Webnucleo Technical Report: Boson Condensate Calculations with libstatmech

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This technical report describes some details of the Bose-Einstein examples in the libstatmech distribution.

1 Bose-Einstein Condensate

At low temperature or high number density, a boson gas tends to collapse into the lowest quantum state (ground state), which is a Bose-Einstein condensate. To calculate thermodynamic quantities in this situation, we need to add the ground state function to the integral and set the integral lower limit to the first excited state energy. These examples demonstrate how to add an user-supplied thermodynamic function and how to set a new integral lower limit.

For our system, we consider ideal bosons in a box with sides of equal length L and volume $V = L^3$. The single-particle states for the bosons are plane waves with momentum $\vec{p} = 2\pi\hbar\vec{n}/L$, where $\vec{n}$ is a vector whose components n_x, n_y, and n_z are 0 or $\pm$integers. The ground state thus has momentum zero, and we consider the energy to be that less the rest mass energy. We may derive the thermodynamic quantities from the grand canonical potential (see, for example, [1])

$$\Omega = k_B T \sum_r \ln\left(1 - e^{\beta(\mu' - \epsilon_r')}\right),$$

where k_B is Boltzmann's constant, T is the temperature, $\beta = 1/k_B T$, μ' is the chemical potential less the rest mass, ϵ_r' is the energy of the single-particle state r less the rest mass, and the sum runs over all single-particle states r. Since we assume uniform density over volume V, the number density is given by

$$n = -\frac{1}{V}\frac{\partial \Omega}{\partial \mu'}.$$

By considering all single-particle states r such that $\epsilon_r = 0$, we thus find the ground-state number density:

$$n_0 = \frac{g}{V}\frac{1}{\exp(-\alpha) - 1}$$

where g is the boson particle's multiplicity and $\alpha = \mu'/kT$, which is always negative. The entropy density is given by

$$s = -\frac{1}{V}\frac{\partial \Omega}{\partial T};$$

hence, the ground-state entropy density is

$$s_0 = -k_B \frac{g}{V}\left[\ln\left(1 - e^{\alpha}\right) + \frac{\alpha}{e^{-\alpha} - 1}\right].$$

Finally, the pressure is

$$P = -\Omega/V;$$

hence, the ground state pressure is

$$P_0 = -\frac{k_B T}{V} g \ln\left(1 - e^{\alpha}\right).$$

Since the ground state single-particle energy is zero and the particles are considered to be non-interacting, the energy density of the ground state is zero.

The boson condensate examples in the libstatmech distribution include these functions, which are then set by the API routine Libstatmech__Boson__updateQuantity(). Once the functions are set, they are applied during quantity calculations.

2 Integral Lower Limit

The non-condensate part of thermodynamic quantity calculations are still computed with the default integrands. Since the ground state quantities are now calculated separately, however, we need to set the integral lower limit to the first excited state energy over $k_B T$. We do this by considering the particle in this state to be non-relativistic:

$$E_1 = \frac{p^2}{2m} = \frac{\hbar^2 (2\pi/\lambda)^2}{2m} = \frac{2(\hbar\pi)^2}{mV^{2/3}}$$

$$x_1 = E_1/kT = \frac{2(\hbar\pi)^2}{mV^{2/3}kT}$$

The new integral lower limit is set in the examples with the API routine Libstatmech__Boson__updateIntegralLowerLimit().

3 Results

We may use the boson example codes in the libstatmech distribution to explore Bose-Einstein condensation in some detail. The examples use both the ground-state boson functions defined above and the default integrands with the lower integral limit x_1. For example, with the function and the integral together the number density is:

$$n = \frac{g}{V}\frac{1}{\exp(-\alpha)-1} + \frac{(kT)^3 g}{2\pi^2(\hbar c)^3}\int_{x_1}^{\infty}\frac{(x+\gamma)\sqrt{x^2+2\gamma x}}{\exp(x-\alpha)-1}\,dx$$

When α (the chemical potential less rest mass over kT) is a large negative number, the function term is small compared to the integral and is negligible. When α is increasing toward zero, the function term starts to dominate. At this point almost all the particles will collapse into the ground state. This happens at low temperatures or high number densities. Figures 1 and 2 below show results from the distribution examples for a system volume $V = 1$ cm for a boson with multiplicity $g = 3$ and a rest mass of $mc^2 = 1$ MeV. Figure 1 shows the ratio of the number of particles N_0 in the ground state relative to the total number of particles N as a function of the total number density of particles in the box of volume V. Since the temperature and volume are fixed, it is clear that adding particles to the system eventually causes condensation in which most of the particles are in the ground state. The number density at which condensation occurs increases for higher temperature because the probability to excite a given boson to the first excited state is higher for higher T.

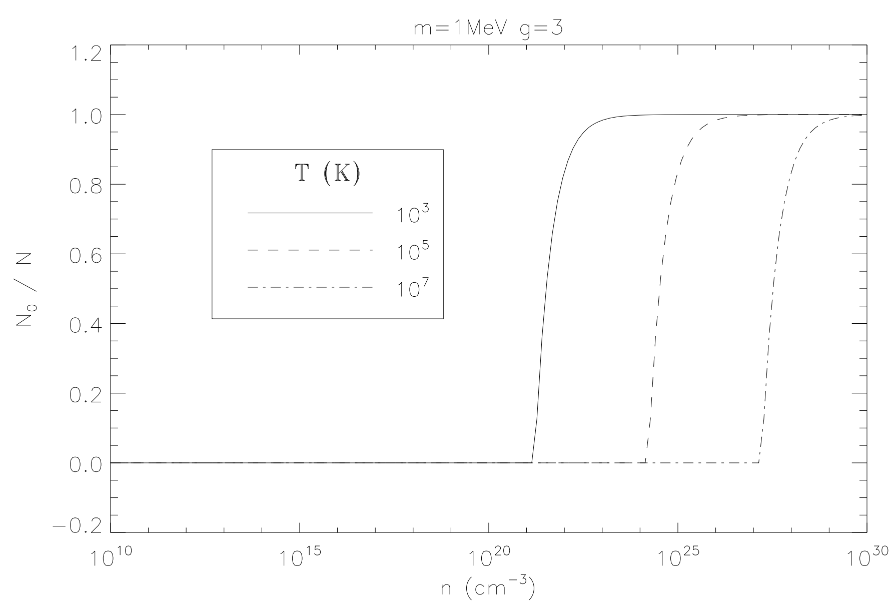

Figure 1: Ground state fraction vs number density at different temperatures. N_0 is the number of particles in the ground state, while N is the total particle number.

Condensation also occurs when the temperature is lowered for fixed number density. Figure 2 shows this for several number densities. As the temperature is lowered, a temperature is reached at which the fraction of particles in the ground state rises quickly. This is the phase transition to the condensate.

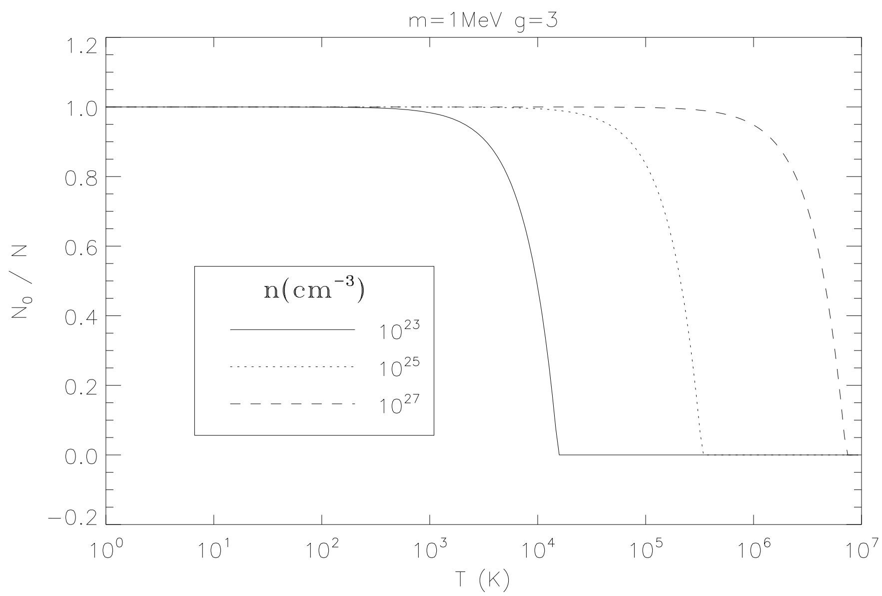

Figure 2: Ground state fraction vs temperature at different number densities. N_0 is the number of particles in the ground state, while N is the total particle number.

The critical temperature T_c at which the phase transition occurs may be computed for non-relativistic bosons to be

$$T_c = \frac{2\pi\hbar^2}{mk_B}\left(\frac{n}{g\zeta(3/2}\right)^{2/3},$$

where $\zeta(3/2)$ is the Riemann zeta function of argument 3/2 [1]. Figure 3 shows N_0/N as a function of T/T_c as computed with a libstatmech example code. It is clear that condensation does indeed occur at T_c. Figure 4 shows the specific heat capacity as a function of T/T_c as computed from a libstatmech example code with $g = 3$ and $mc^2 = 100$ MeV. The cusp in the curve at $T = T_c$ is the signal of the phase transition. As T increases above T_c, the specific heat capacity settles down towards $3k_B/2$, as expected for a non-relativistic, ideal gas.

Figure 5 shows the pressure of an ideal boson gas with $mc^2 = 100$ MeV and $g = 3$ as a function of the number density for a fixed temperature of 100 K. Below the condensation, the pressure is proportional to the number density, as

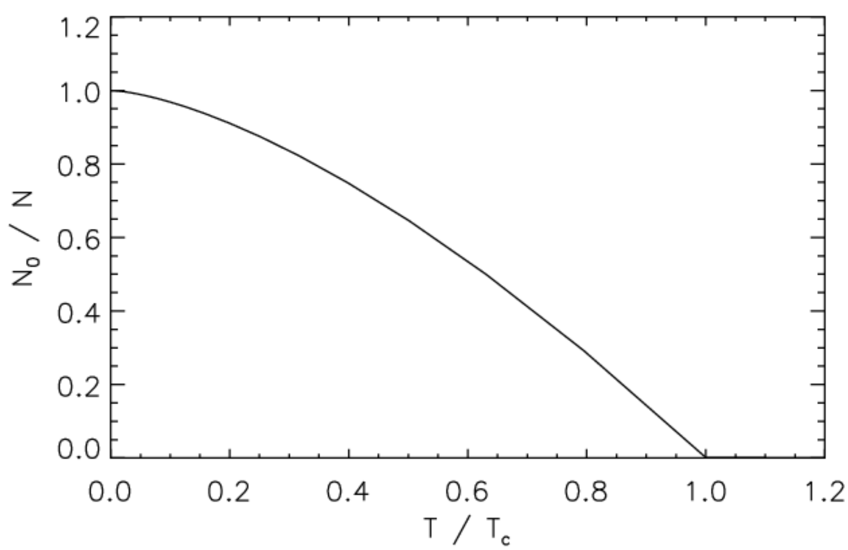

Figure 3: Ground state fraction as a function of the temperature relative to the critical temperature for an ideal boson gas with $mc^2 = 100$ MeV and $g = 3$.

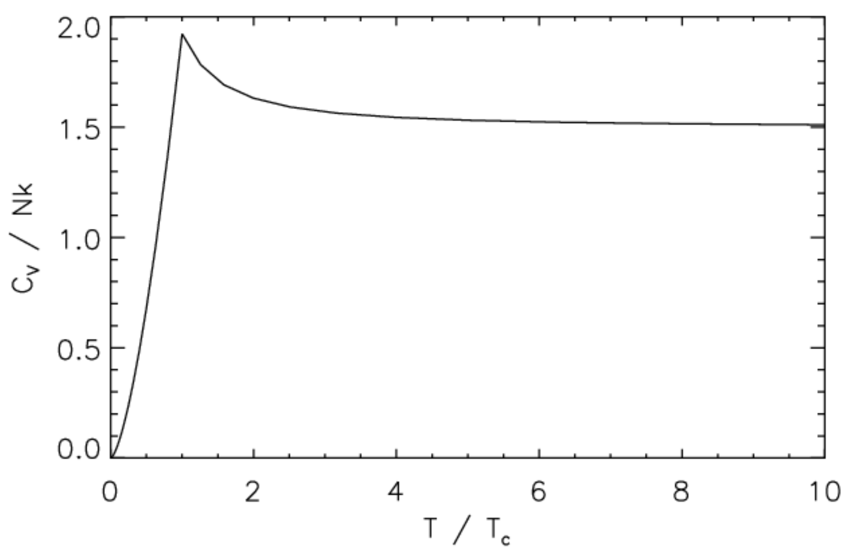

Figure 4: Specific heat capacity as a function of temperature for the ideal boson gas.

expected for an ideal, non-relativistic gas. Once the number density exceeds the critical number density, the pressure becomes constant as a function of number density. This surprising result is due to the fact that, as the number of particles increases towards infinity, the number of particles not in the ground state becomes a constant. To understand this, consider a two-state system with a probability p for a single particle not to be in the ground state. The particles are indistinguishable; therefore, the probability to have m out of a total of N particles not in the ground state is $P(m) = \mathcal{N} p^m$, where $\mathcal{N}$ is a normalization constant. This means that

$$\mathcal{N} \sum_{m=0}^{N} p^m = 1.$$

If $N \to \infty$, then $\mathcal{N} = 1 - p$. The total number of particles not in the ground state for large N is thus

$$\sum_{m>0} (1-p) m p^m = (1-p) p \frac{d}{dp} \sum_{m=0} p^m = (1-p)p/(1-p)^2 = p/(1-p).$$

This becomes a negligible fraction of N as $N \to \infty$. Nevertheless, it is these particles that carry the energy, pressure, and entropy; hence, these quantities become constant as a function of the number density when the condensation occurs.

References

[1] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation*, Oxford University Press, New York, NY, 2003.

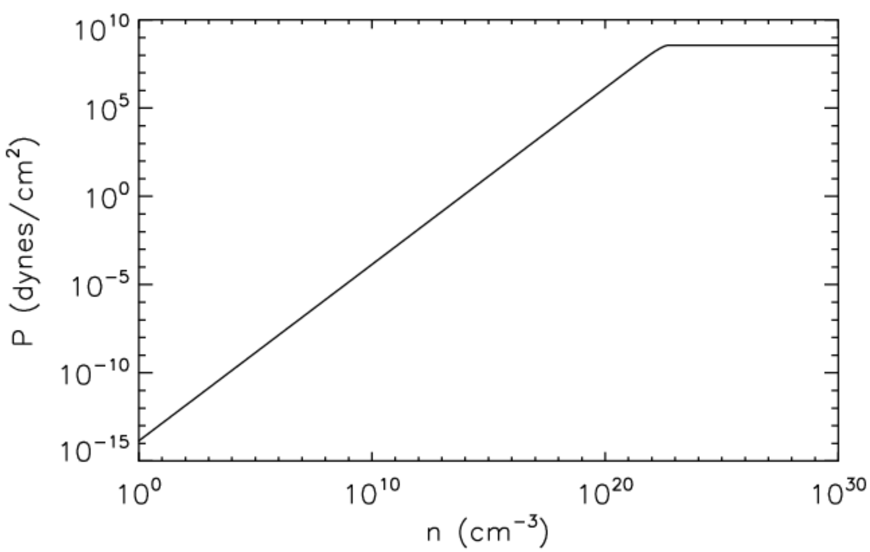

Figure 5: Pressure as a function of number density for an ideal gas of bosons with mass $mc^2 = 100$ MeV and $g = 3$ at $T = 100$ K. Once condensation occurs, the pressure is independent of the number density.