Physics 112
Variation of the chemical potential with T for free bosons in three-dimensions

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As shown in class and a handout [1], the density of single particle states of non-interacting spinless bosons in three dimensions is

$$\rho(\epsilon) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2} \,. \tag{1}$$

The mean occupancy of a *single-particle* state is given by the Bose-Einstein distribution, so the mean *total* number of particles is given by

$$\boxed{N = \int_0^\infty \frac{\rho(\epsilon)}{e^{\beta(\epsilon-\mu)} - 1}\, d\epsilon = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)} - 1}\, d\epsilon \,.} \tag{2}$$

Equation (2) is used to compute the (temperature dependent) chemical potential $\mu(T)$. It is an *implicit* relation. In general, we can not extract $\mu(T)$ outside the integral to get an *explicit* expression for $\mu(T)$.

However, at very high temperatures, which is the classical limit, we *can* obtain $\mu(T)$ explicitly. To do this we neglect the factor of -1 in the denominator of Eq. (2) (which is justified in this limit since μ is large and negative so the exponential dominates). This gives

$$n = \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} e^{\beta\mu_{\rm class}} \int_0^\infty \epsilon^{1/2} e^{-\beta\epsilon}\, d\epsilon \,, \tag{3}$$

where $n \equiv N/V$, in which the factor $e^{\beta\mu_{\rm class}}$ has been pulled out of the integral. Making the substitution $x = \beta\epsilon$ and using the result that $\int_0^\infty x^{1/2} e^{-x}\, dx = \Gamma(3/2) = \sqrt{\pi}/2$, we get

$$e^{-\beta\mu_{\rm class}} = \frac{1}{4\pi^2} \frac{1}{n} \left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} \frac{\sqrt{\pi}}{2} \,. \tag{4}$$

This can be reexpressed as

$$\boxed{\mu_{\rm class}(T) = -\frac{3}{2} k_B T \log\left(\frac{T}{T_Q}\right) ,} \tag{5}$$

where

$$\boxed{T_Q = \frac{\hbar^2}{mk_B}\, 2\pi n^{2/3} \,.} \tag{6}$$

Eqs. (5) and (6) were also obtained in a handout [2]. Note that the high temperature limit corresponds to $T \gg T_Q$.

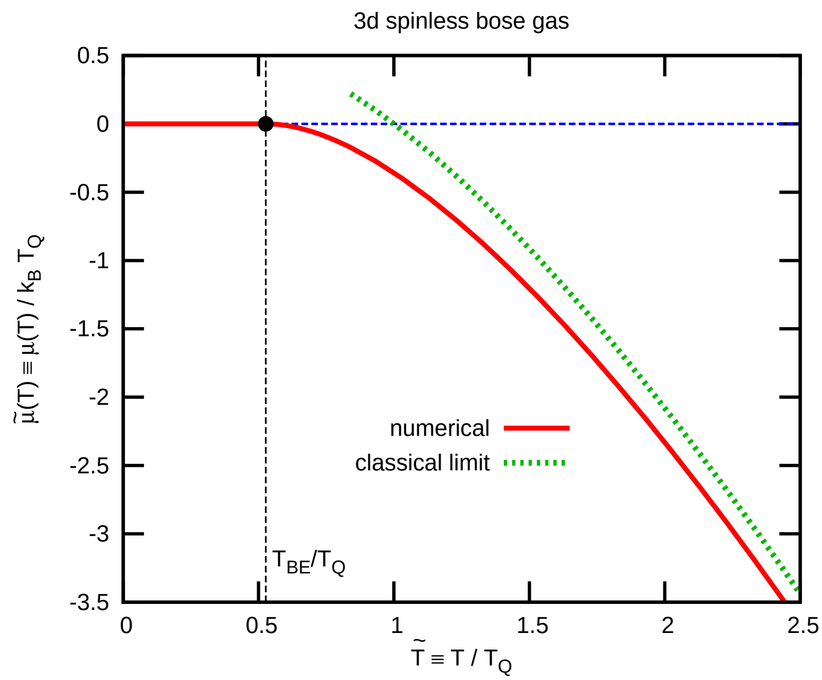

FIG. 1: The solid (red) curve shows $\widetilde{\mu}(T) \equiv \mu(T)/k_B T_Q$ against $\widetilde{T} \equiv T/T_Q$, determined numerically from Eq. (10). The value of $\mu(T)$ is found to vanish at $T = T_{BE}$, the Bose-Einstein condensation temperature, where $\widetilde{T}_{BE} \equiv T_{BE}/T_Q = 0.5272$. In the classical (high-temperature) limit, $\widetilde{\mu}(T)$ is given by Eq. (11). This is shown by the dotted (green) curve. The classical result vanishes at $T = T_Q$ where T_Q is given by Eq. (6).

Taking Eq. (6) to the 3/2-power, and slighly rearranging the factors, gives

$$\frac{\sqrt{\pi}}{2} \, (k_B T_Q)^{3/2} = 4\pi^2 \, n \left(\frac{\hbar^2}{2m} \right)^{3/2} , \tag{7}$$

and substituting into Eq. (2) gives

$$(k_B T_Q)^{3/2} = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\epsilon^{1/2}}{e^{(\epsilon-\mu)/T} - 1} \, d\epsilon \, . \tag{8}$$

Defining

$$\widetilde{\mu} = \frac{\mu}{k_B T_Q} \, , \qquad \widetilde{T} = \frac{T}{T_Q} \, , \tag{9}$$

and $x = \epsilon/k_B T$, Eq. (8) can be written in dimensionless form as

$$\boxed{1 = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}}{e^{(x-\widetilde{\mu})/\widetilde{T}} - 1} \, dx \, .} \tag{10}$$

Equation (10) is the dimensionless form of Eq. (2). I have used Eq. (10) to determine $\widetilde{\mu} \equiv \mu/k_B T_Q$ *numerically* as a function of $\widetilde{T} \equiv T/T_Q$ and show the results by the solid red curve in Fig. 1. The classical (high-T) expression in Eq. (5) can also be put in dimensionless form as

$$\boxed{\widetilde{\mu}_{\rm class}(T) \equiv \frac{\mu_{\rm class}(T)}{k_B T_Q} = -\frac{3}{2} \widetilde{T} \log \widetilde{T},} \tag{11}$$

and this is shown by the dotted (green) curve. At high temperatures, the curve numerically calculated from Eq. (10) approaches the curve obtained from the classical (high-T) limit, Eq. (11).

As the temperature is lowered, $\mu(T)$, as calculated from Eq. (10), becomes less negative until, at a temperature T_{BE}, the Bose-Einstein condensation temperature, it is equal to zero. The value of T_{BE} can be obtained from Eq. (10) by setting $\widetilde{\mu}$ equal to zero. Defining a new integration variable y by $y = x/\widetilde{T}$, Eq. (10) becomes

$$1 = \frac{2}{\sqrt{\pi}} \left(\widetilde{T}_{BE}\right)^{3/2} \int_0^\infty \frac{y^{1/2}}{e^y - 1}\, dy\,, \tag{12}$$

where $\widetilde{T}_{BE} = T_{BE}/T_Q$. The integral is evaluated as follows:

$$\begin{aligned}
\int_0^\infty \frac{y^{1/2}}{e^y - 1}\, dy &= \int_0^\infty \frac{y^{1/2} e^{-y}}{1 - e^{-y}}\, dy \\
&= \int_0^\infty y^{1/2} e^{-y} \left[1 + e^{-y} + e^{-2y} + e^{-3y} + \cdots\right] dy \qquad (13) \\
&= \int_0^\infty y^{1/2} e^{-y}\, dy \left[1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \frac{1}{4^{3/2}} + \cdots\right] \\
&= \Gamma(3/2)\zeta(3/2)\,, \qquad (14)
\end{aligned}$$

where

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t}\, dt \tag{15}$$

is the Gamma function, and

$$\zeta(x) = 1 + \frac{1}{2^x} + \frac{1}{3^x} + \frac{1}{4^x} + \cdots \tag{16}$$

is the zeta function. From Math methods courses we have $\Gamma(3/2) = \sqrt{\pi}/2$. The value of $\zeta(3/2)$ is not known exactly but its numerical value is 2.612. In Eq. (13) we made the substitution $y \to y/2$ in the second term, $y \to y/3$ in the third term, etc. Substituting Eq. (14) into Eq. (12) gives

$$\boxed{\widetilde{T}_{BE} \equiv \frac{T_{BE}}{T_Q} = \left(\frac{1}{\zeta(3/2)}\right)^{2/3} = 0.5272.} \tag{17}$$

This temperature is marked on Fig. 1. From Eqs. (6) and (17) we have

$$\boxed{T_{BE} = 3.313\, \frac{\hbar^2}{m}\, n^{2/3}\,.} \tag{18}$$

As discussed in the corresponding handout for fermions [3], *all* characteristic temperatures for non-interacting gases have the form $(\hbar^2/m)\, n^{2/3}$ times a numerical constant of order unity.

Finally, as discussed in class and in the book, at temperatures below T_{BE} a finite fraction of the particles are in the lowest quantum state (with energy 0). It should be mentioned that, in this region, the chemical potential is actually not quite zero but of order $1/N$. Figure 1 plots $\mu(T)$ in the thermodynamic limit, $N \to \infty$, and so shows $\mu(T)$ equal to zero for $T \le T_{BE}$.

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[1] Physics 112 handout: *"Single particle density of states"*, `http://physics.ucsc.edu/~peter/112/dos.pdf`.

[2] Physics 112 handout: *The "classical" ideal gas*, `http://physics.ucsc.edu/~peter/112/ideal.pdf`.

[3] Physics 112 handout: *Variation of the chemical potential with T for free electrons in three-dimensions*, `http://physics.ucsc.edu/~peter/112/mu_T.pdf`.