Numerical analysis of Bose–Einstein condensation in a three-dimensional harmonic oscillator potential

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Bose–Einstein condensation is the anomalous accumulation of particles in the ground state of a system of bosons, when compared with the population in a system of particles obeying classical statistics. I use undergraduate-level statistical mechanics and a symbolic algebra computer program to study the occupation numbers of the energy levels of a finite number of noninteracting particles confined in a three-dimensional harmonic oscillator potential. I also calculate the heat capacity of the gas. The harmonic oscillator potential simplifies the calculations and approximates the conditions of the recent experiments achieving Bose–Einstein condensation in laser-cooled alkali vapors. © *1998 American Association of Physics Teachers.*

I. INTRODUCTION

The recent achievement of Bose–Einstein condensation of laser-cooled alkali vapors confined in magnetic traps[1–3] is an exciting development that has been well documented in the popular press as well as the scientific literature. The Bose–Einstein condensate has been hailed as a new form of matter, and as the ''molecule of the year'' in 1995 by *Science* magazine.[4] Bose–Einstein condensation is possibly the most theoretically tractable of all phase transitions, and the combination of topical interest and relative simplicity make it a good candidate for inclusion in the undergraduate physics curriculum. Standard textbook treatments of Bose–Einstein condensation[5] investigate a gas of N noninteracting bosons in a rigid container of volume V. This approach, with some extensions, was discussed in a recent ''New Problem'' in this Journal.[6] In this paper I use the quantum statistics that is part of most undergraduate modern physics courses and a computer-based symbolic algebra package to investigate the phenomenon of Bose–Einstein condensation of a fixed number of particles confined in a three-dimensional harmonic oscillator potential. This potential more closely approximates the conditions of the experiments performed to date on alkali atoms, and it simplifies the calculations. (Analytical approximations for this system have been investigated by several authors. Results for the large N limit are discussed in Ref. 7, and results for finite values of N are discussed in Ref. 8.)

Bose–Einstein condensation is an accumulation of population in the ground state of a system of bosons as the temperature of the system is reduced below a critical temperature T_c. Of course the average occupation number of the ground state of any system will increase as the temperature is reduced, independent of whether the system consists of fermions, bosons, or particles assumed to obey classical statistics. The phenomenon of Bose–Einstein condensation is, however, a very abrupt rise in the number of particles at a critical temperature well above the temperature at which classical particles begin to accumulate in the lowest energy state. This condensation is entirely a consequence of the quantum statistics of the Bose–Einstein distribution, and occurs even for ideal noninteracting particles. The effect of the quantum statistics manifests itself when the wave functions of the particles overlap, or in other words, when the de Broglie wavelength of the particles in a gas is of the same order of magnitude as the interparticle separation. (For a general discussion of Bose–Einstein condensation and recent experiments I refer the reader to articles by Burnett[9] and Wieman,[10] while Kleppner[11] offers a personal view of the significance of the experiments.)

Determining the number of particles in the ground state of a simple physical system is in principle a straightforward calculation for any particle statistics. For particles in an isotropic harmonic well the problem is very easy to set up because of the regular spacing of the energy levels and the

easily determined multiplicity of the levels. The mathematical calculations are then easy to handle with a few lines of instructions using a software package like *Mathematica*, *Maple*, or *MathCad*. I review the energy levels of a three-dimensional quantum oscillator in Sec. II, and I discuss the calculation of occupation numbers for classical particles and bosons in Secs. III and IV, respectively. The results of the analysis are most apparent in the graphs of those sections. I then briefly discuss the heat capacity of the gas in Sec. V. Some details of a *Mathematica* program are discussed in Appendix A, and the work in this paper is related to a standard approximation in Appendix B.

II. 3-D HARMONIC OSCILLATOR

The energy levels of a one-dimensional quantum harmonic oscillator are

$$E_{1D} = (j + \tfrac{1}{2})\hbar\omega, \tag{1}$$

where ω is the angular frequency of the classical oscillator and $j \geq 0$ is an integer. For a particle confined in a three-dimensional harmonic potential well the oscillations in the three directions are independent, so the total energy is the sum of three terms of the same form, with independent quantum numbers j_i for each dimension:

$$E_{3D} = (j_x + \tfrac{1}{2})\hbar\omega_x + (j_y + \tfrac{1}{2})\hbar\omega_y + (j_z + \tfrac{1}{2})\hbar\omega_z. \tag{2}$$

For simplicity I will consider an isotropic oscillator, i.e., $\omega_x = \omega_y = \omega_z \equiv \omega$, and I rezero the energy scale at the energy of the ground state with $j_x = j_y = j_z = 0$. With these simplifications the energy becomes

$$E_{3D} = (j_x + j_y + j_z)\hbar\omega. \tag{3}$$

The total energy is thus expressed as an integral number of the units $\hbar\omega$. Simple combinatoric arguments[12] show that there are $(m+2)(m+1)/2$ linearly independent states with an energy $m\hbar\omega$. For example, there are three different states with total energy $\hbar\omega$, six different states with total energy $2\hbar\omega$, and so on.

When there are many noninteracting bosons in the same trap the total energy will simply be the sum of the individual particle energies given by Eq. (3). For bosons there may be many particles occupying the same single-particle state. Those particles in the same harmonic oscillator state are in some sense ''on top of each other'' in that they have exactly the same spatial probability distribution.

III. OCCUPATION NUMBERS FOR CLASSICAL PARTICLES

In this section I review the derivation of the occupation numbers of the energy levels of a three-dimensional quantum harmonic oscillator when the particles are assumed to obey classical statistics. For all of the calculations in this paper I assume a fixed number of noninteracting particles, N, and I assume that the particles are maintained in a heat bath at a temperature T. The particles are assumed to be structureless point particles with no internal energy states. The number of classical particles occupying any distinct single particle state with energy ϵ_l is given by the Boltzmann distribution:

$$(n_l)_{\text{Classical}} = \frac{1}{Ce^{\beta\epsilon_l}}, \tag{4}$$

where $\beta = 1/kT$, and C is a constant that is chosen so that the sum of the occupation numbers of all states is equal to the total number of particles, N, in the well. The total occupation number $\mathcal{N}_m$ of all states with a given energy $m\hbar\omega$ is given by Eq. (4) multiplied by the multiplicity of the energy level, i.e.,

$$(\mathcal{N}_m)_{\text{Classical}} = \frac{(m+2)(m+1)}{2Ce^{m\hbar\omega\beta}}. \tag{5}$$

The only difficulty is determining the normalization constant C. This constant is chosen to satisfy the condition

$$\sum_{m=0}^{\infty} \frac{(m+2)(m+1)}{2Ce^{m\hbar\omega\beta}} = N. \tag{6}$$

For particle numbers N that are not too large it is easy to determine C by numerically solving Eq. (6) using a symbolic algebra package on a personal computer. The constant can then be used by the same package to evaluate the occupation numbers given by Eq. (5). [An alternative approach is to solve Eq. (6) algebraically for C and manipulate the result to obtain a formal expression for the occupation number, but the resulting expression is not transparent or easy to evaluate. And in the case of particles obeying Bose–Einstein statistics treated in the next section such an algebraic solution is not possible.]

Figure 1 is a sample *Mathematica* program that performs this calculation. The first four lines set the values of various constants. The quantity $\hbar\omega$ is set to 1 for convenience, but the symbol **hw** is left in the subsequent expressions so that their meaning is easier to understand. The following 6 lines:

1. define the distribution in terms of the unknown normalization constant c,

2. algebraically sum the occupation numbers,

3. solve for the normalization constant,

4. calculate the numerical values of all the occupation numbers using the normalization constant,

5. extract the value of the ground state occupation number, and

6. plot the occupation numbers as a function of energy.

This program executes in about 30 s on a standard computer with a 486 processor. Further details of the program are discussed in Appendix A.

Figure 2 includes plots of Eq. (5) for at sample of 10 000 particles at three temperatures, and in Fig. 3 I have plotted the number of particles in the ground state as a function of temperature. The occupation numbers illustrated in Fig. 2 show maxima for states with energies greater than zero because of the rapidly rising multiplicity of the energy levels. At high enough m the multiplicity factor in Eq. (5) is dominated by the exponential factor in the denominator, and the occupation numbers decrease with increasing m.

IV. QUANTUM STATISTICS OF BOSONS

The statistics of quantum particles are different than those of classical particles, and the differences will manifest themselves in the occupation numbers of energy levels in gases at very low temperature, or very high density. The origin of the different statistics is the indistinguishability of quantum particles and the requirement that the wave function for bosons by symmetric under particle exchange. The calculation of the occupation numbers proceeds exactly as in the case of clas-

```
hw = 1;                    (* hbar*omega              *)
kt=15;                     (* Boltzmann constant*Temperature *)
n=10000;                   (* Number of atoms         *)
sumlim = 300;              (* Number of terms in sum  *)


dist[c_] := 1/(c*Exp[hw*m/kt]);  (* Boltzmann distribution *)


normsum[c_] := Sum[dist[c]*(m+2)*(m+1)/2,{m,0,sumlim}]
                           (* Define normalization sum    *)


q = FindRoot[normsum[c] == n,{c,0.5}]
                           (* Find normalization constant  *)
{c -> 0.372788}


occnum = Table[N[dist[c/.q] *(m+2)*(m+1)/2],{m,0,sumlim}];
                           (* Calculate occupation numbers *)


Part[occnum,1]            (* Extract ground-state occupation*)
2.68249


ListPlot[occnum,PlotRange->{0,300}];
                           (* Plot occupation numbers     *)
```
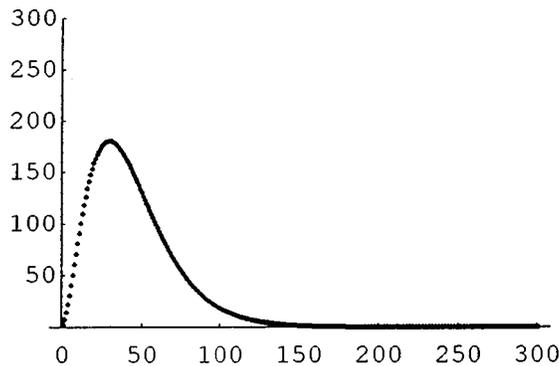

Fig. 1. *Mathematica* code for calculation of occupation numbers of classical particles in an isotropic three-dimensional harmonic oscillator potential.

sical particles, except a different distribution is used. The analog of the Boltzmann distribution for occupation numbers of bosons in single-particle states is the Bose–Einstein distribution,

$$(n_l)_{\text{BE}} = \frac{1}{C'e^{\beta\epsilon_l}-1},\qquad(7)$$

where C' is normalization constant analogous to the constant C in the classical case. The total occupation number in states with an energy $m\hbar\omega$ is then

$$(\mathcal{N}_m)_{\text{BE}} = \frac{(m+2)(m+1)}{2(C'e^{m\hbar\omega}-1)}.\qquad(8)$$

The *Mathematica* code given in Fig. 1 needs to be changed only in the single line where the distribution is defined in order to redo the calculations for bosons.

The energy level occupation numbers that are given by Eq. (8) for a sample of 10 000 bosons are plotted for four temperatures in Fig. 4. For high enough temperatures the results for the energy level occupation numbers given by the quantum statistics are almost indistinguishable from those derived for classical particles in Eq. (5). This is illustrated in the similarity of graphs in Fig. 2 and Fig. 4 for $kT = 25\hbar\omega$. The graphs in Figs. 2 and 4 begin to appear different for temperatures such that $kT \lesssim 19.7\hbar\omega$. The results plotted in Fig. 4 calculated using the Bose–Einstein distribution display a sharp rise in the population in the ground state below this temperature. In Fig. 3 the number of atoms in the ground state of the gas of bosons is plotted versus the temperature of the gas; this graph shows a very sharp rise below $kT = 20\hbar\omega$ compared to the data for classical particles plotted in the same figure. The abrupt rise in the number of bosons in the ground state is the signature of Bose–Einstein condensation. In the limit of large particle numbers the graph of the number of bosons in the ground state acquires a true kink with a discontinuous derivative at the critical temperature T_c. It is worth emphasizing that this condensation occurs even though the particles do not interact, in contrast to the
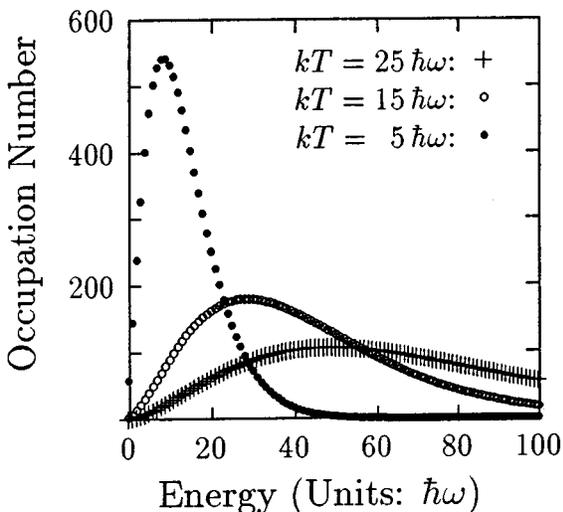
Fig. 2. Occupation numbers of energy states for 10 000 classical particles in an isotropic harmonic oscillator potential at three temperatures: $kT = 25\hbar\omega$, $kT = 15\hbar\omega$, and $kT = 5\hbar\omega$.

case of more familiar phase transitions which are due to intermolecular forces. Bose–Einstein condensation is entirely a consequence of the "extra" -1 in the denominator of the Bose–Einstein distribution, Eq. (7).

V. HEAT CAPACITY OF THE BOSE CONDENSATE

The same program that calculates the occupation number of the energy levels of a gas can easily calculate the average thermal energy of the gas,

$$U = \sum_{m=0}^{\infty} \mathcal{N}_m \epsilon_m = \sum_{m=0}^{\infty} \frac{(m+2)(m+1)}{2(C' e^{m\hbar\omega} - 1)} m\hbar\omega. \qquad (9)$$

The average energy per particle of a gas 10 000 particles as a function of temperature is displayed in Fig. 5.
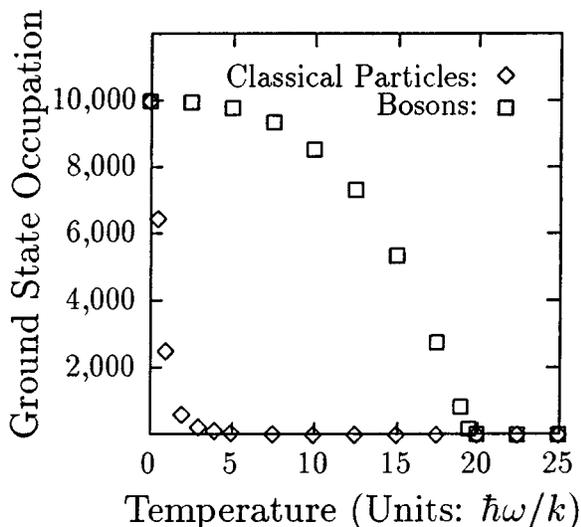

Fig. 3. Occupation number of ground state as a function of temperature for 10 000 classical particles and 10 000 bosons in an isotropic harmonic oscillator potential.
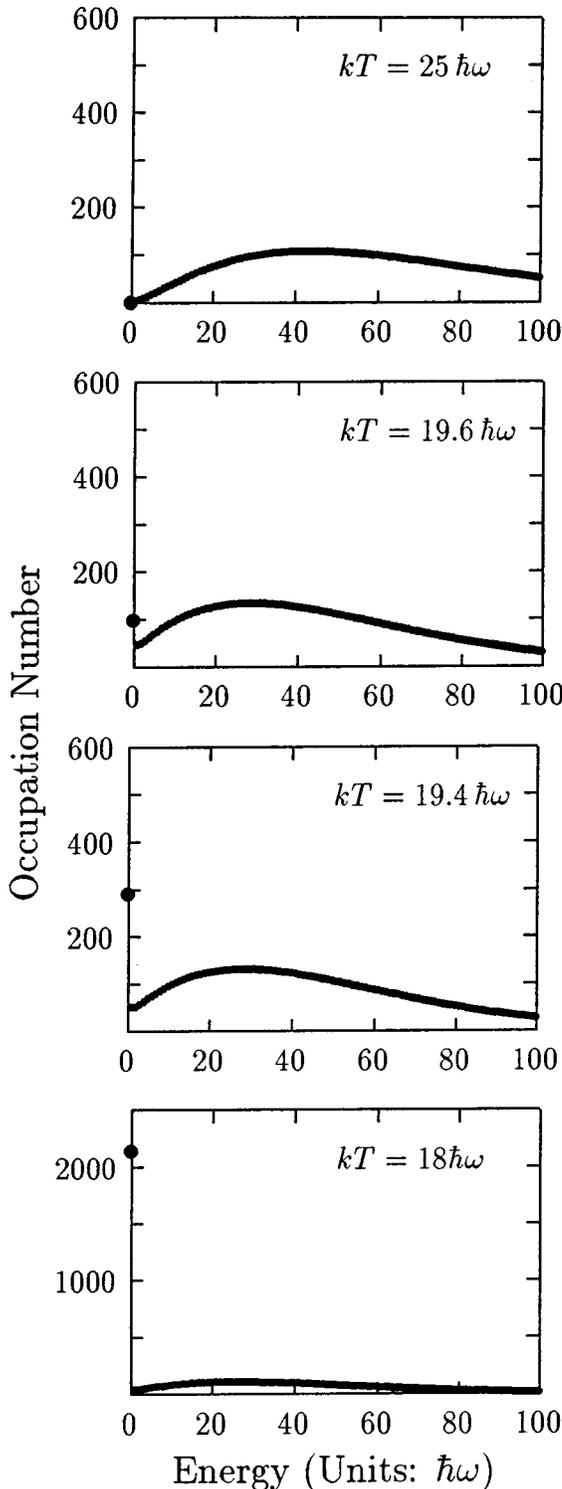

Fig. 4. Occupation numbers of energy states for 10 000 bosons in an isotropic harmonic oscillator potential for $kT = 25\hbar\omega$, $kT = 19.6\hbar\omega$, $kT = 19.4\hbar\omega$, and $kT = 18\hbar\omega$. (Note the change of scale on the lowest graph.)

The heat capacity of gas is defined as

$$C = \frac{dU}{dT}. \qquad (10)$$

(Heat capacity is usually measured at constant volume or at constant pressure. For particles in a harmonic trap neither
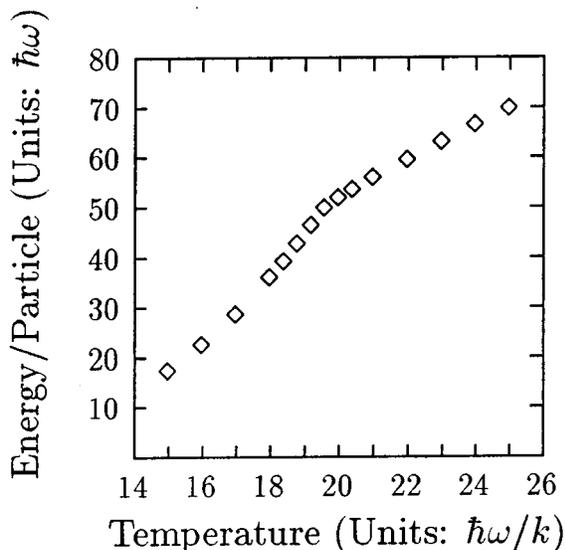
Fig. 5. Average energy per particle as a function of temperature for 10 000 bosons in an isotropic harmonic oscillator potential.

Fig. 6. Heat capacity per particle as a function of temperature for 10 000 bosons in an isotropic harmonic oscillator potential.

concept is really appropriate. For example, the volume occupied by the particles naturally changes as the energy per particle changes, but no work is done by the expansion.) Figure 6 shows the heat capacity determined numerically from the data plotted in Fig. 5. The heat capacity per particle shows the characteristic "lambda" shape at the transition temperature, and approaches the classical value of $3k$ at higher temperatures. (The translational motion of the particles contributes $3k/2$ to the heat capacity per particle, and the potential energy of the harmonic oscillator potential contributes an additional $3k/2$.) A more analytical treatment of the heat capacity in the true thermodynamic limit is given in Refs. 7 and 8.

APPENDIX A: NOTES ON *MATHEMATICA* CODE

While the *Mathematica* code of Fig. 1 is conceptually straightforward, a few constants in the code must be chosen with care. The normalization sum is nominally a sum of an infinite number of terms; in practice the required number of terms in the normalization sum, `sumlim`, will depend on the temperature, and the number of atoms. The sum must include all energy levels that have an appreciable occupation number for the given conditions. The required number can be determined empirically by trying different limits and examining graphs like that produced in the last line of the code in Fig. 1. The displayed graph shows that the occupation number for levels with $E = 300\ \hbar\omega$ is very small, and thus the sum with 300 terms includes all levels with appreciable occupation. For higher temperatures the number of terms would have to be increased. With more atoms in the trap, Bose–Einstein condensation occurs at a higher temperature, and thus more terms must be used in this case. (The critical temperature scales as $N^{1/3}$ as is discussed in Appendix B.)

In determining the normalization constants C (in the case of classical particles) and C' (in the case of bosons) I use the *Mathematica* function `FindRoot` which requires a starting value for its root searching algorithm. In the case of classical particles this choice is not terribly critical, but in the case of
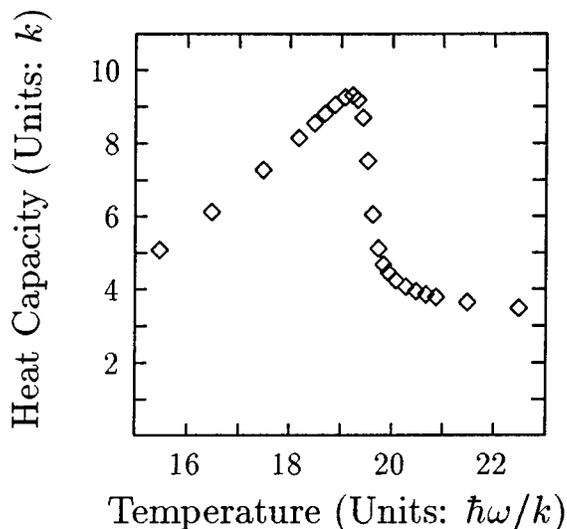
bosons the constant C' gets extremely close to 1 as the temperature nears the critical temperature. (Standard approximation schemes for determining the critical temperature rely on setting C' exactly equal to 1 as is discussed in Appendix B.) If the starting value of the `FindRoot` function is not sufficiently close to 1, the root finding algorithm may actually jump past the root that is close to 1 and find an unphysical value of C' that is less than 1.

APPENDIX B: CONNECTION TO STANDARD APPROXIMATIONS

In conventional introductions to Bose–Einstein condensation the volume in which the particles are contained is considered large enough that the energy states are very closely spaced, and the sum over all energy states like that in Eq. (6) is converted to an integral. The continuum density of states for an isotropic three-dimensional quantum harmonic oscillator is given by

$$f(\epsilon)\ d\epsilon = \frac{\epsilon^2}{2(\hbar\omega)^3}\ d\epsilon, \tag{B1}$$

and it seems that the normalization sum should be replaced by the integral condition

$$\int_0^\infty \frac{\epsilon^2}{(C'e^{\beta\epsilon}-1)}\ d\epsilon = 2N(\hbar\omega)^3. \tag{B2}$$

There is a flaw in this argument because this integral condition is only valid for temperatures above a critical temperature. To see this, imagine that the temperature of the system is lowered. As the temperature decreases, so must the constant C' in order to keep the left side of the equation constant. Examination of the Bose–Einstein distribution, Eq. (7), shows that C' must always be greater than 1 if the occupation numbers are to be positive. Thus, the temperature at which $C' = 1$ is a critical temperature for this integral. The problem is that the ground state with zero energy is completely neglected in the integral of Eq. (B2) because the density of states factor, Eq. (B1), goes to zero at $\epsilon = 0$. The

occupation of the ground state must be explicitly retained in the transition from the sum to an integral, so that below the critical temperature the normalization condition is

$$\frac{1}{C'-1} + \frac{1}{2(\hbar\omega)^3}\int_0^\infty \frac{\epsilon^2}{(C'e^{\beta\epsilon}-1)}\,d\epsilon = N. \tag{B3}$$

Above the critical temperature the number of particles in the ground state is so small that it can be ignored.

The critical temperature is thus determined by evaluating the integral in Eq. (B2) when $C'=1$, and solving for T. This gives

$$kT_c = \left(\frac{2N}{2.404}\right)^{1/3}\hbar\omega. \tag{B4}$$

This result was derived In Ref. 7, along with transition temperatures for other external potentials. For the case of 10 000 particles studied in this paper, this predicts an approximate critical temperature of

$$kT_c \simeq 20.3\hbar\omega, \tag{B5}$$

which is very close to the value determined in Sec. IV.

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[12]The m units of energy must be partitioned between the three independent oscillators. To visualize the problem, represent the units of energy as m indistinguishable particles in a row. There are $(m-1)$ spots between the particles in which to place two ''dividers'' which partition the energy into three sets. The total number of permutations of the particles and dividers is $(M+2)!$. To determine the total number of states this must be divided by $m!2!$ because permuting the energy units energy units amongst themselves and permuting the dividers amongst themselves does not produce a new arrangement. Thus the total number of states is $(m+2)(m+1)/2$.