Is it there a Bose Einstein condensation in the presence of a Gamow state ?

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The Bose-Einstein Condensation (BEC) is a well-known phenomena common to a variety of quantum many-body systems. In this note we address the question of the realization of BEC in presence of quantum unstable states, as it is the case of bosons moving in a central potential which exhibits bound-states and resonances. The formalism needed to include resonances in the calculation of thermodynamical functions is discussed in the text.The explicit calculation of boson occupation factors shows that BEC is inhibited if resonances are present in the boson spectrum.

I. INTRODUCTION

When the motion of non-interacting particles, which obey the Bose-Einstein statistics, is treated at very low temperatures, the dominance of the occupation of the state with zero-momentum (ground state configuration), over that of excited states, becomes more and more manifest as the temperature T goes to zero. In the limit of T=0 all particles occupy the state of zero momentum provided they are massive-particles and that the system has a finite density. The number of particles in the ground state becomes equal to the total number of particles of the system and the chemical potential becomes a negative infinitesimal at the same limit (T=0). This phenomena is exclusively due to the statistics and is known as the Bose-Einstein Condensation (BEC). It was described long-ago [1, 2] and in recent times it has attracted the attention of experimentalists and theoreticians working in different areas of physics. It should be stressed that BEC is not a phase transition, in spite of the similitude between the aspect of the temperature-density domain where it takes place and that of, for instance, regions of the same space limited by critical exponents [3]. It is also well-known that BEC depends on space-dimensions (it does not take place in systems with an even number of dimensions,for instance)[4, 5]. In practically all studies of the phenomena it has been assumed that the configuration space includes states with real values of the energy, that is the case of plane waves, states in a central potential and particles in a box [6]. However, a complete quantum mechanical description of single-particle basis should include also resonances, like Gamow-States, with complex energies [5, 7]. To handle resonances in the context of ordinary quantum mechanics [8, 11] there exist several possibilities, namely: one may extend the Hilbert space representation [12], perform analytic continuations of the spectrum [13–15] or construct hybrid basis with bound, quasi-bound and resonant states [7]. The literature is rich enough in aspects concerning the limitations of each approach and we shall avoid to enumerate them here. The reader may find the details in, for instance, [16]. In the case of the BEC phenomena, the presence of states with complex energy is expected to change the picture. The relations between the density and the temperature, in presence of resonances, may amount to a drastic change in the conditions which determine the manifestation of the BEC.

The paper is organized as follows: In Section II, the conventional formalism of BEC is revisited, and its extension to bases which contain Gamow states is presented in detail. Next, in Section IV we shall discuss the numerical applications of the formalism and present the results. Finally, conclusions are presented in Section V.

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II. FORMALISM

A. Conventional BEC formalism

To start with, let us review the basic concepts related to the BEC mechanism. The grand partition function, which describes a system of N massive bosons which occupy without restrictions a space consisting of an array of levels $\{n_L\}$ of energy ϵ_i is written

$$\mathcal{Z}_D = \sum_{\{n_L\}} e^{-\beta(\epsilon_i\{n_L\}-\mu\{n_L\})} = \prod_j \left(\sum_{n_i=0}^{\infty} e^{-\beta(\epsilon_j-\mu)n_i} \right) = \prod_j \frac{1}{1-e^{-\beta(\epsilon_j-\mu)}} \,, \quad (1)$$

where the sum on configurations is replaced by the direct product of geometric series, each of them of ratio $e^{-\beta(\epsilon_j-\mu)}$, where β is the inverse temperature ($\beta = 1/kT$, being k the Boltzmann constant) and μ is the chemical potential. The total number of bosons, N, is given by the derivative

$$N = \frac{1}{\beta}\frac{\partial}{\partial \mu}\,\log \mathcal{Z}_D\,, \tag{2}$$

leading to the expression

$$N = \sum_j n_j(T)\,, \tag{3}$$

where the boson occupation numbers, $n_j(T)$, have been defined as

$$n_j(T) = \frac{1}{e^{\beta(\epsilon_j-\mu)}-1}\,. \tag{4}$$

Therefore, the calculation of any thermodynamical function requires the explicit knowledge of the occupation factors $n_j(T)$.

B. Unlimited energy spectrum

To start with, we shall assume that the physical system consists of a fixed number of massive bosons moving in a energy space of unlimited plane wave states with discrete energy levels. Then, for such a system we have

$$N = n_{gs}(T) + \sum_{excited} n_j(T), \tag{5}$$

where we have written separately the occupation factor of the ground state $n_{gs}(T)$, which corresponds to $\epsilon_j = 0$, and those of excited energy levels. In terms of the factors of Eq.(4) the expression Eq.(5) takes the form

$$N = \frac{e^{\beta\mu}}{1-e^{\beta\mu}} + \frac{4\pi V}{(2\pi\hbar)^3}\int dp \frac{p^2}{e^{\beta(\epsilon_j-\mu)}-1}, \tag{6}$$

where the replacement of the summation on excited states by an integral on phase space has been applied. Further, by expanding the denominator under the integral in terms of powers of $e^{\beta(\epsilon_j-\mu)}$, one gets

$$N = \frac{e^{\beta\mu}}{1-e^{\beta\mu}} + \frac{V}{(2\pi)^2}\left(\frac{2mk_BT^2}{\hbar}\right)^{3/2}\Gamma(3/2)\sum_{k=0}\frac{e^{(k+1)\beta\mu}}{(k+1)^{3/2}}\,, \tag{7}$$

where

$$\Gamma(a) = \int_0^\infty dw\; w^{a-1}\,e^{-w}\,, \tag{8}$$

is the standard definition of the Gamma function.

This equation determines the value of μ, which in the limit $T \to 0$ goes to $e^{\beta\mu} \to \frac{N}{N+1}$. If we introduce the short hand notation

$$\begin{aligned} \alpha(T) &= \frac{V}{(2\pi)^2}\left(\frac{2mk_BT^2}{\hbar}\right)^{3/2}\Gamma(3/2)\,, \\ \phi(T) &= e^{\beta\mu}\,, \\ \sigma(T) &= \sum_{k=0}\frac{e^{(k+1)\beta\mu}}{(k+1)^{3/2}}\,. \end{aligned} \tag{9}$$

Equation (7) is written

$$(1-\phi(T))N = \phi(T) + (1-\phi(T))\alpha(T)\sigma(T)\,, \tag{10}$$

with solutions, keeping up to second powers of $\phi(T)$, given by

$$\phi(T) = \frac{\alpha(T)+N+1}{\alpha(T)} \pm (1/2)\sqrt{\left(\frac{\alpha(T)+N+1}{\alpha(T)}\right)^2 - \frac{4N}{\alpha(T)}}\,, \tag{11}$$

of which the solution with negative sign in front of the square root gives the correct physical solution, which obeys the limit $\phi(T) \to \frac{N}{N+1}$ as $T \to 0$. From this result, the number of particles in excited states and in the unlimited energy space is written

$$N_{excited} = \alpha(T)\phi(t)\,. \tag{12}$$

As $T \to 0$ only the ground state will be fully occupied. As the temperature increases the occupation of the ground , state decreases and it vanishes at a certain critical temperature T_c. The explicit structure of this temperature dependence is easily extracted from the previous equations by taking the ratio of the expression of Eq.(7) at $T \leq T_c$ and it at $T = T_c$, namely

$$N_{gs} = N\left(1 - \frac{\alpha(T)}{\alpha(T_c)}\right) = N\left(1 - \left(\frac{T}{T_c}\right)^{(3/2)}\right)\,, \tag{13}$$

which is the famous result known as the Bose-Einstein Condensation (BEC).

C. Limited energy spectrum

When the energy spectrum is truncated at a certain value ϵ_{max} the function $\Gamma(3/2)$ of Eq.(7) should be replaced by the incomplete gamma function

$$\gamma(3/2, \epsilon_{max}/k_BT) = \int_0^{\epsilon_{max}/k_BT} dw\; w^{1/2}e^{-w}\,, \tag{14}$$

whose analytic expression is written

$$\begin{aligned} \gamma(3/2, \epsilon_{max}/k_BT) = {} & \frac{\sqrt{\pi}}{2}\,\mathrm{erf}\left(\sqrt{\frac{\epsilon_{max}}{k_BT}}\right) \\ & - \sqrt{\frac{\epsilon_{max}}{k_BT}}\,e^{-(\frac{\epsilon_{max}}{k_BT})}\,. \end{aligned} \tag{15}$$

Then, in the notation of the previous subsection, the number of particles in excited states is given by

$$N_{excited} = \frac{\alpha(T)\phi(T)}{\Gamma(3/2)}\gamma(3/2, \epsilon_{max}/k_BT)\,. \tag{16}$$

D. Resonances (Gamow States)

Let us assume that the spectrum, in addition to a given number of discrete states, has an unstable quantum state, with resonant energy $\epsilon_0 > \epsilon_M$ and decay width γ. The unstable quantum state belongs to the type of states generically known as Gamow states [13]. In order to disentangle the effects of both types of states we shall calculate the total density ρ as the sum of two terms ρ_D and ρ_G, which are the densities corresponding to the discrete (D) and unstable (G) sectors of the basis, respectively. In non-relativistic quantum mechanics, a quantum resonance can be represented by a vector state which has a Breit-Wigner energy distribution up to some approximation. An exact Breit-Wigner energy distribution will correspond with a vector state $|\psi\rangle$ such that its decay probability $P(t) = \langle\psi|e^{-itH}|\psi\rangle$ is an exponential for all times $t \geq 0$. This is not possible if $|\psi\rangle$ is a normalizable vector in a Hilbert space for the following reasons: i.) Since the spectrum of the Hamiltonian that produces the decay H has to be bounded from below, no vector may have the Breit-Wigner energy distribution (also called the Cauchy distribution), which is non-zero for all real values; ii.) For small values of t, $P(t)$ cannot be exponential (Zeno effect) and iii.) For large values of t, $P(t)$ has also structural deviations from the exponential decay law for small as well as large values of the time t.

Nevertheless, these deviations are difficult to detect, Zeno times are very small and deviations for large values of time occur when almost the whole sample has decayed. Therefore, for most practical purposes the exponential decay is a good approximation for the decay probability in most physical situations. However and as noted in the previous paragraph, no normalizable vector state may decay exponentially for all values $t \geq 0$.

Resonances are characterized by the value of two parameters [7–9], the resonance energy ϵ_0 and the width $\gamma > 0$. In 1958, Nakanishi proposed [10] that a vector representing an exponentially decay state, $|\psi^G\rangle$, should be an eigenvector of the Hamiltonian responsible for the decay with a complex eigenvalue of the form $H|\psi^G\rangle = (\epsilon_0 - i\gamma/2)\,|\psi^G\rangle$, so that $e^{-itH}\,|\psi^G\rangle = e^{-i\epsilon_0 t}\,e^{-\gamma t}|\psi^G\rangle$, which implies that it decays exponentially for all positive values of time. An immediate difficulty arises after this description: The Hamiltonian H should be self adjoint and self adjoint operators do not have complex eigenvalues. At least in Hilbert space. The solution is to extend the Hilbert space in order to accommodate the Gamow vector into a well defined mathematical structure, see [7] and references thereof. This is the rigged Hilbert space, which is a triplet of states $\Phi \subset \mathcal{H} \subset \Phi^\times$, where $\mathcal{H}$ is the Hilbert space. We may always construct a rigged Hilbert space such that [7, 9]: i.) The Gamow vector $|\psi^G\rangle$ is in the bigger space $\Phi^\times$. ii.) The Hamiltonian H can be extended to $\Phi^\times$, so that the eigenvalue equation $H|\psi^G\rangle = (\epsilon_0 - i\gamma/2)\,|\psi^G\rangle$ holds in $\Phi^\times$. iii.) Also, the equation $e^{-itH}\,|\psi^G\rangle = e^{-i\epsilon_0 t}\,e^{-\gamma t}|\psi^G\rangle$ is well defined in $\Phi^\times$. iv.) Finally, one may find a particular representation of $\Phi \subset \mathcal{H} \subset \Phi^\times$ such that $|\psi^G\rangle$ has a Breit-Wigner energy distribution [7, 9].

E. Particle number calculation for a limited energy space and resonances

If in addition to the upper limit of the energy, ϵ_{max}, we include a resonance in the spectrum, as explained in the previous subsection, of energy ϵ_G and width γ_G, its projection on the real energy axis takes the form

$$D(\epsilon, \epsilon_G, \gamma_G) = \frac{\gamma_G}{\pi} \frac{1}{(\epsilon - \epsilon_G)^2 + (\gamma_G/2)^2}\,. \qquad (17)$$

The contribution of this state to the number of particles in excited states is given by the integral

$$N_{excited} = \int_{\epsilon_G - \gamma_G/2}^{\epsilon_G + \gamma_G/2} d\epsilon\; D(\epsilon, \epsilon_G, \gamma_G) \frac{1}{e^{\beta(\epsilon - \mu)} - 1}\,, \qquad (18)$$

which, after some straightforward steps yields

$$N_{excited} = \alpha(T)\phi(t)\frac{4}{\pi}\left(\frac{\epsilon_G}{k_B T}\right)^{(1/2)} e^{-\frac{\epsilon_G}{k_B T}}/\Gamma(3/2)\,, \qquad (19)$$

provided $\gamma_G/2$ is much smaller than ϵ_G.

To conclude with the analysis of the results for the particle number density note that Eq.(19) vanishes if $\epsilon_G \to \infty$ and Eq.(16) coincides with Eq.(12) when $\epsilon_{max} \to \infty$.

III. MEAN VALUE OF THE ENERGY

Proceeding with the study of the thermal response of a system of massive bosons with real and complex energies, we shall, in this section, calculate the mean energy of the system under the conditions described in the previous section, namely: for unlimited and limited energy spectrum and for the case where a resonance is included in the spectrum.

A. Mean Energy for the unlimited spectrum

The mean value of the energy is written

$$\langle E - \mu\rangle = -\frac{\partial log Z}{\partial \beta} = \sum_j \frac{(\epsilon_j - \mu)}{e^{\beta(\epsilon_j - \mu)} - 1}\,. \qquad (20)$$

By transforming the sum into an integral on space and momentum, and using the variables introduced previously when calculating the number of particles, the mean energy acquires the expression:

$$\langle E - \mu\rangle = \frac{V}{(2\pi)^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} e^{\beta\mu} k_B T(\Gamma(5/2) - \beta\mu\Gamma(3/2))\,. \qquad (21)$$

Then, replacing the functions Γ by their values the mean energy is given by

$$\langle E - \mu\rangle = \frac{V}{(2\pi)^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} e^{\beta\mu}\frac{\sqrt{\pi}}{2}\left(\frac{3}{2}k_B T - \mu\right), \qquad (22)$$

which is further written in the form

$$\frac{\langle E-\mu\rangle}{\langle N\rangle} = \left(\frac{3}{2}k_BT - \mu\right) , \quad (23)$$

after using the known expression for the average number of particles.

B. Mean Energy for the limited spectrum

Following the same sort of replacements of the sum on energy levels by integrations in phase space the expression for the mean energy, when the energy ϵ_j of the states belonging to the spectrum is limited to a certain cut-off value ϵ_{max} such that $\epsilon_j \leq \epsilon_{max}$, is easily obtained. The explicit expression for it is the following:

$$\langle E-\mu\rangle = \frac{V}{(2\pi)^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} e^{\beta\mu}k_BT \times \\ (\gamma(5/2,\eta_{max}) - \beta\mu\gamma(3/2,\eta_{max})) , \quad (24)$$

with, as before

$$\gamma(a,\eta_{max}) = \int_0^{\eta_{max}} dw\, w^{a-1}\, e^{-w} , \quad (25)$$

being $\eta_{max} = \epsilon_{max}/k_BT$. It just amounts to the use of incomplete gamma functions $\gamma(r,\eta_{max})$, with $a = 3/2$ and $a = 5/2$, instead of the regular gamma functions $\Gamma(a)$ which appear in the case of the unlimited value $\eta_{max} \to \infty$. In addition, we may use the expression of the incomplete gamma functions to write Eq.(24), leading to the following expression:

$$\frac{\langle E-\mu\rangle}{\langle N\rangle} = \left(\frac{3}{2}k_BT - \mu\right) \mathrm{erf}\left(\sqrt{\eta_{max}}\right) \\ - \frac{2}{\sqrt{\pi}}\sqrt{\eta_{max}}\left(\frac{1}{2} + \eta_{max}\right) e^{-\eta_{max}} . \quad (26)$$

C. Mean energy associated to the resonance

The expression of the mean energy for the region of the spectrum where the resonance is located is written

$$\langle E-\mu\rangle = \frac{\gamma_G}{\pi}\int_{\epsilon_G-\frac{\gamma_G}{2}}^{\epsilon_G+\frac{\gamma_G}{2}} d\epsilon \frac{(\epsilon-\mu)}{(e^{\beta(\epsilon-\mu)}-1)}\frac{1}{(\epsilon-\epsilon_G)^2+\frac{\gamma_G^2}{4}} , \quad (27)$$

making use of the explicit expression given in Eq.(17). To calculate this integral we shall write it in the complex plane making use of the identity

$$\frac{1}{(\epsilon-\epsilon_G)^2+\frac{\gamma_G^2}{4}} = -\frac{i}{\gamma_G}\left(\frac{1}{\epsilon-\epsilon_G-\frac{i\gamma_G}{2}} - \frac{1}{\epsilon-\epsilon_G+\frac{i\gamma_G}{2}}\right) \quad (28)$$

and expanding, as done before, the exponential in the denominator

$$\frac{1}{(e^{\beta(\epsilon-\mu)}-1)} = \sum_{n=0}^{\infty} e^{-(n+1)\beta(\epsilon-\mu)} . \quad (29)$$

Then, calling $z_0(\pm) = \epsilon_G - \mu \pm i\frac{\gamma_G}{2}$ and $z = \epsilon - \mu$, the integral of Eq.(27) becomes

$$-\frac{i}{\gamma_G}\sum_{n=0}^{\infty}\int dz e^{-(n+1)\beta z}\left(\frac{z}{z-z_0(+)} - \frac{z}{z-z_0(-)}\right) \quad (30)$$

The result of it, by applying Cauchy's residues theorem is just

$$\frac{4\pi}{\gamma_G}\sum_{n=0}^{\infty} e^{-(n+1)\beta(\epsilon_G-\mu)}((\epsilon_G-\mu)\cos\alpha_n + \gamma\sin\alpha_n) \quad (31)$$

with $\alpha_n = (n+1)\frac{\beta\gamma_G}{2}$.

Finally, by multiplying Eq.(31) by the remaining factor $\frac{\gamma_G}{\pi}$ one obtains the contribution to the mean value of the energy given by the resonance.

As a limiting value, assuming that $\frac{\beta\gamma_G}{2}$ is much smaller than 1, which is to say that the factor k_BT is much greater γ_G, this mean value takes the form

$$\langle E-\mu\rangle \approx 4(\epsilon_G-\mu)e^{-\beta(\epsilon_G-\mu)} . \quad (32)$$

IV. RESULTS

To begin with the discussion of our results we shall show those obtained by the use of the formalism introduced in subsection II B. Figure 1 shows the conventional BEC mechanism. It is then evident that for the unlimited energy space the ground state occupancy dominates the picture until the inversion of the population takes place at a certain critical temperature. As discussed in the text this is not the signature of a phase transition but just the inversion of the population of levels with the complete depopulation of the ground state.

The situation changes when the energy space is truncated and a resonance is added to it. The formalism was presented in subsections II C and II E. The results shown in Figure 2 indicated that the BEC mechanism is prevented. The fractional occupancy shown by the lower curve of Figure 2 does not exhibit the crossing characteristic of the BEC (see Figure 1) but rather it grows up at a lower pace.

Since the effect of the inclusion of the resonance is hidden because the excited state occupancy includes also its contribution, we have taken them separately. To better illustrate the effect we have worked out the solution for a two level model space to which a resonance is added, as explained next.

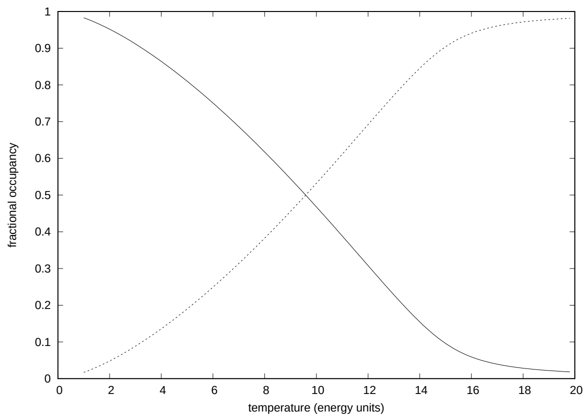

FIG. 1. Occupation factors as a function of the temperature. The fraction of particles in the ground state (solid line) and in excited states (dashed-line) for a system with a finite number of bosons occupying an unrestricted number of energy levels is shown as a function of the temperature (given in units of energy). The results have been obtained by solving the equations given in subsection II B, as explained in the text.

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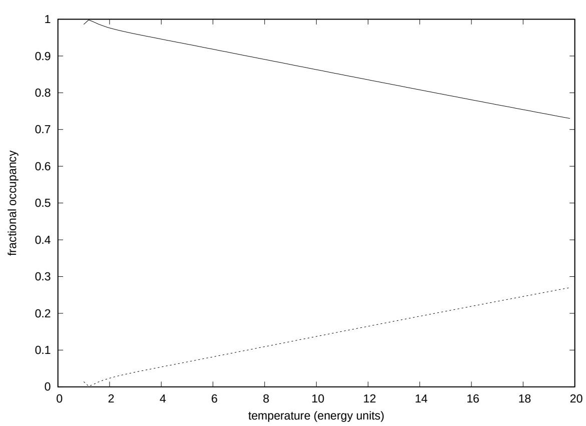

FIG. 2. Occupation factors as a function of the temperature. The fraction of particles in the ground state (solid line) and in excited states (dashed-line) for a system with a finite number of bosons occupying a restricted number of energy levels, to which it has been added a resonance, is shown as a function of the temperature (given in units of energy). The results have been obtained by solving the equations given in subsection II E, as explained in the text.

A. Two level model

We have taken a system consisting of two levels separated in energy by an energy gap ϵ_0, each level having a degeneracy Ω and a number of bosons N_b. To this space we add a resonance at an energy ϵ_G with a width γ_G. For the sake of the calculations we have fixed these values at $\epsilon_0 = 4, \epsilon_G = 3 * \epsilon_0, \gamma_G = \epsilon_G/100$ (all these values are given in arbitrary energy units, the same as for the absolute temperature) and fixed the degeneracy of the levels at the value $\Omega = 2000$. The number of bosons was fixed at $N_b = 200$. The solution for the number of particles occupying each level is rather easily obtained, by applying the procedure described in the previous subsections. The results of the calculations, for the two level model configuration, are shown in Figure 3. At lower temperatures the majority of the bosons occupy the ground state, but as the temperature increases the sum of the number of bosons in the first two levels differs significantly from the initial value N_b. The difference in the number of particles, that is $N_b - N_{gs} - N_{excited}$ is precisely equal to the number of bosons which reach the resonance. Physically it means that the Gamow state is acting as a doorway for the emission of particles from the system, preventing the occurrence of the Bose-Einstein condensation.

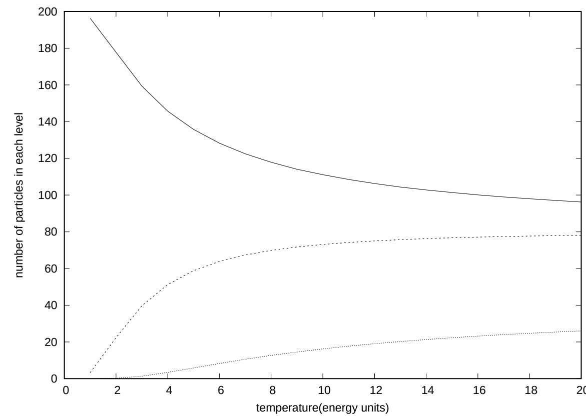

FIG. 3. Number of particles, for each level, for a system consisting of two discrete levels plus a resonance. The upper and middle curves show the number of particles which occupy the ground state and the excited state of the two-level model, and the lower curve shows the number of particles which goes to the resonance, respectively, as discussed in subsection IV A.

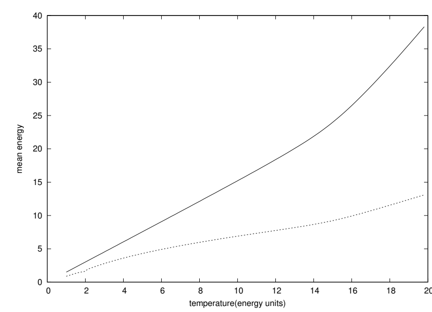

FIG. 4. Mean energy per particle, as a function of the temperature. The results for the unrestricted energy spectrum (Eq.(23)) are represented by a solid line. Those for the restricted spectrum (Eq.(26)) are show with dashed lines.

Figure 4 shows the results for the mean energy per particle, both for the unrestricted and the restricted energy spectra. The features of these results, as a function of the temperature, are consistent with the fact that the BEC is not a phase transition, otherwise there should be an abrupt change in both curves at a certain critical value of the temperature. Instead, when the temperature is above $k_B T_c \approx 14$ energy units the solution for the unrestricted goes almost linear while for the solution for the restricted energy spectrum the curve saturates.

V. CONCLUSIONS

In this work we have addressed the question related to the effects associated to the presence of resonances in a system of massive bosons at finite temperature. The path chosen to investigate it consisted of the inclusion in the spectrum of a resonance (i.e: a Gamow state). The statistical treatment shows that:

1.- The BEC does not take place when resonance states are present in the energy spectrum. They act as doorways from where the particles escape. In other words, the replacement of the continuum by one or more resonances inhibits the BEC mechanism.

2.- Similarly, other thermodynamical functions in the presence of a resonant state will depart from their ordinary values.

Both features may be of relevance in dealing with physical systems where the resonances are indeed a component of the spectrum, like, for instance, the atomic nucleus and other quantum many particle systems.

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