

# A computational introduction to quantum statistics using harmonically trapped particles

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## Abstract

In a 1997 paper Moore and Schroeder argued that the development of student understanding of thermal physics could be enhanced by computational exercises that highlight the link between the statistical definition of entropy and the second law of thermodynamics [Am. J. Phys. **65**, 26 (1997)]. I introduce examples of similar computational exercises for systems in which the quantum statistics of identical particles plays an important role. I treat isolated systems of small numbers of particles confined in a common harmonic potential, and use a computer to enumerate all possible occupation-number configurations and multiplicities. The examples illustrate the effect of quantum statistics on the sharing of energy between weakly interacting subsystems, as well as the distribution of energy within subsystems. The examples also highlight the onset of Bose-Einstein condensation in small systems.

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## I. INTRODUCTION

In a 1997 paper in this journal Moore and Schroeder argued that the development of student understanding of thermal physics could be enhanced by computational exercises that highlight the link between the statistical definition of entropy and the second law of thermodynamics.<sup>1</sup> The first key to their approach was the use of a simple model, the Einstein solid, for which it is straightforward to develop an exact formula for the number of microstates of an isolated system. The second key was the use of a computer, rather than analytical approximations, to evaluate these formulas. This approach, using the micro-canonical ensemble appropriate for an isolated system, highlights the role of probability in determining the thermal properties of a system. (The use of the Einstein solid as a pedagogical tool was developed further in an introductory text by Moore<sup>2</sup> and a more advanced text by Schroeder.<sup>3</sup>) In this paper I adopt the approach of Moore and Schroeder, and apply it to simple systems in which the quantum statistics of identical particles plays an important role. The examples are designed to amplify that connection between the statistical definition of entropy and temperature, as developed by Moore and Schroeder, while illustrating the profound effect of the statistics of identical particles. They also provide students with a connection to the vibrant field of trapped ultra-cold atoms. (For an overview of the field, see, for example, Ref. 4 and Ref. 5.)

The examples considered in this paper demonstrate the breakdown of classical equipartition, the different occupation-number distributions for bosons, fermions, and distinguishable particles, and the onset of Bose-Einstein condensation. The goal of the approach used in this paper is not the derivation of analytical results using sophisticated mathematics. Rather, it is the use of an unsophisticated technique — the explicit counting of the states of an isolated system with the aid of a computer — to help students gain insight into the effects of quantum statistics on thermal properties, thereby extending the pedagogical treatment of Moore and Schroeder.

I first consider a gas with a fixed number of weakly-interacting particles trapped together in a one-dimensional harmonic potential. This potential has the advantage that the multiplicity for a collection of distinguishable classical particles is identical to that of the Einstein solid considered by Moore and Schroeder. The deviations from the thermal properties explored in Ref. 1 are thus directly traceable to the quantum statistics of identical particles.

In order to highlight the unequal sharing of energy between fermions and bosons at a common temperature, as well as the different energy distributions for the two kinds of particles, the one-dimensional systems I consider consist of mixtures of both bosons and fermions in a common potential. I then consider a gas of particles trapped in a three-dimensional isotropic harmonic trap, and explore how the increased density of states (due to the degeneracy of the energy levels) leads to the onset of Bose-Einstein condensation.

## II. TRAPPED PARTICLES IN ONE DIMENSION

### A. States and Multiplicities

The energy levels and multiplicities of the Einstein solid considered by Moore and Schroeder are identical to those of  $N$  non-interacting distinguishable particles of mass  $m$  confined together in a one-dimensional harmonic oscillator potential characterized by the angular frequency  $\omega$ . The energy of any individual particle is

$$E_i = m_i \hbar \omega \equiv \epsilon m_i, \quad (1)$$

where the index  $i$  labels the particle, and  $m_i$  is a non-negative integer. The total energy of the gas of  $N$  trapped particles is thus

$$U = \sum_{i=0}^N m_i \epsilon \equiv q \epsilon, \quad (2)$$

where  $q$  is another non-negative integer. (I have ignored the zero-point energy, which plays no role in the statistical mechanics of the system.) As in the case of the Einstein solid discussed in Ref. 1, the multiplicity for  $N$  trapped distinguishable particles with  $q$  units of energy is

$$\Omega^{\text{D}}(N, q) = \binom{q + N - 1}{q} = \frac{(q + N - 1)!}{q!(N - 1)!}. \quad (3)$$

The difference between the gas of trapped particles and the Einstein solid arises when the particles are identical, i.e., indistinguishable. In the case of the Einstein solid the particles are distinguished by their positions in the lattice (with the assumption that the interparticle spacing is large compared to the spatial extent of a single-particle wavefunction); in the case of trapped particles, all particles occupy the same space near the minimum of the potential, and the quantum statistics of identical particles must be considered.

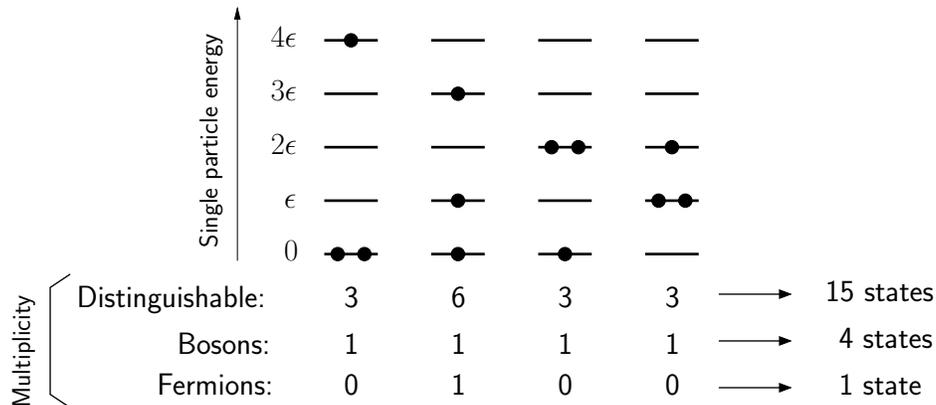


FIG. 1: Possible occupation-number configurations of 3 particles with total energy  $4\epsilon$  in a one-dimensional harmonic oscillator potential. The number of distinct states for each configuration is given for distinguishable particles, bosons, and fermions. (For simplicity I have assumed that all of the fermions have the same spin orientation, so that at most one fermion may occupy a state.)

For low-energy closed systems with small numbers of particles it is straightforward to demonstrate the effect of quantum statistics on occupation numbers by writing down all possible ways the units of energy can be distributed between the available states. A particular distribution, with  $n_0$  units of energy in the ground state,  $n_1$  units in the first excited state, etc., is known as an occupation-number configuration, and can be written as the set of integers  $\{n_0, n_1, n_2, \dots\}$ . The enumeration of configurations “by hand” is the basis for problems in several undergraduate texts. For example, Griffiths<sup>6</sup> presents problems based on small numbers of particles in square well potentials, and Schroeder<sup>7</sup> leads students to investigate particles in the one-dimensional harmonic potential considered in this paper. The strategy used in this paper is identical to that used to solve these textbook problems, so students who have completed exercises like these should be ready to appreciate how a computer can be used to extend this kind of investigation to larger systems with more energy.

Before turning to larger systems, I first review the results of a typical textbook exercise by considering the case of 3 particles in a harmonic potential with 4 units of energy. The possible occupation-number configurations for this situation are illustrated in Fig. 1. The multiplicity for distinguishable particles is  $\Omega^{(D)} = 15$ , consistent with Eq. (3). The multiplicity for bosons,  $\Omega^{(B)} = 4$ , is less than the multiplicity for distinguishable particles, because without labels on the particles there are fewer distinct ways to arrange them, and the multiplicity

for fermions,  $\Omega^{(F)} = 1$ , is smaller still, because of the prohibition on multiply occupied states articulated in the Fermi exclusion principle. (To keep things simple, I am assuming that all of the fermions have the same spin orientation, so that only one fermion can occupy any single-particle state.)

The number of energy units per particle in the example of Fig. 1 is only  $4/3$ , which means that a large fraction of the configurations for distinguishable particles and bosons have multiply-occupied states. In the limit in which the number of energy units per particle is large, the fraction of configurations with multiply occupied levels goes to zero, and the multiplicity for distinguishable particles is larger than the multiplicity for identical particles by the factor  $N!$ . In this limit the entropy of a system of distinguishable particles differs from the entropy of a system of identical particles by the constant additive term  $\ln(N!)$ , and the thermodynamics of bosons, fermions, and distinguishable particles are identical. The quantum statistics of identical particles will only reveal itself at energies for which classical statistics predicts a significant probability of multiple occupation.

The enumeration of all possible states “by hand” that is possible for small systems quickly becomes a daunting task as the number of particles grows. In the following paragraphs I discuss algorithms for determining the multiplicities  $\Omega^{(B)}$  and  $\Omega^{(F)}$  for arbitrary numbers of bosons and fermions respectively. These algorithms are well-suited to implementation on a computer, so that students can go beyond standard textbook exercises and gain further insight into the thermodynamic properties of identical particles in larger systems.

For identical bosons there is one state for each of the possible occupation-number configurations,  $\{n_0, n_1, n_2, \dots\}$ . Each of the possible configurations with  $q$  units of energy must satisfy the condition

$$q = 0 \times n_0 + 1 \times n_1 + 2 \times n_2 + \dots = \sum_{i=0}^{\infty} i \times n_i, \quad (4)$$

subject to the constraint that the total number of particles is fixed, i.e.,

$$\sum_{i=0} n_i = N. \quad (5)$$

The conditions that must be satisfied for possible configurations can be mapped to the well-studied problem in number theory of finding integer partitions. A partition of a given non-negative integer is a set of non-negative integers that sum to the given integer. For example, the integer 4 can be written as the sums  $3 + 1$ ,  $2 + 2$ ,  $2 + 1 + 1$ , and  $1 + 1 + 1 + 1$ ,

and the integer partitions of 4 are denoted (4), (3, 1), (2, 2), (2, 1, 1), and (1, 1, 1, 1). The conditions given in Eq. (4) will be satisfied if the set of occupation numbers  $n_1, n_2, n_3, \dots$  are chosen in the following manner:  $n_1$  is given by the number of times a 1 appears in a given integer partition,  $n_2$  is given by the number of times a 2 appears, etc. The occupation of the ground state,  $n_0$  can then be determined using the particle number constraint expressed in Eq. (5), giving  $n_0 = (N - \sum_{i>0} n_i)$ . As an example, the integer partitions of 4 map to the following occupation-number configurations for bosons:

$$(4) \longrightarrow \{n_0 = 3, n_1 = 0, n_2 = 0, n_3 = 0, n_4 = 1\}, \quad (6a)$$

$$(3, 1) \longrightarrow \{n_0 = 2, n_1 = 1, n_2 = 0, n_3 = 1, n_4 = 0\}, \quad (6b)$$

$$(2, 2) \longrightarrow \{n_0 = 2, n_1 = 0, n_2 = 2, n_3 = 0, n_4 = 0\}, \quad (6c)$$

$$(2, 1, 1) \longrightarrow \{n_0 = 0, n_1 = 2, n_2 = 1, n_3 = 0, n_4 = 0\}, \quad (6d)$$

$$(1, 1, 1, 1) \longrightarrow \{n_0 = 0, n_1 = 4, n_2 = 0, n_3 = 0, n_4 = 0\}. \quad (6e)$$

The (1, 1, 1, 1) partition does not yield a possible configuration for three particles, because the number of parts in this partition is greater than the number of particles, violating the constraint of Eq. (5). The multiplicity of states with three particles and 4 units of energy is thus the number of integer partitions of 4 with a number of parts less than or equal to 3.

Generalizing this example gives the multiplicity of a general state with  $q$  units of energy, and  $N$  particles as

$$\Omega^{(B)}(N, q) = p(q \mid \text{number of parts} \leq N), \quad (7)$$

where  $p$  is a function giving the number of integer partitions of  $q$  with the number of parts less than or equal to  $N$ . Routines for enumerating and counting integer partitions are standard features of modern computer algebra systems, and are also available in many low-level programming languages.<sup>8</sup> For example, in *Mathematica*<sup>®</sup> the integer partitions of  $q$  with the number of parts less than or equal to  $n$  are enumerated with the command `IntegerPartitions[q,n]`, and the number of partitions can be counted with `Length[IntegerPartitions[q,n]]`. This makes the determination of the number of states of identical bosons straightforward, in much the same way that Eq. (3) enables the counting of states of distinguishable particles.

The case of fermions is a little more subtle. Not all boson configurations given by the simple “integer partition method” can be realized for fermions, because such a listing yields many configurations with multiply occupied single-particle states ( $n_i > 1$ ). For

one-dimensional systems, however, the enumeration of “legal” configurations of fermions is just as easy as it is for bosons, because there is a one-to-one correspondence between the bosonic states with energy  $q\epsilon$ , and the fermionic states with energy  $U_{T=0}^{(F)} + q\epsilon$ , where  $U_{T=0}^{(F)} = N(N-1)\epsilon/2$  is the total energy of fermions at  $T = 0$ . (A further discussion of this correspondence can be found in Appendix A, and in Ref. 9.) Therefore

$$\begin{aligned}\Omega^{(F)}(N, q) &= \Omega^{(B)}(N, q - q_{T=0}^{(F)}) \\ &= p(q - N(N-1)/2 \mid \text{number of parts} \leq N),\end{aligned}\tag{8}$$

where  $q_{T=0}^{(F)} \equiv E_{T=0}^{(F)}/\epsilon$  is the total number of units of energy for fermions at  $T = 0$ . This means that the multiplicity calculation for fermions requires the same algorithm as the calculations for bosons.

## B. Interacting Systems, Entropy, and Temperature

Moore and Schroeder considered weakly interacting systems of distinguishable particles. Equations (3), (7), and (8), giving the multiplicities for distinguishable particles, identical bosons, and identical fermions respectively, provide the tools that enable a student to repeat the same kind of calculations in a system in which the identity of the particles plays an important role. In this section I will consider two weakly interacting sub-systems in a common potential, with particle numbers  $N_1$  and  $N_2$ , energies  $q_1\epsilon$  and  $q_2\epsilon$ , multiplicities  $\Omega_1$  and  $\Omega_2$ , and entropies  $S_1 = k \ln \Omega_1$  and  $S_2 = k \ln \Omega_2$ .

As a simple example, let subsystem 1 contain 3 distinguishable particles, and subsystem 2 contain 3 identical bosons, and assume that the total energy to be shared between the systems is  $6\epsilon$ . This is the same introductory example considered in Ref. 1, except for the fact that in my example subsystem 2 is composed of bosons. The multiplicities for all possible energy distributions are listed in Fig. 2; the multiplicities for two subsystems of distinguishable particles are also given for comparison.

If subsystems 1 and 2 are both distinguishable particles, the most likely distribution of energy is that in which the 6 units of energy are shared equally between the two subsystems, with 3 units of energy in each. In addition, the expected value of the energy in each subsystem, when averaged over all energy distributions, is also  $3\epsilon$ . When subsystem 2 is made up of bosons this is no longer the case, and the expected value of the energy in

$$N_1 = N_2 = 3 \quad q_{\text{total}} = 6$$

$q_1$	$\Omega_1^{(D)}$	$q_2$	$\Omega_2^{(B)}$	$(\Omega_2^{(D)})$	$\Omega_{\text{total}} = \Omega_1^{(D)}\Omega_2^{(B)}$	$(\Omega_1^{(D)}\Omega_2^{(D)})$
0	1	6	7	(28)	7	(28)
1	3	5	5	(21)	15	(63)
2	6	4	4	(15)	24	(90)
3	10	3	3	(10)	30	(100)
4	15	2	2	(6)	30	(90)
5	21	1	1	(3)	21	(63)
6	28	0	1	(1)	28	(28)

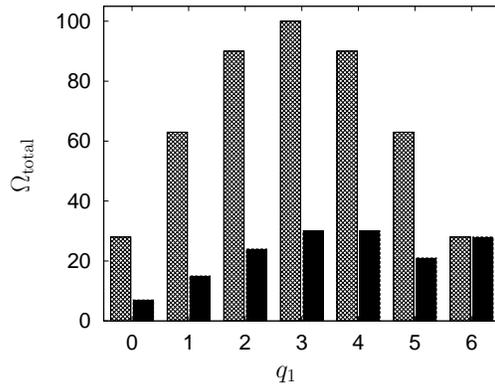


FIG. 2: Explicit multiplicities for a small system comprising two subsystems, each with 3 particles. The system has 6 units of energy, which are divided between the subsystems. The case of 3 distinguishable particles and 3 bosons is illustrated with the solid bars in the graph. For comparison, the case in which all 6 particles are distinguishable, which is the same case considered in Fig. 1 of Ref. 1, is also illustrated with the shaded bars in the graph, and in parentheses in the table. Energy is not shared equally between the interacting subsystems of bosonic and distinguishable particles.

subsystem 1 of distinguishable particles is a little more  $3.5\epsilon$ ; the effect of the quantum statistics is that the subsystem of bosons “gives up” energy to the system of distinguishable particles (on average). Students can repeat this kind of calculation for small numbers of fermions and distinguishable particles.

For larger systems I use a computer to calculate the information that is displayed for a small system in the table of Fig. 2. The entropies for interacting subsystems of 20 distinguishable particles and 20 identical bosons with total energy  $U = 80\epsilon$  are displayed in Fig. 3. (The *Mathematica* notebook used to generate the data for this system is available at [URL will be inserted by AIP]; representative code is listed in Appendix B). The entropies are plotted as a function of  $q_D$ , the number of units of energy in the subsystem of distinguishable particles. As in the small system of 6 particles discussed above, the maximum entropy does not occur at the value of  $q_D$  that gives equal energy per particle in the two subsystems. The maximum in  $S_{\text{total}}$  occurs at  $q_D = 64$ , which means that in the most likely distribution the bosons have only 20% of the total energy. The maximum occurs when the distribution

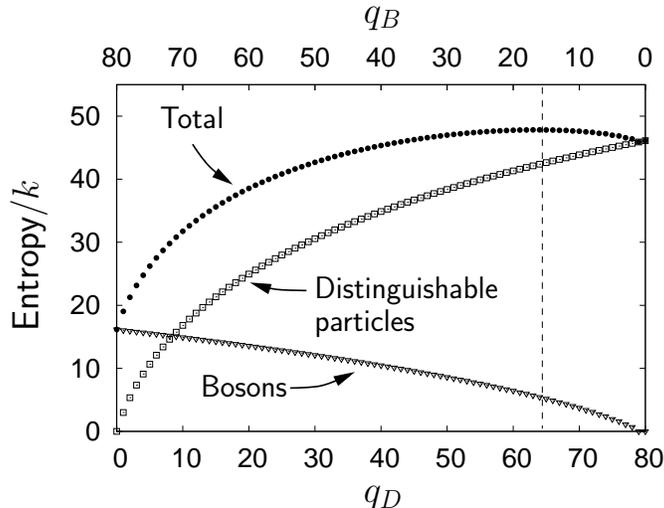


FIG. 3: Entropies for a system of 20 distinguishable particles and 20 bosons, with a total energy  $U_{\text{total}} = 80\epsilon$ . The entropies are plotted as functions of the number of units of energy in the subsystem of distinguishable particles. (The number of units of energy in the system of bosons is indicated along the top of the graph.) The dashed vertical line highlights the most likely distribution of energy, with 64 units of energy in the subsystem of distinguishable particles, and 16 units of energy in the subsystem of bosons.

of energy between subsystems is such that the slopes of graphs of  $S_D$  and  $S_B$  have equal magnitudes, but opposite signs. This reinforces the concept that temperature is determined by the derivative of the entropy with respect to energy, i.e.,

$$\frac{1}{T} = \frac{dS}{dU}. \quad (9)$$

(This relationship is usually developed for constant-volume rigid-wall containers, or in contexts in which volume isn't a relevant variable. In contrast, a gas of trapped particles expands as energy is added, but this definition of temperature is still applicable because no work is done by the system as it expands, as long as the effective spring constant is held constant; see Ref. 10.) Approximate temperatures of the subsystems, as given by the relationship

$$\frac{1}{T} \simeq \frac{S(q+1) - S(q-1)}{2\epsilon} = \frac{k}{\epsilon} \left( \frac{\ln [\Omega_{\text{total}}(q+1)] - \ln [\Omega_{\text{total}}(q-1)]}{2} \right), \quad (10)$$

are illustrated in Fig. 4, showing that these two subsystems equilibrate at a temperature just below that given by  $kT = 4\epsilon$ .

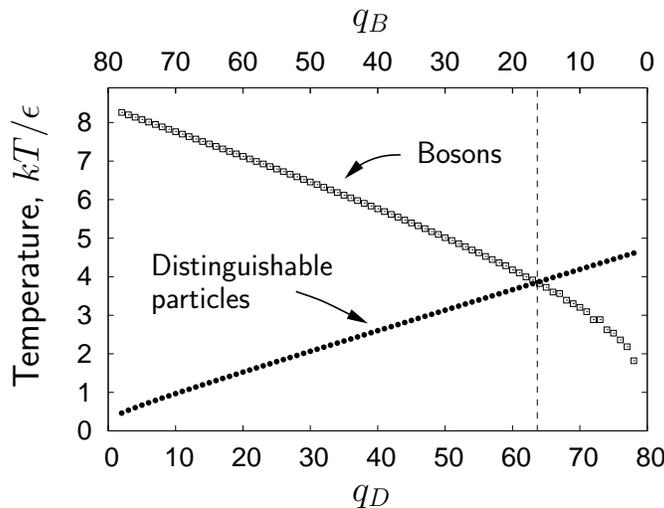


FIG. 4: Temperatures of the subsystems of 20 distinguishable particles and 20 identical bosons, with a total energy  $U = 80\epsilon$ . The temperatures are plotted as functions of the number of units of energy in the subsystem of distinguishable particles. (The number of units of energy in the subsystem of bosons is indicated along the top of the graph.) The dashed vertical line highlights the point at which the two temperatures are equal.

Students can explore the effect of the average energy per particle on the division of energy between the two subsystems. As the total number of particles in each subsystem is reduced, thereby raising the energy per particle, the division of energy between the two subsystems approaches the 50:50 split expected for classical particles. This demonstrates that the effect of the quantum statistics of identical particles decreases as the energy per particle increases, because the accompanying probability of double occupancy decreases.

I will leave the case of interacting fermions and distinguishable particles as an exercise for students, and consider next a subsystem of 20 fermions exchanging energy with 20 bosons, with a total energy of  $270\epsilon$ . The total energy must be larger than in the previous example, because it must be greater than the zero-point energy of the fermions,  $U_{T=0}^{(F)} = 190\epsilon$ . The only change in the method of calculation from the previous example is in the determination of multiplicities, i.e., the substitution of Eq. (8) for Eq. (7). Repeating the same kinds of calculations previously carried out on a system with less energy gives the results illustrated in Figs. 5 and 6. The total entropy is maximized when the sub-system of bosons has energy  $40\epsilon$  and the system of fermions has  $230\epsilon$ , and this occurs when the approximate equilibrium

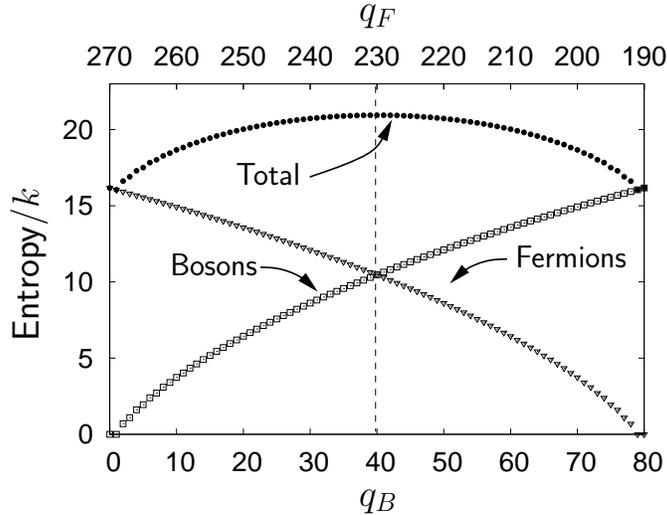


FIG. 5: Entropies for a system of 20 identical fermions and 20 bosons, with a total energy  $U_{\text{total}} = 270\epsilon$ . The entropies are plotted as functions of the number of units of energy in the subsystem of bosons. (The number of units of energy in the subsystem of fermions is indicated along the top of the graph.) The dashed vertical line highlights the most likely distribution of energy, with 40 units of energy in the subsystem of bosons, and 230 units of energy in the subsystem of fermions.

temperature calculated using Eq. (10) is given by  $kT = 5.76\epsilon$ . Note that at this temperature the 80 units of energy *above* the zero-point energy of the fermions are shared equally between the two sub-systems

These examples highlight the important role of quantum statistics in determining how entropy changes when thermal energy is exchanged between subsystems. Equilibrium is achieved when the entropy changes in the two subsystems balance upon exchange of energy, indicating an extremum in the total entropy. In these examples we see the breakdown of classical equipartition, as the average energy per particle is *not* the same in the two subsystems when they reach thermal equilibrium.

### C. Thermodynamic Distribution Functions

The results of the preceding section demonstrate the effect of quantum statistics on the equilibrium distribution of energy between interacting subsystems. In this section I investigate the distribution of energy between particles within a single system. In other

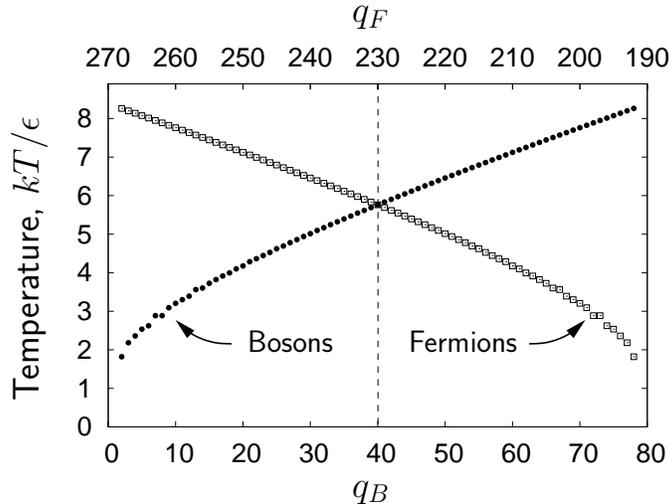


FIG. 6: Temperature of subsystems of 20 identical fermions and 20 bosons, with a total energy  $U = 270\epsilon$ . The temperatures are plotted as functions of the number of units of energy in the subsystem of bosons. (The number of units of energy in the subsystem of fermions is indicated along the top of the graph.) The dashed vertical line highlights point at which the two temperatures are equal.

words, I address the question “Given a system of  $N$  harmonically trapped particles with total energy  $q\epsilon$ , what is the average number of particles with a given single-particle energy?”

In the previous section it was only necessary to count the number of microstates in order to determine the most likely distribution of energy between two subsystems; for bosons and fermions this entailed the counting of integer partitions. In order to determine the expected number of particles with a given energy within a system, it is necessary to go one step farther: each integer partition must be converted into an explicit occupation-number configuration,  $\{n_0, n_1, n_2, \dots\}$ , like those illustrated for a small system in Fig. 1. Once all occupation-number configurations are known, expected occupation number of a single-particle energy level  $\bar{n}_m$  can be determined as the average of the occupation number in all configurations, with weighting factors given by the multiplicities  $g_i$  of each configuration:

$$\bar{n}_m = \frac{\sum_i (n_m)_i g_i}{\sum_i g_i}, \quad (11)$$

where  $(n_m)_i$  is the number of particles with energy  $m\epsilon$  in the  $i^{\text{th}}$  configuration, and the sum is over all configurations. (For identical particles the sum simplifies because  $g_i = 1$  for all

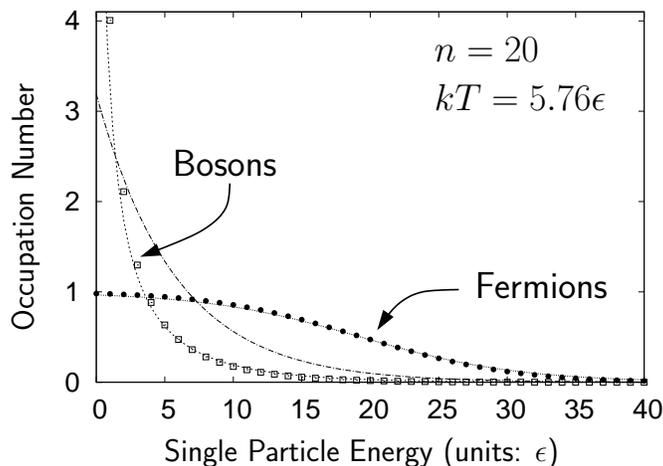


FIG. 7: Average occupation numbers for a closed system of 20 trapped bosons with energy  $E_B = 40\epsilon$ , and a system of 20 trapped fermions with energy  $E_F = 270\epsilon$ . The systems both have a temperature given by  $kT = 5.76\epsilon$ . For comparison, the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac distributions for 20 particles at this temperature are illustrated with continuous lines.

allowed configurations.)

As was noted previously, enumeration of integer partitions is a standard part of many computation packages, and it is straightforward to convert an integer partition into an occupation-number configuration (an example is given in the *Mathematica* listing in Appendix B). With an explicit listing of all configurations, it is easy to evaluate Eq. (11) for all values of  $m$  to generate a distribution of occupation numbers.

Two distributions of occupation numbers are illustrated in Fig. 7: one is the distribution for a system of 20 bosons with energy  $U^{(B)} = 40\epsilon$ , and the other is for a system of 20 fermions with an energy  $U^{(F)} = 230\epsilon$ . I have chosen these two systems because, as was demonstrated in the previous section, they both have the same temperature  $kT = 5.76\epsilon$ .

At this temperature the occupation numbers are very different for bosons and fermions. In the thermodynamic limit, occupation numbers will be given by the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac distributions for distinguishable particles, identical bosons, and identical fermions respectively. For comparison, these three distributions for 20 particles in equilibrium with a heat bath at temperature  $kT = 5.76\epsilon$  are also plotted in Fig. 7. Although the explicit enumeration of microstates discussed in this paper is limited to small

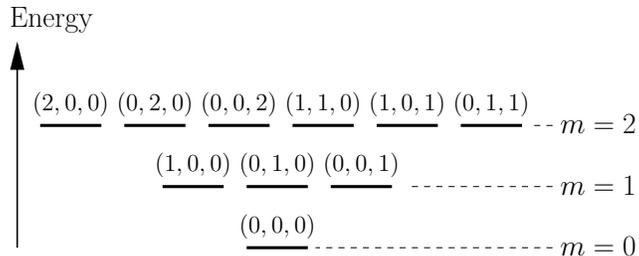


FIG. 8: The lowest energy single-particle states of an isotropic harmonic oscillator potential. The quantum numbers of the levels are indicated as  $(m_x, m_y, m_z)$ .

numbers of particles, the agreement with the distributions appropriate in the large- $N$  limit is striking.

### III. TRAPPED PARTICLES IN THREE DIMENSIONS AND THE APPROACH TO BOSE-EINSTEIN CONDENSATION

In this section I present results for occupation-number distributions for particles in three-dimensional traps. In three-dimensional isotropic harmonic potentials the allowed single-particle energies are the same as they are in one dimension, but the levels in three-dimensional potentials are degenerate. As in the one-dimensional case, the single-particle states have energies given by  $E_i = m_i \hbar \omega = m_i \epsilon$ , but now the integer coefficient  $m_i$  is the sum of three other positive integers corresponding to the units of excitation in the independent one-dimensional oscillators associated with the  $x$ ,  $y$ , and  $z$  directions. The lowest energy single-particle states of an isotropic three-dimensional potential are illustrated in Fig. 8. The number of single-particle states with energy  $m\epsilon$  is given by<sup>11</sup>

$$d_m = \frac{(m+1)(m+2)}{2}. \quad (12)$$

The degeneracy of the levels of this potential is a manifestation of the increased density of states in higher dimensions that exists even when the potentials are not isotropic, or harmonic. This increased density of states leads to Bose-Einstein condensation when the temperature is low enough. The techniques used in this paper are limited to small numbers of particles, so it is not possible to see that Bose-Einstein condensation exhibits the features of a true phase transition, but it is possible to see a relatively abrupt rise in the ground

state occupation at low temperatures.

To calculate the occupation-number distribution I again use Eq. (11) to average over all configurations. Because the energy level spacing is the same in both one and three dimensions, the set of possible occupation-number configurations  $\{n_0, n_1, n_2, \dots\}$  for a given particle number  $N$  and total energy  $q\epsilon$  will be the same in both cases, and configurations can be generated as in previous sections. The complication that arises in three dimensions is due to the degeneracy of the levels, which leads to multiple distinct states in each occupation-number configuration, whereas in one-dimension the multiplicity  $g_i$  of each configuration of bosons or fermions is 1. As a simple example, consider three particles with energy  $2\epsilon$  in the occupation-number configuration  $\{n_0 = 2, n_1 = 0, n_2 = 1\}$ . It is straightforward to examine Fig. 8 and list all possible states to see that there are 6 distinct states for bosons, and 18 for distinguishable particles; for the configuration  $\{n_0 = 1, n_1 = 2\}$  there are again 6 states for bosons, but 27 for distinguishable particles.

The combinatoric problem of determining the multiplicity  $g$  of occupation-number configurations in the general case has been covered in undergraduate texts (see, for example, Ref. 12). For  $N$  particles with occupation numbers  $\{n_0, n_1, n_2, \dots, n_m, \dots\}$  in single-particle levels with degeneracy  $d_m$ , the multiplicities for identical bosons and distinguishable particles are given by

$$g^{(B)} = \prod_m \binom{n_m + d_m - 1}{n_m}, \quad (13)$$

and

$$g^{(D)} = N! \prod_m \frac{(d_m)^{n_m}}{n_m!}, \quad (14)$$

where the product is over all values of  $m$  corresponding to occupied single-particle states (unoccupied states all contribute factors of unity).

In this section I investigate a system of 20 identical bosons in a three-dimensional trap, and compare it to a system of 20 distinguishable particles. (I do not consider interacting subsystems of particles in this section.) All possible configurations are generated by computer using the integer-partition method, and the occupation numbers from these configurations are used in Eqs. (13) or (14), along with degeneracy factors from Eq. (12), to determine appropriate multiplicities for each configuration. Counting the number of all possible states for a given system energy gives the total multiplicity necessary for calculating entropy. The ground state occupation number is calculated from the configurations and multiplicities

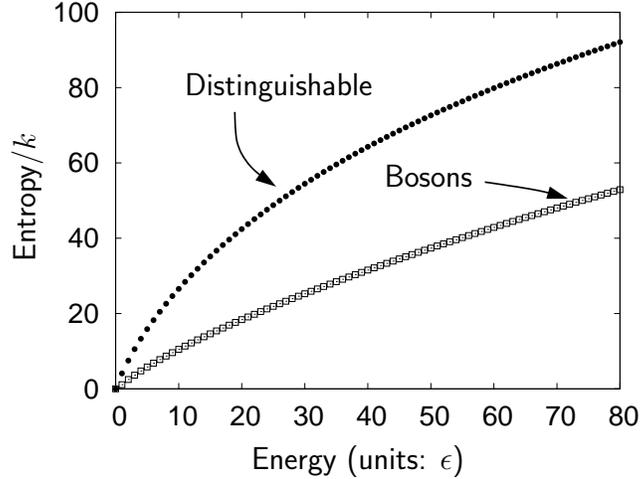


FIG. 9: Entropy as a function of system energy for 20 bosons and for 20 distinguishable particles in a three-dimensional harmonic trap.

using Eq. (11) with  $m = 0$ . Sample *Mathematica* code is included in Appendix B.<sup>13</sup>

Figure 9 shows a comparison of the entropies of the two kinds of particles as a function of the energy of the system. At high energies (and corresponding low probability of multiple occupation of any single state), the figure shows the gradual approach to the limit in which the entropy graphs have the same slope, with the entropy of the distinguishable particles being larger by the constant additive term  $\ln(20!)$ , as was discussed in Section II A.

The ground state occupation as a function of energy is illustrated in the upper graph of Fig. 10, and the ground state occupation as a function of temperature is illustrated in the lower graph. The top graph shows the expected increase in ground state occupation as the energy decreases, but it exhibits no obvious features that might indicate the onset of condensation into the ground state. In sharp contrast, the accumulation of bosons in the ground state as a function of temperature, illustrated in the lower graph, displays a relatively sharp rise below the temperature  $T = 2.5\epsilon/k$ , and the graph exhibits a change in curvature below this temperature.

Although the techniques used in this paper are limited to very small particle numbers, the results do exhibit features that can be considered small- $N$  precursors of Bose-Einstein condensation. In the limit of large particle numbers, the ground-state occupation exhibits an abrupt rise at a critical temperature,  $T_c$ , that is characteristic of a true phase transition.

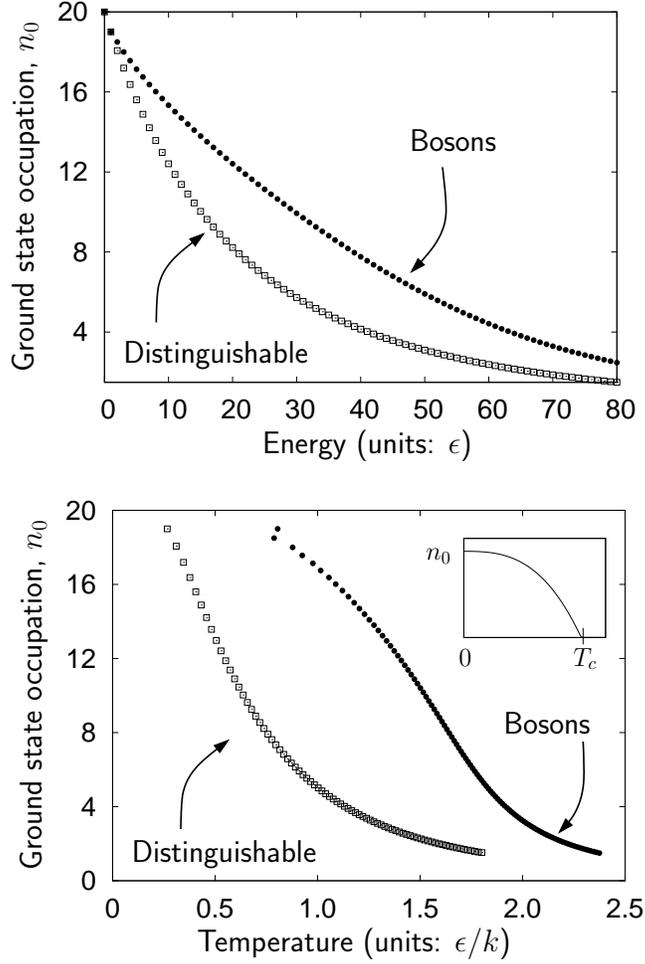


FIG. 10: Ground state occupation for 20 bosons, and for 20 distinguishable particles in three-dimensional harmonic trap. The upper graph shows the occupation as a function of energy, and the lower graph shows the occupation as a function of temperature. For comparison, the lower graph also contains an inset of a typical ground state occupation as function of temperature in the large- $N$  limit.

For comparison with the results of this paper, a typical graph of condensate fraction as a function of temperature for large  $N$  is displayed in an inset graph in Fig. 10.

Further insight into the striking difference in the shapes of the occupation-number graphs in Fig. 10 is revealed in the relationship between energy per particle and temperature that is plotted in Fig. 11. At temperatures above  $T = \epsilon/k$  for distinguishable particles, and above about  $T = 2.5\epsilon/k$  for bosons, the energy per particle increases linearly with temperature,

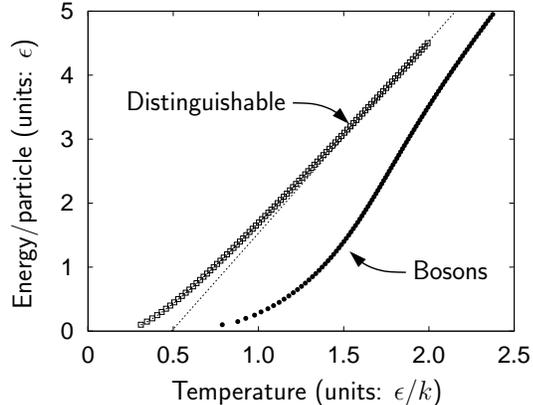


FIG. 11: Temperature as a function of energy for 20 bosons and for 20 distinguishable particles in a three-dimensional harmonic trap.

giving  $\Delta E = 3Nk\Delta T$  as expected from equipartition for a classical system of trapped particles. Below  $T = 2.5\epsilon/k$  the energy is small enough that multiply occupied states are likely. (Examination of Fig. 8 shows that there are only 10 available states with energy less than or equal to  $2\epsilon$ , and only 30 available states with energy less than or equal to  $3\epsilon$ .) When multiple occupation becomes likely, the effects of quantum statistics become evident in the multiplicity and entropy, with corresponding manifestations in the temperature. The result is that near the critical temperature, small changes in the temperature of a bosonic system result in a larger change in energy than would be predicted for the corresponding system of classical particles.

In the limit in which the trap frequency is small enough that the density of states can be treated as a continuum, and the number of particles is large, the approximate critical temperature is given by the condition  $kT_c = (2N/2.404)^{1/3}\hbar\omega$ ,<sup>14</sup> or  $kT_c \simeq 2.5\epsilon$  for the 20 particles considered in this section. This is consistent with the temperature at which the ground state occupation for bosons starts to rise in Fig. 11. It is also consistent with the results for small numbers of particles given by the numerical techniques of Ref. 15.

#### IV. DISCUSSION

Modern pedagogical treatments of introductory statistical mechanics bring to the forefront the probabilistic underpinnings of thermal physics. The study of equilibrium statistical

mechanics in a closed system is conceptually very simple: enumerate all possible states and see which one is most likely to “win.” The techniques used in this paper take advantage of this simplicity, and highlight the influence of quantum statistics on the thermal properties of a simple system. These techniques can be used to develop exercises that extend the treatment of Moore and Schroeder<sup>1</sup> for more advanced classes, and thereby enhance student understanding of the concepts of temperature, entropy, total energy, and the distribution of energy. Although the computational techniques introduced in this paper are limited to very small numbers of particles, the consequences of the quantum statistics are very evident, and the thermal properties of systems with as few as 20 particles already exhibit features characteristic of much larger systems.

### **Appendix A: Correspondence between boson and fermion configurations in one dimension**

As a demonstration of the correspondence between the occupation-number configurations of bosons and fermions in a one-dimensional harmonic potential, consider the configuration of bosons illustrated on the left in Fig. 12. To find the corresponding fermionic state, start with lowest-energy fermionic state with the same number of particles as in the bosonic configuration, i.e., the fermion configuration at temperature  $T = 0$ . (This configuration is indicated with open dots in the figure.) I have put a set of labels on all of the dots in both diagrams in order of decreasing energy — this is to facilitate the following discussion, and does not represent any distinguishability of particles. The next step is to raise the energy of each of the particles in the fermion configuration by exactly the energy of the particle with the same label in the boson configuration — particles A, B, and C are all raised by three units, and D and E are both raised by one unit. No states with double occupancy are created by this procedure, and the final energy of the fermion configuration is equal to the energy at  $T = 0$  plus the energy of the boson configuration. This procedure assigns a unique fermionic state to every state of bosons, and the process can be reversed, giving a one-to-one correspondence between states of  $N$  bosons with energy  $q\epsilon$ , and states of  $N$  fermions with energy  $q\epsilon + U_{T=0}^{(F)}$ . The multiplicities of these two sets of states must thus be the same.

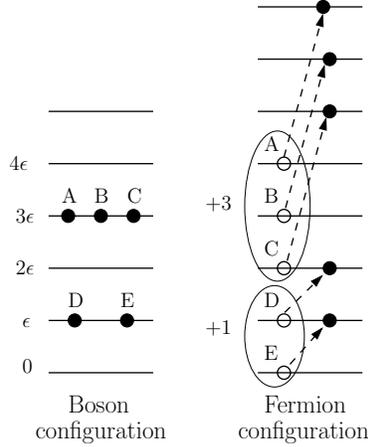


FIG. 12: Correspondence between boson and fermion configurations of particles in a one-dimensional harmonic potential.

## Appendix B: Mathematica code samples

### 1. Generating data for Figs. 3 & 4; sharing of energy in 1D traps (Section IIB)

Multiplicities for Distinguishable Particles, Bosons, and Fermions

```
OmegaD[q_,n_] := Binomial[q+n-1, q] (* Eq. 3 *)
```

```
OmegaB[q_,n_] := Length[IntegerPartitions[q, n]] (* Eq. 7 *)
```

```
OmegaF[q_,n_] := Length[IntegerPartitions[q-n(n-1)/2, n]] (* Eq. 8 *)
```

Entropies for Distinguishable Particles, Bosons, and Fermions

```
sD[q_,n_] := Log[OmegaD[q, n]]
```

```
sB[q_,n_] := Log[OmegaB[q, n]]
```

```
sF[q_,n_] := Log[OmegaF[q, n]]
```

System parameters:

```
nB = 20; (* Number of bosons *)
```

```
nD = 20; (* Number of distinguishable particles *)
```

```
u = 80; (* Total energy *)
```

Boson entropy vs. energy in bosons:

```
entropyBvqB = Table[q, sB[q, nB],{q, 0, u}];
```

Switch independ. variable to the energy in disting. particles (plotted in Fig. 3):

```
entropyBvqD =  
  Table[entropyBvqB[[i, 1]], entropyBvqB[[Length[entropyBvqB]+1-i,2]],  
        {i, 1, Length[entropyBvqB]}];
```

Distinguishable particle entropy vs. energy in distinguishable particles (plotted in Fig. 3):

```
entropyDvqD = Table[{q, sD[q, nD]},{q, 0, u}];
```

Total entropy vs. energy in distinguishable particles (plotted in Fig. 3):

```
entropyTotalvqD =  
  Table[{q, entropyBvqD[[{q+1, 2}] + entropyDvqD[[{q+1, 2}]],{q, 0, u}];
```

Boson temp. vs. energy in bosons, and vs. energy in distinguishable particles [Eq. (10)]  
(plotted in Fig. 4):

```
tBvqB = Table[i-1, 2/(entropyBvqB[[i+1,2]] - entropyBvqB[[i-1,2]])),  
             {i, 3, Length[entropyBvqD]-2}];  
tBvqD = Table[{u-tBvqB[[i,1]],tBvqB[[i, 2]]}, {i, 1, Length[tBvqB]}];
```

Distinguishable particle temperature vs. energy in distinguishable particles [Eq. (10)]  
(plotted in Fig. 4):

```
tDvqD = Table[i-1, 2/(entropyDvqD[[i+1, 2]] - entropyDvqD [[i-1, 2]]),  
             {i, 3, Length[entropyDvqD] - 2}];
```

## 2. Generating data for Fig. 7; occupation number distributions (Section II C)

### a. Distribution for bosons

Generate *Mathematica* List containing integer partitions for bosons:

```
nB = 20;      (* Number of particles *)  
q = 40;      (* Number of Energy units *)  
ipListB = IntegerPartitions[q, nB];
```

Convert integer partitions to occupation number configurations [see above Eq. (11)]:

```
configListB = Table[0, {i, 1, Length[ipListB]}, {j, 1, q+1}];  
For[i=1, i<= Length[ipListB], ++i,  
  {configListB[[i]] = BinCounts[ipListB[[i]], {0, q+1, 1}],  
  configListB[[i, 1]] = nB - Length[ipListB[[i]] ]}];
```

Calculate boson distribution by averaging over all configurations:

```
s = Sum[configListB[[i]], {i, 1, Length[configListB]}/Length[ipListB];  
distB = Table[{i-1, s[[i]]}, {i, 1, Length[s]}];
```

### b. Distribution for fermions

Generate *Mathematica* List containing integer partitions for fermions:

```
nB = 20;          (* Number of particles *)  
q = 230;         (* Number of Energy units *)  
eF0 = nF(nF-1)/2; (* Energy of fermions at T=0 *)  
qF = q - eF0;    (* Energy to be used when calculation partitions [Eq. (8)] *)  
ipListF = IntegerPartitions[qF, nF];
```

Initialize list of integer partitions with occupation numbers for  $T = 0$ :

```
configListF = Table[If[i<=nF, 1, 0], {i, 1, nF+q+eF0}, {j, 1, Length[ipListF]}];
```

Convert boson to fermion partitions. Use procedure of Appendix A. Start with most energetic particle at  $T = 0$ , and bump it up by the largest energy in the integer partition. Continue moving down ladder of energies as illustrated in Fig. 12:

```
For[i=1, i<= Length[configListF], ++i, {  
  For[j=1, j<= Length[ipListF[[i]]], j++, {configListF[[i, nF + 1 - j]] = 0,  
  configListF[[i, nF+1-j+ipListF[[i, j]] ] ] = 1}}];
```

Calculate fermion distribution by averaging over all configurations:

```
s = Sum[configListF[[i]], {i, 1, Length[configListF]}/Length[ipListF];  
distF = Table[{i-1, s[[i]]}, {i, 1, Length[s]}];
```

### 3. Generating data for Figs. 9 & 10; particles in a 3D trap (Section III)

Multiplicities for  $n$  distinguishable particles ( $\Omega_{\text{Dsingle}}$ ) or bosons ( $\Omega_{\text{Bsingle}}$ ) in a single occupation-number configuration contained in list  $ll$ , [Eqs. (13) & (14)]:

```

OmegaDsingle[n_, ll_] := Factorial[n] Product[((m+1)(m+2)/2^ll[[m+1]]/
  Factorial[ll[[m+1]]], {m, 0, Length[ll]-1}]
OmegaBsingle[n_, ll_] := Product[Binomial[ll[[m+1]] + (m+1)(m+2)/2 - 1, ll[[m+1]]],
  {m, 0, Length[ll]-1}]

```

System parameters:

```

n = 20;      (* Number of particles *)
q = 30;      (* Number of units of energy *)
ex0 = 0;     (* Initialize expected value of gnd. st. occupation *)
OmegaT = 0;  (* Initialize total multiplicity *)

```

Generate list of integer partitions for  $n$  particles with  $q$  units of energy. Convert each partition to an occupation-number configuration. Calculate multiplicity of configuration. Determine contribution of partition to ground state occupation:

```

ipList = IntegerPartitions[q, n];      (* Create list of integer partitions *)
For[i=1, i<= Length[ipList], ++ii,
  {configList = BinCounts[ipList[[i]], {0, q+1, 1}],
  configList[[1]] = n - Length[ipList[[i]]],
  Omega1 = OmegaBsingle[n, configList]      (* Multiplicity of configuration *),
  ex0 += Omega1*configList[[1]]      (* Increment gnd. st. occupation, Eq. (11) *),
  OmegaT += Omega1      (*Increment total multiplicity *)}]
Print["Entropy = ", Log[OmegaT]/N]
Print["Ground state occupation = ", ex0/OmegaT/N]

```

Output:

```

Entropy = 25.2562
Ground state occupation = 9.93635

```

## Acknowledgments

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<sup>1</sup> T. A. Moore and D. V. Schroeder, “A different approach to introducing statistical mechanics,” *Am. J. Phys.* **65**, 26–36 (1997).

<sup>2</sup> T. A. Moore, *Six Ideas That Shaped Physics, Unit T: Some Processes are Irreversible*, 2<sup>nd</sup> ed. (McGraw-Hill, Boston, 2003).

<sup>3</sup> D. V. Schroeder, *An Introduction to Thermal Physics* (Addison-Wesley, San Francisco, 2000).

<sup>4</sup> F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, “Theory of Bose-Einstein condensation in trapped gases,” *Rev. Mod. Phys.* **71**, 463–512 (1999).

<sup>5</sup> C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2001).

<sup>6</sup> D. J. Griffiths, *Introduction to Quantum Mechanics*, 2<sup>nd</sup> ed. (Pearson Prentice Hall, Upper Saddle River, NJ, 2005), Problem 5.23.

<sup>7</sup> See problems 7.10, 7.16, and 7.17 in Ref. 3.

<sup>8</sup> The enumeration of integer partitions is a standard function in commercial software packages like *Mathematica* and *Maple*. Examples of open-source routines for enumeration of integer partitions can be found in the complete mathematical software system *Sage* (<http://www.sagemath.org/>), the Python library for symbolic mathematics, *SymPy* (<http://www.sympy.org/>), and in individual functions for inclusion in Python code (<http://code.activestate.com/recipes/218332-generator-for-integer-partitions/>). All calculations in this paper have been done in both *Mathematica* and Python, but because the state of open-source software is rapidly evolving, examples in this paper are given in *Mathematica* versions.

<sup>9</sup> J. Arnaud, J. M. Boé, L. Chusseau, and F. Philippe, “Illustration of the Fermi-Dirac statistics,”

Am. J. Phys. **67**, 215–221 (1999).

- <sup>10</sup> M. Ligare, “Classical thermodynamics of particles in harmonic traps,” Am. J. Phys. **78**, 815–819 (2010).
- <sup>11</sup> 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 amongst themselves and permuting the dividers amongst themselves does not produce a new arrangement. Thus the total number of states is  $(m + 2)(m + 1)/2$ .
- <sup>12</sup> A derivation of the general multiplicity formulas can be found in Section 5.4.2 of Ref. 6.
- <sup>13</sup> The determination of the integer partitions and evaluation of Eqs. (13) & (14) requires considerable computer time for the larger values of the energy considered in this paper. Numerical tabulations of the results are available from the author.
- <sup>14</sup> V. Bagnato, D. E. Pritchard, and D. Kleppner, “Bose-Einstein condensation in an external potential,” Phys. Rev. A **35**, 4354–4358 (1987).
- <sup>15</sup> M. Ligare, “Numerical analysis of Bose-Einstein condensation in a three-dimensional harmonic oscillator potential,” Am. J. Phys. **66**, 185–190 (1998).