where the canonical partition function \( Z_N = 1/p_N \) is

\[
Z_N = \sum_{n_0=0}^{N} \left(\frac{N - n_0 + \mathcal{H}/\eta - 1}{N - n_0}\right) \left(\frac{\eta}{1 + \eta}\right)^{N-n_0}. \tag{5.19}
\]

The master equation (5.17) for \( p_{n_0} \), and the analytic approximate expressions (5.18) and (5.19) for the condensate distribution function \( p_{n_0} \) and the partition function \( Z_N \), respectively, are among the main results of the condensate master equation approach. Now we are able to present the key picture of the theory of BEC fluctuations, that is the probability distribution \( p_{n_0} \), Fig. 7. Analogy with the evolution of the photon number distribution in a laser mode (from thermal to coherent, lasing) is obvious from a comparison of Fig. 7 and Fig.
4. With an increase of the number of atoms in the trap, $N$, the picture of the ground-state occupation distribution remains qualitatively the same, just a relative width of all peaks becomes narrower.

![Graphs showing central moments for ideal Bose gas in an isotropic harmonic trap with $N=200$ atoms.](image)

**Fig. 6.** The first four central moments for the ideal Bose gas in an isotropic harmonic trap with $N = 200$ atoms as calculated via the solution of the condensate master equation (solid lines - quasithermal approximation, Eq. (5.18); dash lines - low temperature approximation, Eq. (5.8)). Dots are “exact” numerical result obtained in the canonical ensemble.

The average number of atoms condensed in the ground state of the trap is

$$\langle n_0 \rangle = N - \mathcal{H} + p_0 \eta (N + \mathcal{H}/\eta).$$  \hspace{1cm} (5.20)

The squared variance and higher central moments can be also calculated analytically, e.g.,

$$\Delta n_0^2 = (1 + \eta)\mathcal{H} - p_0 (\eta N + \mathcal{H}) \left( N - \mathcal{H} + 1 + \eta \right) - p_0^2 (\eta N + \mathcal{H})^2.$$  \hspace{1cm} (5.21)
Fig. 7. Probability distribution of the ground-state occupation, $p_{n_0}$, at the temperature $T = 0.2, 0.5, 0.8$ and $1.0 T_c$ in an isotropic harmonic trap with $N = 200$ atoms as calculated from the solution of the condensate master equation (5.2) in the quasithermal approximation, Eq. (5.18), (solid line) and the “exact” numerical dots obtained in the canonical ensemble.

where

$$p_0 = \frac{1}{Z_N} \frac{(N + \mathcal{H}/\eta - 1)!}{N!(\mathcal{H}/\eta - 1)!} \left(\frac{\eta}{1 + \eta}\right)^N$$

(5.22)

is the probability that there are no atoms in the condensate.

The first four central moments for the Bose gas in a harmonic trap with $N = 200$ atoms are presented in Fig. 6 as the functions of temperature in different approximations. It is clearly seen that the analytic results based on quasithermal distribution are indistinguishable from the exact numerical results for the mean, and the second and the fourth moments. The results for the third moment are however quantitatively somewhat different. The success of the master equation approach is that the analytic expressions are available for the partition function as well as the condensate distribution function that mimic the exact solution to a remarkable degree for a mesoscopic ideal Bose gas.

As a final point, we mention that a laser phase transition analogy exists via the $P$-representation of the density matrix [DeGiorgio and Scully (1970), Graham and Haken (1970)]

$$\rho = \int \frac{d^2 \alpha}{\pi} P(\alpha, \alpha^*) |\alpha > < \alpha|,$$

(5.23)
where $|\alpha >$ is a coherent state. The steady-state solution of the Fokker-Planck equation for laser near threshold is [Scully and Zubairy (1997)]

$$P(\alpha, \alpha^*) = \frac{1}{\mathcal{N}} \exp \left[ \left( \frac{A-C}{A} \right) |\alpha|^2 - \frac{B}{2A} |\alpha|^4 \right]$$

(5.24)

which clearly indicates a formal similarity between

$$\ln P(\alpha, \alpha^*) = -\ln \mathcal{N} + (1 - \mathcal{H}/(N + 1)) n_0 - (1/2(N + 1)) n_0^2$$

(5.25)

for the laser equation and the Ginzburg-Landau type free energy [Scully and Zubairy (1997), DeGiorgio and Scully (1970), Graham and Haken (1970)]

$$G(n_0) = \ln p_{n_0} \approx \text{const} + a(T)n_0 + b(T)n_0^2,$$

(5.26)

where $|\alpha|^2 = n_0$, $a(T) = -(N - \mathcal{H})/N$ and $b(T) = 1/2N$ for large $N$ near $T_c$.

### 5.4 Squeezing, Noise Reduction and BEC fluctuations

The term “squeezing” originates from the studies of a noise reduction in quantum optics. In the present BEC context this aspect of (quantum) optical physics is relevant to the characteristic function for the total number of atoms in the two, $\mathbf{k}$ and $-\mathbf{k}$, modes squeezed by Bogoliubov coupling. A detailed derivation of the characteristic function for the fluctuations of the number of atoms in the two excited modes squeezed by the Bogoliubov coupling is presented in [Kocharovsky et al. (2000b)], it utilizes known results for the squeezed states of the radiation field and is given by

$$\Theta_{\pm k}(u) \equiv Tr \left\{ e^{iu(\beta_k^+ \beta_{-k} + \beta_{-k}^+ \beta_k)} e^{-\varepsilon_k(b_k^+ b_k + b_{-k}^+ b_{-k})/T} (1 - e^{-\varepsilon_k/T})^2 \right\}$$

$$= \frac{(z(A_k) - 1)(z(-A_k) - 1)}{(z(A_k) - e^{iu})(z(-A_k) - e^{iu})},$$

(5.27)

where

$$A_k = \frac{V}{\bar{n}_0 U_k} \left( \varepsilon_k - \frac{\hbar^2 k^2}{2M} - \frac{\bar{n}_0 U_k}{V} \right), \quad z(A_k) = \frac{A_k - e^{\varepsilon_k/T}}{A_k e^{\varepsilon_k/T} - 1},$$

(5.28)

$\varepsilon_k$ is the energy of Bogoliubov quasiparticles

$$\varepsilon_k = \sqrt{\left( \frac{\hbar^2 k^2}{2M} + \frac{\bar{n}_0 U_k}{V} \right)^2 - \left( \frac{\bar{n}_0 U_k}{V} \right)^2},$$

(5.29)
\( M \) is the atomic mass, \( V \) is the condensate volume, \( U_k \) is the atom-atom scattering energy. In Eq. (5.27) \( \hat{\beta}_k \) are bare canonical ensemble quasiparticles which are related to Bogoliubov quasiparticles \( \hat{b}_k \) by the canonical transformation

\[
\hat{\beta}_k = u_k \hat{b}_k + v_k \hat{b}^+_k, \quad \hat{\beta}^+_k = u_k \hat{b}^+_k + v_k \hat{b}^-_k,
\]

(5.30)

where \( u_k \) and \( v_k \) are Bogoliubov amplitudes

\[
u_k = \frac{1}{\sqrt{1-A^2_k}}, \quad v_k = \frac{A_k}{\sqrt{1-A^2_k}}.
\]

(5.31)

The characteristic function for the distribution of the total number of the excited atoms is equal to the product of the coupled-mode characteristic functions, \( \Theta_n(u) = \prod_{k\neq 0, mod(\pm k)} \Theta_{\pm k}(u) \), since different pairs of \((k, -k)\)-modes are independent to the first approximation. The product \( \Pi \) runs over all different pairs of \((k, -k)\)-modes.

By doing all calculations via the canonical-ensemble quasiparticles we automatically take into account all correlations introduced by the canonical-ensemble constraint. The important conclusion is that for square well trap the ground state occupation fluctuations are not Gaussian even in the thermodynamic limit. It is more convenient, in particular, for the analysis of the non-Gaussian properties, to solve for the cumulants \( \kappa_m \) which are defined as coefficients in Taylor expansion \( \ln \Theta_n(u) = \sum_{m=1}^{\infty} \kappa_m (iu)^m / m! \), where \( \Theta_n(u) \) is the characteristic function \( \Theta_n(u) = Tr \{ e^{iu\hat{\rho}} \} \). There are simple relations between \( \kappa_m \) and central moments \( \mu_m \), in particular,

\[
\kappa_1 = \bar{n}, \quad \kappa_2 = \mu_2, \quad \kappa_3 = \mu_3, \quad \kappa_4 = \mu_4 - 3\mu_2^2.
\]

(5.32)

The “generating cumulants” \( \bar{\kappa}_m \) are simply related to the cumulants \( \kappa_m \) by

\[
\kappa_1 = \bar{\kappa}_1, \quad \kappa_2 = \bar{\kappa}_2 + \bar{\kappa}_1, \quad \kappa_3 = \bar{\kappa}_3 + 3\bar{\kappa}_2 + \bar{\kappa}_1, \quad \kappa_4 = \bar{\kappa}_4 + 6\bar{\kappa}_3 + 7\bar{\kappa}_2 + 3\bar{\kappa}_1.
\]

(5.33)

For Gaussian distribution \( \kappa_m = 0 \), for \( m = 3, 4, \ldots \).

The explicit formula for all cumulants in the dilute weakly interacting Bose gas was obtained in [Kocharovsky et al. (2000b)]:

\[
\bar{\kappa}_m = \frac{1}{2} (m-1)! \sum_{k \neq 0} \left[ \frac{1}{(z(A_k) - 1)^m} + \frac{1}{(z(-A_k) - 1)^m} \right].
\]

(5.34)
For the ideal gas the answer is

\[ \tilde{\kappa}_m = (m - 1)! \sum_{k \neq 0} \frac{1}{(\epsilon_k/T - 1)^m}. \]  

(5.35)

In comparison with the ideal Bose gas, Eq. (5.35), for the interacting particles we have effectively a mixture of two species of atom pairs with \( z(\pm A_k) \) instead of \( \exp(\epsilon_k/T) \).

It is important to emphasize that the first equation in (5.34), \( m = 1 \), is a non-linear self-consistency equation,

\[ N - \bar{n}_0 = \kappa_1(\bar{n}_0) \equiv \sum_{k \neq 0} \frac{1 + A_k^2 \epsilon_k/T}{1 - A_k^2(\epsilon_k/T - 1)}. \]  

(5.36)

to be solved for the mean number of ground-state atoms \( \bar{n}_0(T) \), since the Bogoliubov coupling coefficient \( A_k \), and the energy spectrum \( \epsilon_k \), are themselves functions of the mean value \( \bar{n}_0 \). Then, all the other equations in (5.34), \( m \geq 2 \), are nothing else but explicit expressions for all cumulants, \( m \geq 2 \), if one substitutes the solution of the self-consistency equation (5.36) for the mean value \( \bar{n}_0 \).

The Eq. (5.36), obtained for the interacting Bose gas in the canonical-ensemble quasiparticle approach, coincides precisely with the self-consistency equation for the grand-canonical dilute gas in the so-called first-order Popov approximation (see a review in [Shi and Griffin (1998)]). The latter is well established as a reasonable first approximation for the analysis of the finite-temperature properties of the dilute Bose gas and is not valid only in a very small interval near \( T_c \), given by \( T_c - T < a(N/V)^{1/3}T_c \ll T_c \), where \( a = MU_0/4\pi\hbar^2 \) is a usual s-wave scattering length. The analysis of the Eq. (5.36) shows that in the dilute gas the self-consistent value \( \bar{n}_0(T) \) is close to that given by the ideal gas model, and for very low temperatures goes smoothly to the value given by the standard Bogoliubov theory [Lifshitz and Pitaevskii (1981), Abrikosov et al. (1963), Fetter and Walecka (1971)] for a small condensate depletion, \( N - \bar{n}_0 \ll N \). This is illustrated by Fig. 8 in which we show the first four cumulants. Near the critical temperature \( T_c \) the number of excited quasiparticles is relatively large, so that along with the Bogoliubov coupling other, higher order effects of interaction should be taken into account to get a complete theory. Note that the effect of a weak interaction on the condensate fluctuations is very significant, see Fig. 8, even if the mean number of condensed atoms changes by relatively small amount.
Fig. 8. Temperature scaling of the first four cumulants, the mean value \( \bar{n}_0/N = N - \kappa_1/N \), the variance \( \sqrt{\kappa_2/N} = \langle (n_0 - \bar{n}_0)^2 \rangle^{1/2}/N^{1/2} \), the third central moment \( -\kappa_3/N^{1/2} = \langle (n_0 - \bar{n}_0)^3 \rangle^{1/3}/N^{1/2} \), the fourth cumulant \( |\kappa_4|^{1/4}/N^{1/2} = |\langle (n_0 - \bar{n}_0)^4 \rangle - 3\kappa_2^2|/N^2 \), of the ground-state occupation fluctuations for the dilute weakly interacting Bose gas with \( U_0 N^{1/3}/\varepsilon_1 V = 0.05 \) (thick solid lines), as compared with the ideal gas (thin solid lines) and with the “exact” numerical result in the canonical ensemble (dot-dashed lines) for the ideal gas in the box; \( N = 1000 \). For the ideal gas the thin solid lines are almost indistinguishable from the “exact” dot-dashed lines in the condensed region, \( T < T_c(N) \). Temperature is normalized by the standard thermodynamic-limit critical value \( T_c(N) \) that differs from the finite-size value \( T_c(N) \), as is clearly seen in graphs.

6 Hybrid approach to condensate fluctuations

We now show how to combine ideas from the canonical ensemble quasiparticle formalism of [Kocharovsky et al. (2000b)] (which works well for an interacting gas at temperature not too close to \( T_c \) when \( \sqrt{\mu_2} \ll \bar{n}_0 \)) with the physics of the master equation approach (in the spirit of the quantum theory of the laser) [Kocharovsky et al. (2000a)], in order to obtain essentially perfect quantitative agreement with the exact numerical solution of the canonical partition function at all temperatures for the fluctuation statistics of the Bose gas. Such a hybrid technique was proposed in [Svidzinsky and Scully (2006)].

We recall the master equation for the condensate probability distribution for
a non-interacting Bose gas ((5.2)

\[
\frac{1}{\kappa} p_{n_0} = -K_{n_0} (n_0 + 1) p_{n_0} + K_{n_0} n_0 p_{n_0 - 1} - H_{n_0} n_0 p_{n_0} + H_{n_0 + 1} (n_0 + 1) p_{n_0 + 1},
\]

(6.1)

The detailed balance condition yields

\[
\frac{p_{n_0 + 1}}{p_{n_0}} = \frac{K_{n_0}}{H_{n_0 + 1}}.
\]

(6.2)

Since the occupation number of the ground state cannot be larger than \(N\) there is a canonical ensemble constraint \(p_{N+1} = 0\) and, hence, \(K_N = 0\). In contrast to \(p_{n_0}\), the ratio \(p_{n_0+1}/p_{n_0}\) as a function of \(n_0\) shows simple monotonic behavior. We approximate \(K_{n_0}\) and \(H_{n_0}\) by a few terms of the Taylor expansion near the point \(n_0 = N\)

\[
K_{n_0} = (N - n_0)(1 + \eta) + \alpha (N - n_0)^2,
\]

(6.3)

\[
H_{n_0} = \mathcal{H} + (N - n_0)\eta + \alpha (N - n_0)^2.
\]

(6.4)

The parameters \(\mathcal{H}, \eta\) and \(\alpha\) are independent of \(n_0\); they are functions of the occupation of the excited levels. We derive them below by matching the first three central moments in the low temperature limit with the result of [Kocharovsky et al. (2000b)]. We note that the detailed balance equation (6.2) is the Padé approximation [Baker (1996)] of the function \(p_{n_0+1}/p_{n_0}\). Padé summation has proven to be useful in many applications, including condensed-matter problems and quantum field theory.

Equations (6.2)-(6.4) yield an analytical expression for the condensate distribution function

\[
p_{n_0} = \frac{1}{Z_N} \frac{(N - n_0 - 1 + x_1)! (N - n_0 - 1 + x_2)!}{(N - n_0)! (N - n_0 + (1 + \eta)/\alpha)!},
\]

(6.5)

where \(x_{1,2} = (\eta \pm \sqrt{\eta^2 - 4\alpha \mathcal{H}})/2\alpha\) and \(Z_N\) is the normalization constant determined by \(\sum_{n_0=0}^{N} p_{n_0} = 1\). In the particular case \(\eta = \alpha = 0\) Eq. (6.5) reduces to Eq. (5.8) obtained in the low temperature approximation.

Using the distribution function (6.5) we find that, in the validity range of [Kocharovsky et al. (2000b)] (at low enough \(T\)), the first three central moments \(\mu_m \equiv \langle (n_0 - \bar{n}_0)^m \rangle\) are

\[
\bar{n}_0 = N - \mathcal{H}, \quad \mu_2 = (1 + \eta)\mathcal{H} + \alpha \mathcal{H}^2,
\]

(6.6)
\[
\mu_3 = -\mathcal{H}(1 + \eta + \alpha \mathcal{H})(1 + 2\eta + 4\alpha \mathcal{H}).
\]  
(6.7)

Eqs. (6.6), (6.7) thus yield

\[
\mathcal{H} = N - \bar{n}_0, \quad \eta = \frac{1}{2} \left( \frac{\mu_2}{\mu_2} - 3 + \frac{4\mu_2}{\mathcal{H}} \right),
\]  
(6.8)

\[
\alpha = \frac{1}{\mathcal{H}} \left( \frac{1}{2} - \frac{\mu_2}{\mathcal{H}} - \frac{\mu_3}{2\mu_2} \right).
\]  
(6.9)

On the other hand, the result of [Kocharovsky et al. (2000b)] for an interacting Bogoliubov gas is (see Appendix for derivation of \(\bar{n}_0\) and \(\mu_2\))

\[
\bar{n}_0 = N - \sum_{k \neq 0} \left[ (u_k^2 + v_k^2) f_k + v_k^2 \right],
\]  
(6.10)

\[
\mu_2 = \sum_{k \neq 0} \left[ (1 + 8u_k^2v_k^2)(f_k^2 + f_k) + 2u_k^2v_k^2 \right],
\]  
(6.11)

\[
\mu_3 = -\sum_{k \neq 0} \left( u_k^2 + v_k^2 \right) \left[ (1 + 16u_k^2v_k^2)(2f_k^3 + 3f_k^2 + f_k) + 4u_k^2v_k^2(1 + 2f_k) \right],
\]  
(6.12)

where \(f_k = 1/\left[ \exp(\varepsilon_k/k_B T) - 1 \right] \) is the number of elementary excitations with energy \(\varepsilon_k\) present in the system at thermal equilibrium, \(u_k\) and \(v_k\) are Bogoliubov amplitudes. Substitute for \(\bar{n}_0, \mu_2\) and \(\mu_3\) in Eqs. (6.8), (6.9) their expressions [Kocharovsky et al. (2000b)] (6.10)-(6.12) yields the unknown parameters \(\mathcal{H}, \eta\) and \(\alpha\). The beauty of the present “matched asymptote” derivation is that the formulas for \(\mathcal{H}, \eta\) and \(\alpha\) are applicable at all temperatures, i.e. not only in the validity range of [Kocharovsky et al. (2000b)]. The distribution function (6.5) together with Eqs. (6.8), (6.9) provides complete knowledge of the condensate statistics at all \(T\). Taking \(v_k = 0\) and \(u_k = 1\) in (6.10)-(6.12) we obtain the ideal gas limit.

Figure 9 shows the average condensate particle number \(\bar{n}_0\), its variance, third and fourth central moments \(\mu_m\) and fourth cumulant \(\kappa_4\) as a function of \(T\) for an ideal gas of \(N = 200\) particles in a harmonic trap. Solid lines are the result of the present approach which is in remarkable agreement with the “exact” dots at all temperatures both for \(\mu_m\) and \(\kappa_4\). Central moments and cumulants higher than fourth order are not shown here, but they are also remarkably accurate at all temperatures. Results of [Kocharovsky et al. (2000b)] are given by dashed lines which are accurate only at sufficiently low \(T\). Deviation of higher order cumulants (\(m = 3, 4, \ldots\)) from zero indicates that the fluctuations are not Gaussian.
Clearly the present hybrid method passes the ideal gas test with flying colors. We note the excellent agreement with the exact analysis for the third central moment and fourth cumulant $\kappa_4$ given in Fig. 9.

Next we apply this technique to $N$ interacting Bogoliubov particles confined in a box of volume $V$. The interactions are characterized by the gas parameter $an^{1/3}$, where $a$ is the s-wave scattering length and $n = N/V$ is the particle density. The energy of Bogoliubov quasiparticles $\varepsilon_k$ depends on $\bar{n}_0$, hence, the equation $\bar{n}_0 = \sum_{n_0=0}^{N} n_0 p_{n_0}$ for $\bar{n}_0$ must be solved self-consistently. In Fig. 10 we plot $\bar{n}_0$, the variance $\Delta n_0$, third and fourth central moments as a function of $T$ for an ideal and interacting ($an^{1/3} = 0.1$) gas in the box. Solid lines show the result of the present approach, while [Kocharovsky et al. (2000b)] is represented by dashed lines. The present results agree well for all $\mu_m$ with [Kocharovsky et al. (2000b)] in the range of its validity. Near and above $T_\text{c}$ [Kocharovsky et al. (2000b)] becomes inaccurate. However, the results of the present method are expected to be accurate at all $T$. Indeed, in the limit $T \gg T_\text{c}$ the present results (unlike [Kocharovsky et al. (2000b)]) merge with those for the ideal gas. This is physically appealing since at high $T$ the kinetic energy becomes much larger than the interaction energy and the gas behaves ideally. Similar to the ideal gas, the interacting mesoscopic BEC $\bar{n}_0(T)$ exhibits a smooth transition when passing through $T_\text{c}$.

One can see from Fig. 10 that the repulsive interaction stimulates BEC, and yields an increase in $\bar{n}_0$ at intermediate temperatures, as compared to the ideal gas. This effect is known as “attraction in momentum space” and occurs for energetic reasons [Leggett (2001)]. Bosons in different states interact more strongly than when they are in the same state, and this favors multiple occupation of a single one-particle state.

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Appendix

7 Mean condensate particle number and its variance for weakly interacting BEC

In the framework of Bogoliubov theory the particle operator can be expressed in terms of the quasiparticle creation and annihilation operators as

$$
\hat{\beta}_k = u_k \hat{b}_k + v_k \hat{b}_{-k}^+, \quad \hat{\beta}_k^+ = u_k \hat{b}_k^+ + v_k \hat{b}_{-k},
$$

(7.1)
Fig. 9. Average condensate particle number $\langle n_0 \rangle$, its variance $\Delta n_0 = \sqrt{\langle (n_0 - \bar{n}_0)^2 \rangle}$, third and fourth central moments $\langle (n_0 - \bar{n}_0)^m \rangle$ ($m = 3, 4$) and fourth cumulant $\kappa_4$ as a function of temperature for an ideal gas of $N = 200$ particles in a harmonic trap. Solid lines (CNB5) show the result of the hybrid approach. [Kocharovsky et al. (2000b)] yields dashed lines (CNB3). Dots are “exact” numerical simulation in the canonical ensemble. The temperature is normalized by the thermodynamic critical temperature for the trap $T_c = \hbar \omega N^{1/3}/k_B \zeta(3)^{1/3}$, where $\omega$ is the trap frequency.

where $u_k$ and $v_k$ are Bogoliubov amplitudes. The total number of particles out of the condensate is given by the expectation value of the operator

$$\hat{N}_{out} = \sum_{k \neq 0} \beta_k^+ \beta_k = \sum_{k \neq 0} \left[ u_k^2 \hat{b}_k^+ \hat{b}_k + v_k^2 \hat{b}_k \hat{b}_k^+ + u_k v_k (\hat{b}_k \hat{b}_{-k} + \hat{b}_k^+ \hat{b}_{-k}^+) \right].$$

(7.2)

Using the particle number constraint $\hat{n}_0 + \hat{N}_{out} = N$ we obtain

$$\bar{n}_0 = N - \langle \hat{N}_{out} \rangle = N - \sum_{k \neq 0} \left[ (u_k^2 + v_k^2) f_k + v_k^2 \right],$$

(7.3)

where $f_k = \langle \hat{b}_k^+ \hat{b}_k \rangle = 1/[\exp(\varepsilon_k/k_B T) - 1]$ is the number of elementary excitations with energy $\varepsilon_k$ present in the system at thermal equilibrium.
moments as a function of temperature for an ideal (\(a n^{1/3} = 0\)) Bose gas of \(N = 200\) particles in a box. Solid lines are the result of the hybrid approach. [Kocharovsky et al. (2000b)] yields dashed lines (CNB3). The temperature is normalized by the thermodynamic critical temperature for the box \(T_c = 2\pi h^2 n^{2/3} / k_B M \zeta(3/2)^{2/3}\), where \(M\) is the particle mass.

In a similar way one can calculate particle fluctuations [Giorgini et al. (1998)]. Using Eq. (7.2) we have

\[
\hat{N}_{\text{out}}^2 = \sum_{k \neq 0} \hat{\beta}_k^+ \hat{\beta}_k \sum_{q \neq 0} \hat{\beta}_q^+ \hat{\beta}_q = \sum_{k, q \neq 0} \left[ u_k^2 v_q^2 (\hat{b}_k^+ \hat{b}_q \hat{b}_q^+ \hat{b}_k) + u_k^2 v_q^2 (\hat{b}_q \hat{b}_k^+ \hat{b}_q^+ \hat{b}_k) + u_k^2 v_q^2 (\hat{b}_q \hat{b}_k \hat{b}_q^+ \hat{b}_k^+) + u_k^2 v_q^2 (\hat{b}_q \hat{b}_k^+ \hat{b}_q \hat{b}_k^+) \right] + \sum_{k, q \neq 0} \left[ v_k^2 u_q^2 (\hat{b}_k^+ \hat{b}_k \hat{b}_q \hat{b}_q^+) + v_k^2 u_q^2 (\hat{b}_k \hat{b}_k^+ \hat{b}_q \hat{b}_q^+) + v_k^2 u_q^2 (\hat{b}_k \hat{b}_k^+ \hat{b}_q \hat{b}_q^+) \right]
\]

\(\text{(7.4)}\)

To calculate the expectation value of the terms with four quasiparticle operators appearing in \(\langle \hat{N}_{\text{out}}^2 \rangle\) we use Wick’s theorem which holds for the operators of statistically independent excitations. In particular, nonzero averages come from the terms with \(q = \pm k\). Using Wick’s theorem we obtain

\[
\langle \hat{b}_k^+ \hat{b}_k \hat{b}_k^+ \hat{b}_k \rangle = 2 f_k^2 + f_k, \quad \langle \hat{b}_k^+ \hat{b}_k \hat{b}_k^+ \hat{b}_k \rangle = f_k^2,
\]

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\[
< \hat{b}_k \hat{b}_k^+ \hat{b}_k \hat{b}_k^+ > = 2 f_k^2 + 3 f_k + 1, \quad < \hat{b}_k \hat{b}_k^+ \hat{b}_{-k} \hat{b}_{-k}^+ > = (f_k + 1)^2, \\
< \hat{b}_k^+ \hat{b}_k \hat{b}_k^+ > = < \hat{b}_k \hat{b}_k^+ \hat{b}_k > = 2 f_k^2 + 2 f_k, \\
< \hat{b}_k^+ \hat{b}_{-k} \hat{b}_{-k}^+ > = < \hat{b}_{-k} \hat{b}_{-k}^+ \hat{b}_{-k} > = f_k^2 + f_k, \\
< \hat{b}_k \hat{b}_{-k} \hat{b}_{-k}^+ > = < \hat{b}_{-k} \hat{b}_{-k}^+ \hat{b}_k > = (f_k + 1)^2, \\
< \hat{b}_k^+ \hat{b}_{-k} \hat{b}_k \hat{b}_{-k}^+ > = < \hat{b}_{-k}^+ \hat{b}_k \hat{b}_{-k} \hat{b}_{-k}^+ > = f_k^2,
\]

and therefore

\[
< \hat{N}_{out}^2 > = \sum_{k \neq \pm q \neq 0} [u_k^2 u_q^2 f_k f_q + v_k^2 v_q^2 (f_k + 1)(f_q + 1) + 2u_k^2 v_q^2 f_k(f_q + 1)] +
\]

\[
\sum_{k \neq 0} [u_k^4 (\hat{b}_k^+ \hat{b}_k^+ \hat{b}_k^+ \hat{b}_k^+ > + \hat{b}_k^+ \hat{b}_k^+ \hat{b}_{-k}^+ \hat{b}_{-k})] + v_k^4 (\hat{b}_k \hat{b}_k^+ \hat{b}_{-k}^+ \hat{b}_{-k} > + \hat{b}_k \hat{b}_{-k}^+ \hat{b}_{-k}^+ \hat{b}_{-k} >) +
\]

\[
u_k^2 v_k^2 (\hat{b}_k^+ \hat{b}_k^+ \hat{b}_k^+ \hat{b}_k^+ > + \hat{b}_k^+ \hat{b}_k^+ \hat{b}_{-k}^+ \hat{b}_{-k} > + \hat{b}_{-k} \hat{b}_{-k}^+ \hat{b}_{-k}^+ \hat{b}_{-k} > + \hat{b}_{-k} \hat{b}_{-k}^+ \hat{b}_{-k}^+ \hat{b}_{-k} >) =
\]

\[
\sum_{k \neq \pm q \neq 0} [u_k^2 u_q^2 f_k f_q + v_k^2 v_q^2 (f_k + 1)(f_q + 1) + 2u_k^2 v_q^2 f_k(f_q + 1)] +
\]

\[
\sum_{k \neq 0} [u_k^4 (3f_k^2 + f_k) + v_k^4 (3f_k^2 + 5f_k + 2) + u_k^2 v_k^2 (10f_k^2 + 10f_k + 2)] . \tag{7.5}
\]

From the other hand

\[
< \hat{N}_{out} >^2 = \sum_{k \neq 0 \neq q} [(u_k^2 + v_k^2) f_k + v_k^2] \left[ (u_q^2 + v_q^2) f_q + v_q^2 \right] . \tag{7.6}
\]

Using the particle number constraint together with Eqs. (7.5) and (7.6) and \( u_k^2 - v_k^2 = 1 \) we find the following answer for the squared variance of condensate fluctuations [Giorgini et al (1998)]

\[
\mu_2 \equiv < \hat{n}_0 > - < \hat{n}_0 >^2 = < \hat{N}_{out} > - < \hat{N}_{out} >^2 =
\]

\[
\sum_{k \neq 0} [(1 + 8u_k^2 v_k^2)(f_k + f_k) + 2u_k^2 v_k^2] . \tag{7.7}
\]

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