The relativistic Bose gas

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Abstract. The quantum statistical mechanics of an ideal relativistic Bose gas of massive particles is discussed. The thermodynamic functions of the system are obtained from the exact expression for the logarithm of the grand partition function. The correct procedure for carrying out the non-relativistic and ultra-relativistic limits is presented. The limitations and errors of previous calculations which relied on the binomial expansion of the density of states are pointed out. It is shown that the behaviour of the system in the limit of zero temperature is dominated by the non-relativistic effects.

1. Introduction

Ideal gases are a valuable tool in obtaining information about a great many physical situations. In weakly interacting systems they provide a qualitative understanding of several important features and also serve as a basis for the development of a perturbative scheme. The quantum statistics of ideal gases has been used extensively to describe both fermion and boson systems. Electrons in metals, liquid helium and superconductors are just a few examples where a non-relativistic treatment has been successfully used in explaining some remarkable features such as the existence of a Fermi surface in metals and the occurrence of a phase transition (Bose–Einstein condensation) in both helium and superconductors (condensation of Cooper pairs). Astrophysical systems, however, require a fully relativistic treatment. The most notable examples are white dwarfs and neutron stars. In the former, the degeneracy pressure of an electron gas stabilises the star against gravitational collapse, while it has been conjectured that pion condensation occurs in the interior of neutron stars.

Even though the quantum statistical mechanics of the ideal relativistic boson gas has received considerable attention in the past (in fact, the birth of quantum statistics is marked by Bose's derivation of Planck's law of blackbody radiation and the first analyses of a relativistic gas of massive particles go way back to Jüttner (1928) and Glaser (1935) and, more recently, to Landsberg and Dunning-Davies (1965)), it is our opinion that certain difficulties concerning the ultra-relativistic regime of the system deserve a careful discussion in order to avoid unreliable procedures contained in the earlier works. Quite recently, Kuzmin and Shaposhnikov (1979) have explored the cosmological implications of a massive primordial photon gas thus turning the study of the behaviour of boson gases in the extreme conditions of the ultra-relativistic limit into a matter of current interest. Here we present a treatment of the problem which reproduces all the known results and allows us to detect mistakes and correct the results of previous analyses of the ultra-relativistic limit. In § 2 the formalism and the exact formulae for the thermodynamic functions are shown. In § 3 we show how the different

approximations of the exact results are correctly obtained with the help of the relations among the three relevant lengths of the system. For this purpose a generalised thermal wavelength is introduced. In § 4 the behaviour of the ultra-relativistic gas is obtained. This approach has led us to conclude that the massless particle gas is the only truly ultra-relativistic system at any temperature or, equivalently, that the behaviour of a massive particle gas at very low temperature ($k_B T \ll mc^2$) is of a non-relativistic nature.

2. The formalism and exact results

We begin by writing the logarithm of the grand partition function of the ideal boson gas as an integral transform of the single particle partition function $Z_1(\beta)$ (Goulart Rosa and Grandy 1973)

$$\ln \Xi = \frac{-1}{2i} \int_{\alpha-i\infty}^{\alpha+i\infty} t^{-1} \cot(\pi t) \exp(\beta \xi t) Z_1(\beta t) \, dt \tag{1}$$

where $\beta^{-1} = k_B T$, ξ is the chemical potential, $\alpha \in (0, 1)$. In order to calculate $Z_1(\beta) = \sum_j \exp(-\beta E_j)$ let us consider the gas contained in a cubic box of volume $V = L^3$. According to quantum mechanics, the particle energy takes the discrete values

$$E^2 = (\hbar c k)^2 + m^2 c^4,$$
$$k_i = 2\pi n_i / L \qquad n_i = 0, \pm 1, \pm 2, \ldots \qquad i = 1, 2, 3, \tag{2}$$

where we have imposed periodic boundary conditions on the wavefunctions. The number of states with energy between E and $E + dE$ is then given by

$$D(E) = \frac{4\pi V g}{(hc)^3} [E^2 - m^2 c^4]^{1/2} E \tag{3}$$

where $g = (2S + 1)$ is the spin degeneracy. Replacing the summation over the particle states index j by an integration involving the density of states, we obtain

$$Z_1(\beta) = (4\pi V g / \lambda_c^3)(K_2(u)/u) \tag{4}$$

where $\lambda_c = h/mc$ is the Compton wavelength, $u = \beta mc^2$ and K_2 is the modified Bessel function. The expression for $D(E)$ contains only the bulk term and as usual this is justified in the limit of large volumes; in doing so we have discarded *ab initio* all questions concerning boundary effects on the behaviour of the system. (The sensitivity of the Bose–Einstein condensation to boundary conditions, in the non-relativistic case, was shown by Landau and Wilde (1979). They show that whereas periodic Dirichlet, Neumann and 'repulsive wall' conditions lead to the same density of condensate, the 'attractive wall' conditions lead to a different answer.)

We recall that the modified Bessel functions $K_\nu(t)$ are regular functions throughout the t-plane cut along the negative axis and are real and positive when $\nu > -1$ and $t > 0$. The asymptotic expansion for large argument and the ascending series from which one can obtain the behaviour in the limit of $t \to 0$ are, respectively:

$$K_\nu(t) \sim (\pi/2t)^{1/2} \exp(-t) \left[1 + \frac{4\nu^2 - 1}{8t} + \frac{(4\nu^2 - 1)(4\nu^2 - 9)}{2!(8t)^2} + \ldots \right] \tag{5}$$

$$K_\nu(t) = \tfrac{1}{2}(t/2)^{-\nu} \sum_{k=0}^{\nu-1} \frac{(\nu-k-1)!}{k!} \left(\frac{-t^2}{4}\right)^k + (-1)^{\nu+1} \ln(t/2) I_\nu(t)$$

$$+ \tfrac{1}{2}(-t/2)^\nu \sum_{k=0}^{\infty} \{\psi(k+1) + \psi(k+\nu+1)\} \frac{(t/2)^{2k}}{k!(\nu+k)!} \tag{6}$$

where $\psi(k)$ is the logarithmic derivative of the gamma function $\Gamma(k)$ and

$$I_\nu(t) = (t/2)^\nu \sum_{k=0}^{\infty} \frac{(t/2)^{2k}}{k! \Gamma(\nu+k+1)}. \tag{7}$$

Bearing in mind that the energy in equation (2) contains the particle rest energy, we note that the familiar non-relativistic (ultra-relativistic) one-particle partition function is regained from equation (4) if we substitute K_2 by the first term of equation (5) (equation (6)). Corrections to these limits can be obtained retaining higher order terms in the asymptotic and ascending series for $K_2(t)$. We will return to discuss this point later on with more details since this is the crux of the problem.

The integral resulting from the substitution of equation (4) into equation (1) can be evaluated by closing the straight line contour to the right with a semi-arc of a circle. Because of the analytic behaviour of the K_ν, the integrand of equation (1) is an analytic function on the right half t-plane except at $t = n$; $n = 1, 2, 3, \ldots$ where it has simple poles due to the factor $\cot(\pi t)$. The application of Cauchy's theorem gives the following expression for $\ln \Xi$:

$$\ln \Xi = \frac{4\pi Vg}{\lambda_c^3 u} \sum_{n=1}^{\infty} (e^{\beta\xi n}/n^2) K_2(nu). \tag{8}$$

From the requirement that the integral along this semi-circle vanishes when the radius goes to infinity, one derives that $\xi \leqslant mc^2$. This condition on ξ coincides with the physical requirement that the chemical potential should never exceed the minimum energy of the particles so that the occupation number be always positive. Other quantities of interest, such as the entropy, the pressure, the average number of particles present in the system, are obtained from the thermodynamic potential Ω by suitable partial differentiation, e.g.

$$\Omega \equiv -\ln \Xi/\beta = -PV \tag{9a}$$

$$S \equiv -\left(\frac{\partial\Omega}{\partial T}\right)_{V,\xi} = k_B \frac{4\pi Vg}{\lambda_c^3 u} \sum_{n=1}^{\infty} \frac{e^{\beta\xi n}}{n^2} [2K_2(nu) - \beta\xi n K_2(nu) - nu K_2'(nu)] \tag{9b}$$

$$P \equiv -\left(\frac{\partial\Omega}{\partial V}\right)_{T,\xi} = \frac{4\pi\beta^{-1}g}{\lambda_c^3 u} \sum_{n=1}^{\infty} \frac{K_2(nu) e^{\beta\xi n}}{n^2} \tag{9c}$$

$$\bar{N} \equiv -\left(\frac{\partial\Omega}{\partial\xi}\right)_{T,V} = \frac{4\pi Vg}{\lambda_c^3 u} \sum_{n=1}^{\infty} \frac{K_2(nu) e^{\beta\xi n}}{n} \tag{9d}$$

$$\bar{E} \equiv TS - PV + \xi\bar{N} = \frac{4\pi Vg}{\lambda_c^3 u} \beta^{-1} \sum_{n=1}^{\infty} \frac{e^{\beta\xi n}}{n^2} [K_2(nu) - nu K_2'(nu)] \tag{9e}$$

$$U \equiv \bar{E} - \bar{N}(mc^2) = \frac{4\pi Vg}{\lambda_c^3 u} \beta^{-1} \sum_{n=1}^{\infty} \frac{e^{\beta\xi n}}{n^2} [K_2(nu) - nu K_2'(nu) - nu K_2(nu)]. \tag{9f}$$

Below the critical temperature we must add to equation (9a) the contribution

$$\Omega_0 = (1/\beta) \ln\{1 - \exp[-\beta(mc^2 - \xi)]\}$$

from the zero momentum state which is lost when one transforms the summation into an integral over the energy in $Z_1(\beta)$. This formalism has been recently used to discuss the case of a boson gas confined in an Einstein universe (Aragão de Carvalho and Goulart Rosa 1980).

3. Special cases

The formulae in the previous section are exact and well known (Glaser 1935). This being the case, it is important to investigate how these expressions approach their classical limit, so as to identify the purely quantum-mechanical contributions to the thermodynamic functions. Furthermore, we can compute their non-relativistic and ultra-relativistic limits, thus obtaining simplified formulae which have been used in a large number of physical applications.

There are three characteristic lengths in the system: the Compton wavelength, the average distance between particles $\bar\lambda \equiv (V/\bar N)^{1/3}$ and the thermal wavelength $\lambda_T \equiv h/\bar p$ where $\bar p$ is the average momentum (in modulus):

$$\bar p \equiv \frac{Vg}{Z_1(\beta)h^3} \int d^3p \, |p| \, e^{-\beta E_p}, \qquad Z_1(\beta) = g \sum_p e^{-\beta E_p}. \tag{10}$$

In the non-relativistic approximation $E_p = p^2/2m$ the thermal de Broglie wavelength is recovered $[2\lambda_T/\pi = (h^2/2\pi m k_B T)^{1/2}]$. The use of the photon dispersion relation in equation (10) gives $\lambda_T = hc/3k_B T$. The relationships between these lengths will alone specify the different regimes of the system.

The classical limit of the expressions must correspond to a physical situation in which the average distance between particles in the gas by far exceeds the thermal wavelength ($\bar\lambda \gg \lambda_T$). It is clear that in this case the wavefunctions of the particles in the gas will have little overlap, allowing for a classical treatment. If, however, $\bar\lambda \lesssim \lambda_T$ there will be considerable overlap and quantum-mechanical effects become very important. We will see that the classical limit corresponds to restricting the sums over n appearing in equations (9) to just one term ($n = 1$). In this limit we recover the Boltzmann distribution and the condition $\bar\lambda \gg \lambda_T$ is satisfied.

Non-relativistic and ultra-relativistic limits are purely kinematical ones which can be taken whether we are dealing with a fully quantum expression or its classical form. They correspond to cases in which $\bar pc$ is either much smaller or much greater than mc^2. We can characterise those limits by comparing the thermal wavelength λ_T of the system with the Compton wavelength λ_c associated with each particle: (i) $\lambda_T \gg \lambda_c \to$ non-relativistic; (ii) $\lambda_T \ll \lambda_c \to$ ultra-relativistic.

Before we proceed to treat each case individually, two comments are in order: (a) by forming all possible combinations with the parameters $\bar\lambda$, λ_T and λ_c we can discuss the limiting cases of interest: these are shown in figure 1; (b) taking appropriate limits in the expressions of § 2 allows us to have complete control over the corrections to these limits, whereas this information is lost if we start out using asymptotic dispersion relations such as $E = p^2/2m$ or $E = pc$. In our calculations we have avoided performing any disfiguring approximation on the dispersion relation (equation (2)).
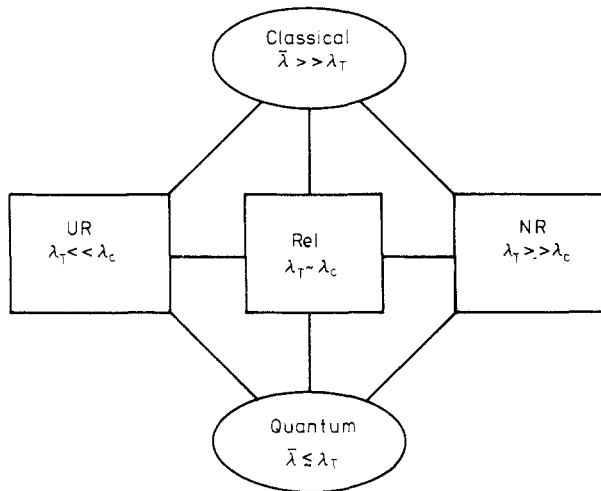
Figure 1.

3.1. The Boltzmann limit

The classical limit of the system is obtained by retaining only the first term in the expressions for the thermodynamic functions. This can be shown if we consider, for instance, the particle number $\bar{N}$. As is well known, the Boltzmann distribution can be obtained by expanding the Bose–Einstein distribution $n_i = X_i(1 - X_i)^{-1}$ for $X_i \ll 1$, $X_i = \exp \beta(\xi - E_i)$ and keeping the first term only. There $\bar{N}$ will be written as:

$$\bar{N} = \sum_i \bar{n}_i \simeq e^{\beta \xi} \sum_i e^{-\beta E_i} = e^{\beta \xi}(4\pi Vg/\lambda_c^3)(K_2(u)/u) \tag{11}$$

which is the first term in equation $(9d)$. The higher order terms of the fugacity series are to be associated with quantum corrections to the classical expressions.

The argument u of the modified Bessel functions is simply related to the ratio of λ_T and λ_c, i.e. $u = (8/\pi)(\lambda_T^{NR}/\lambda_c)^2$ or $u = (3\lambda_T^{UR}/\lambda_c)$, where λ_T^{NR} and λ_T^{UR} are, respectively, the non-relativistic and the ultra-relativistic forms of λ_T. If $u \gg 1$ the asymptotic expansion for K_2 can be used, resulting in an expansion for the thermodynamic functions in powers of u^{-1} where the first terms are the familiar non-relativistic expressions and the others are relativistic corrections. On the other hand, for $u \ll 1$ the ascending power series for K_2 will produce a perturbative expansion in powers of u where the first term will be the massless particle gas expression.

One word of caution must be said concerning the way of carrying out this limiting operation in the expressions for entropy, energy and, in general, for the derivatives with respect to temperature of the free energy. The recurrence relation for K_2 and its derivative must be used before using the asymptotic expansion for large arguments or, in other words, as a general rule all approximations shall be carried out only as the last step in our calculations.

4. The quantum limit

We shall now extend the same procedures for carrying out the NR and UR limits to the exact quantum expressions for the thermodynamic functions. Let us consider first the

NR limit. We stress the fact that the summation index n in equations (9) appears also in the argument of the Bessel functions multiplying the parameter $u = mc^2/k_B T$ and that a large value for u can be obtained lowering the temperature and/or increasing the mass. This already suggests that, for a fixed non-zero mass and in the limit of very low (zero) temperature, non-relativistic effects cannot be neglected. The non-relativistic limit is easily obtained replacing each K_2 appearing in the fugacity series of the thermodynamic functions by their asymptotic expansions. The presence of the exponential term in equation (5), and the fact that the asymptotic expansion becomes an even better representation the larger the value of n, make the expansion converge for all allowed values of ξ. The summation over n can be carried out and written in terms of the Bose–Einstein function $F_\sigma(\alpha)$.

$$\ln \Xi = \left(\frac{2\pi}{u}\right)^{3/2} \frac{Vg}{\lambda_c^3} [F_{5/2}(\alpha) + \tfrac{15}{8} u^{-1} F_{7/2}(\alpha) + \tfrac{105}{128} u^{-2} F_{9/2}(\alpha) + O(u^{-3})] \tag{12}$$

where

$$\alpha \equiv \beta(mc^2 - \xi)$$

$$F_\sigma(\alpha) = \sum_{n=1}^{\infty} n^{-\sigma} e^{-\alpha n} \qquad \alpha \geqslant 0 \tag{13}$$

$$F_\sigma(0) = \zeta(\sigma)$$

and $\zeta(z)$ is the Riemann zeta function. There is no novelty in the above expression and it is just a duplication of Glaser's result. Even so we stress the important fact that this is the equation which gives the correct zero temperature ($u \to \infty$) behaviour of the massive boson gas. The non-observance of this simple fact would lead us to reproduce the results of the literature together with their unsurmountable difficulties.

The UR limit is a little more subtle as we will now see. To obtain an expression for $\ln \Xi$ in this approximation we make use in equation (8) of equations (6) and (7). For very small values of $t = nu$, only the first few terms in the ascending series for K_2 are important and keeping them should result in an expansion for $\ln \Xi$ in terms of u. There is no problem in carrying out the summation over the fugacity index in the equation for $\ln \Xi$ provided we restrict the chemical potential further in order to have convergence of the sums. Actually for a given value of $nu \ll 1$ only the first terms in equations (6) and (7) will give significant contributions. But as n keeps increasing, deviations from the approximate expression for K_2 start to occur and higher order terms should be taken into account. However, this can be remedied by choosing the value of $\xi < 0$ such that the exponential factor $\exp \beta n\xi$ is very small so that the higher order contributions are negligible; the closer ξ is to the origin, the poorer is the ability of the exponential term to guarantee the convergence and higher order terms of the expansion for K_2 must be taken into account. The leading terms of the resulting expression are once again represented in terms of the Bose–Einstein functions.

$$\ln \Xi = \frac{8\pi Vg}{(\lambda_c u)^3} \left\{ F_4(\alpha') - \frac{1}{4} u^2 F_2(\alpha') + \frac{1}{16} u^4 \left[F_0(\alpha')(A - \ln u) \right.\right.$$

$$\left.\left. - \sum_{p=1}^{\infty} \exp(-p\alpha') \ln p \right] + O(u^6) \right\} \tag{14}$$

where $A = [\psi(1) + \psi(3)]/2 + \ln 2$ and $\alpha' = -\beta\xi$.

In the limit of zero mass only the first term survives, yielding the familiar expression for the photon gas.

Comparison of our results with those of Glaser and Landsberg and Dunning-Davies (hereafter LDD) is best achieved through the average number of particles:

$$\bar{N} = \frac{8\pi Vg}{(\lambda_c u)^3} \left\{ F_3(\alpha') - \frac{1}{4} u^2 F_1(\alpha') + \frac{u^4}{16} \left[F_{-1}(\alpha')(A - \ln u) \right. \right.$$

$$\left. \left. - \sum_{p=1}^{\infty} \exp(-p\alpha')p \ln p \right] + \mathrm{O}(u^6) \right\}. \tag{15}$$

Several remarks are in order: In their approximate expression for $\bar{N}$, LDD have found a linear term—$F_2(\alpha)u$—and taking their calculations one step further a positive quadratic term $\frac{1}{4}u^2 F_1(\alpha)$ is obtained. The argument of the Bose–Einstein function in their expression is $\alpha = \beta(mc^2 - \xi)$; recalling that $F_\sigma(0) = \zeta(\sigma)$ and $\zeta(1) = \infty$ we immediately see that any analysis of the behaviour of the system at and below the critical temperature which takes into consideration other terms than the photon contribution must be wrong. Moreover, for higher order correction terms the divergence of the coefficient (B–E functions) is even worse at $T \leq T_c$. This is not surprising since their approximate expression is obtained by binomial expansion of the density of states and then performing an integration term by term over the (forbidden) region $[0, 2u]$ of the energy spectrum which lies outside the radius of convergence of the expansion.

The difference between our results can be seen clearly noting that their expression for $\bar{N}$ can also be obtained from equation $(9d)$, expanding both the exponential and the Bessel functions for small arguments and then carrying out the summation over n. This procedure is unacceptable as we have remarked before and leads to the unwanted divergences.

Both LDD and Glaser's techniques for discussing the UR limit are based on the binomial expansion of the density of states followed by the thermal average integration. Even so, their results are not in agreement. In Glaser's work the restriction of a non-positive chemical imposed in order to avoid a divergence in the first correction to the photon term is the result also of unjustified approximations. In his evaluation of the integral $\int_{n\epsilon_0/k_B T}^{\infty} \exp(-\alpha)\,d\alpha$ the factor $\exp(n\epsilon_0/kT)$ which should appear in the answer is approximated by one before carrying out the summation over n. Its inclusion would shift again the upper bound for ξ from zero to mc^2 and thus lead to a divergent second-order term in $\bar{N}$.

In conclusion we can say that all of the above discrepancies can be traced back to the fact that their approximations are made at the level of the density of states. Clearly that procedure destroys some of the characteristic features of the exact density of states in the low-energy part of the spectrum such as the value of the function $D(E)$ and the sign of the curvature at $E_{\min} = mc^2$. It is known (Rino *et al* 1977) that Bose–Einstein condensation and the low-temperature behaviour of the system are determined by the shape of the density of states in the neighbourhood of $E_{\min}$. Therefore, any modification of the function in this region will bring drastic changes in the low-temperature behaviour of the system. No matter how small the mass, the density of states is a concave function below $E = (3/2)^{1/2} mc^2$ being zero and having an infinite derivative at $E_{\min} = mc^2$. Thus, carrying out approximations which change these characteristics of the non-relativistic region of $D(E)$ will not produce the correct results

to describe the system in the limit of low temperature. From what we have discussed so far it is now clear that equation (14) does not describe the critical region $\xi = mc^2$ of the system, except for the case $m = 0$ where its first term is equal to the exact expression for the photon gas. In this case the critical temperature is obtained by setting $\alpha' = -\beta\xi = 0$ in the equation for the average particle number:

$$(8\pi g\zeta(3))(k_B T_c/hc)^3 = \bar{N}/V$$

which states nothing but that $\lambda_T^{UR} \simeq \bar{\lambda}$. (In the NR limit the criticality condition can also be expressed as $\lambda_T^{NR} = \bar{\lambda}$, also up to a number.)

For massive and highly dense gases, considering that the leading corrections are of second order, we expect that the photon term gives an accurate description of the behaviour of the system in the critical region $T \lesssim T_c$, e.g. the number of particles in the condensate is given by

$$\bar{N}_0 = \bar{N}[1 - (T/T_c)^3].$$

However, as $k_B T_c$ is lowered and approaches the region where the density of states changes convexity, the deviations and corrections to the photon terms become important. Although no simple analytical expression for this region can be obtained we want to indicate how the exact equation can be correctly approximated and numerically evaluated to describe this situation. Besides setting $\xi = mc^2$ we can split the summation over n into two: the first going from $n = 1$ to $nu \simeq 1$ where $u = \lambda_T/\lambda_c$ so we can approximate K_2 by its small argument expansion. The number of terms to be considered will depend of course on the precise nature of the calculation. From $n = u^{-1}$ to infinity we use the asymptotic expansion for K_2. These two terms essentially give the amount of mixture of UR and NR effects respectively.

For $k_B T_c$ well below the minimum energy the NR limit applies and we get the well known results, e.g.

$$\bar{N}_0 = \bar{N}[1 - (T/T_c)^{3/2}], \qquad 0 \leqslant T \leqslant T_c$$

where we have remarked that this equation is also correct in the zero temperature limit.

5. Discussion

The expressions for the thermodynamic functions of the relativistic Bose gas are derived from the exact expression for the free energy of the system. The non-relativistic and ultra-relativistic limits are carried out directly from the exact results avoiding the procedure of expanding the density of states as in previous works. The discrepancies between our results and those by Glaser and Landsberg and Dunning-Davies are traced back to unjustified approximations involving the expansion and truncation of the density of states before the evaluation of the thermal averages. The realisation that previous results were also inappropriate to discuss the system below its critical temperature has led us to investigate its degenerate behaviour. We also show that the behaviour of the gas made up of massive particles in the limit of zero temperature is always non-relativistic. Upon completion of this paper we became aware of the work by Bechmann *et al* (1979) which treated the same system.

Acknowledgments

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