Calculating and visualizing the density of states
for simple quantum mechanical systems

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Abstract

We present a graphical approach to understanding the degeneracy, density of states, and cumulative state number for some simple quantum systems. By taking advantage of basic computing operations we define a straightforward procedure for determining the relationship between discrete quantum energy levels and the corresponding density of states and cumulative level number. The density of states for a particle in a rigid box of various shapes and dimensions is examined and graphed. It is seen that the dimension of the box, rather than its shape, is the most important feature. In addition, we look at the density of states for a multi-particle system of identical bosons built on the single-particle spectra of those boxes. A simple model is used to explain how the \( N \)-particle density of states arises from the single particle system it is based on.

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I. INTRODUCTION

The concept of the density of states (DOS) is used in many areas of physics. For example, it is important for reaction rates in nuclear physics, the calculation of specific heat capacities, black-body radiation, phonon spectra, and so on. The DOS arises naturally and early in statistical physics. To calculate average quantities in statistical physics, one could do an integral over phase space, but this is typically very complex. The alternative is to express the variable of interest in terms of the energy of the system. The volume element in phase space is replaced by a weighting factor in an energy integral, which is often much easier to work with. This weighting factor is the density of states and is the subject of this paper.

Consider the problem of calculating $\langle f \rangle$, the expected outcome of a measurement of some physical quantity $f$. If you know the allowed quantum states of the system and can calculate $f_i$, the value of $f$ in the $i$th state, then $\langle f \rangle = \sum_i f_i P_i$, where $P_i$ is the probability of the system being in the $i$th state. This is sometimes referred to as a sum over microstates. It is often easier to write $f$ as a function of energy and perform a sum over the allowed energies. We then have $\langle f \rangle = \sum_i f(\epsilon_i) P(\epsilon_i)$, where the probability of the system being on the energy level $\epsilon$ is given by $P(\epsilon) = d_\epsilon \frac{e^{-\beta \epsilon}}{Z}$. Here $Z = \sum_j e^{-\beta \epsilon_j}$ is the partition function, $\beta = \frac{1}{kT}$, and $d_\epsilon$ is the degeneracy of the level or number of states with energy $\epsilon$. If the system has an energy $\epsilon$, then each of these $d_\epsilon$ states is equally likely. Now, for our expected value of $f$ we have

$$\sum_i f_i P_i \rightarrow \sum \epsilon d_\epsilon f(\epsilon) P(\epsilon).$$ (1)

In a system where $\epsilon$ is continuous (or effectively so), the sum becomes an integral and $d_\epsilon$ is replaced by $g(\epsilon)$—the DOS—a measure of how many states there are in a small range $d\epsilon$ around $\epsilon$. The DOS $g(\epsilon)$ is no longer an absolute number of states; it is now a weighting factor in an integral over energy. We must be careful here because $g(\epsilon)$ is often confused with the level density; indeed, the terms are often used interchangeably. We use the term “level” to mean an allowed value of energy and the DOS is the level density multiplied by a degeneracy factor.

In this paper we present a procedural approach to obtain the DOS for systems that arise in modern physics and statistical mechanics courses. In the next section we apply the procedure to a single particle in a rigid box. In Sec. III the procedure for visualizing the DOS is summarized and the effect of the shape of the box on the DOS is examined. Section IV
addresses systems of \(N\) noninteracting bosons, where \(N\)-particle spectra are calculated and the dependance of their DOS on \(N\) is compared with a simple model.

II. VISUALIZING THE DENSITY OF STATES FOR A PARTICLE IN A BOX

The particle in a box is one of the first examples students encounter in quantum mechanics. It is simple enough to solve from scratch by hand and exhibits much of the salient nonclassical behavior. Furthermore, it serves as a basic template for a host of interesting topics: scattering, double-well potentials, and perturbation theory to name a few. We will discuss the DOS in the context of a particle in a box of various dimensions. First we introduce the concept of degeneracy via numerical results for the spectrum. This leads naturally to the idea of a cumulative state number from which the DOS naturally follows. Then an analytic approach to obtaining the DOS is presented.

We start with a (nonrelativistic) particle of mass \(M\) inside a box. We assume the box is rigid, by which we mean that the potential energy is infinite outside the box and zero inside the box. In a one-dimensional box of length \(L\) the energy levels are given by \(\epsilon_n = \epsilon_0 n^2\), where \(\epsilon_0 = \frac{\pi^2\hbar^2}{2ML^2}\) and the quantum number \(n\) is an integer. In a two-dimensional square box with sides of length \(L\), the energy levels are given by \(\epsilon_n = \epsilon_0 (n_x^2 + n_y^2)\), where \(n_x\) and \(n_y\) are the quantum numbers corresponding to the two spatial dimensions. In the three-dimensional case of a cubical box of side length \(L\), we have \(\epsilon_n = \epsilon_0 (n_x^2 + n_y^2 + n_z^2)\).

It is natural to associate each quantum number with a number line and each integer value with a point along this line. In two dimensions the pair of quantum numbers defines a plane or two-dimensional space called \(n\)-space. This space could also be called momentum space by using the identity \(p_x = \hbar k_x = n_x\pi\hbar/L\). The energy depends on the sum of the squares of \(n_x\) and \(n_y\). One way of thinking about the distribution of these energies is to locate them in \(n\)-space. Using the horizontal axis for \(n_x\) and the vertical axis for \(n_y\), we can write all energy values at their corresponding grid points. This is done in Fig. 1 where at each pair of quantum numbers \((n_x, n_y)\) the energy is written (in units of \(\epsilon_0\)); for example, at grid points \((n_x, n_y) = (1, 3)\) and \((3, 1)\) we see a “10.” Suppose \(n\) is the radius of a circle in \(n\)-space such that \(n^2 = n_x^2 + n_y^2\). Rewriting the energy as \(\epsilon_n = \epsilon_0 n^2\) we see that in \(n\)-space a given energy (in units of \(\epsilon_0\)) corresponds to a circle of radius \(\sqrt{\epsilon/\epsilon_0}\). (The radius \(n\) is related to the magnitude of the momentum vector by \(|\vec{p}| = n\pi\hbar/L\). In Fig. 1 the circles
corresponding to energies “36” and “65” are shown as dotted curves with radii \( \sqrt{36} = 6 \) and \( \sqrt{65} \approx 8 \), respectively.

When energies correspond to more than one independent state we say they are “degenerate.” If we make a list of all energies corresponding to the various quantum numbers \((n_x, n_y)\) and order them by energy, we can make a plot of the “number of states with energy \( \epsilon \)” vs \( \epsilon \). This quantity is \( d_\epsilon \), the degeneracy of the energy \( \epsilon \), and for discrete spectra it is an integer. A plot of \( d_\epsilon \) is a series of spikes, of height \( d_\epsilon \), at each allowed \( \epsilon \).

To further illustrate this idea, imagine a hypothetical single-particle spectrum where the lowest nine energies are \( \{\epsilon\} = \{2, 2, 3, 3, 3, 5, 5, 5\} \). We have plotted \( d_\epsilon \) vs \( \epsilon \) for this system in Fig. 2 (upper left panel). At this point it is helpful to introduce the cumulative state number \( N(\epsilon) \), defined as the number of states with energy \( \leq \epsilon \); its graph is a staircase where each step has a height \( d_\epsilon \) and a width determined by the gap to the next energy (lower left panel of Fig. 2). In other words, given an ordered list of energies \( \{\epsilon_i\} \) we have \( N(\epsilon) = i \) for \( \epsilon_i < \epsilon < \epsilon_{i+1} \).

A plot of the spikes \( d_\epsilon \) gives a visual measure of the degeneracies of the energies. These degeneracies are quite delicate in the sense that most perturbations to the potential will break them and the picture for \( d_\epsilon \) will change dramatically. Each \( d_\epsilon \)-high spike will turn into a cluster of \( d_\epsilon \) separate spikes, each one unit high. The spacing of the spikes will be determined by the strength of the perturbation. The corresponding change in \( N(\epsilon) \) is that each step in the unperturbed system that was \( d_\epsilon \) high will now become a series of short steps, each one unit high (upper and lower right panels of Fig. 2). It is hoped that Figs. 1 and 2 will be a useful starting point for student discussion.

A smooth DOS function \( g(\epsilon) \) is useful because at higher energies one is interested in the number of states in an interval, or the density of spikes along the \( \epsilon \)-axis. The DOS and cumulative state number are related by \( g(\epsilon)d\epsilon = dN(\epsilon) \), so the DOS is recognized as the slope of \( N(\epsilon) \). We must be careful here because the slope of a staircase is infinite at each step, so we mean slope in an averaging sense.

To get \( g(\epsilon) \) from \( N(\epsilon) \) we can take a numerical derivative using a finite difference scheme,

\[
g(\epsilon) = \frac{dN(\epsilon)}{d\epsilon} = \frac{N(\epsilon + \delta\epsilon/2) - N(\epsilon - \delta\epsilon/2)}{\delta\epsilon}.
\]

(2)

It is worth saying explicitly that if the energies are put into bins of width \( \delta\epsilon \), with center \( \epsilon \), then \( g(\epsilon) = \) (number of states in bin)/(width of bin).
Now that we have a numerical representation for $g(\epsilon)$, we would like to get an analytic expression for $g(\epsilon)$ that is valid for the statistical region where the DOS is large and well approximated by a smooth function. We will do this for the rigid box potentials where $\epsilon = n^2$ (in units of $\epsilon_0$). In $n$-space the states with energy in an interval $d\epsilon$ centered on $\epsilon$ correspond to a set of points in a spherical shell of thickness $dn$ with all-positive coordinates. In Fig. 1 the number of states between the quarter circles of radius $n$ and $n + dn$ is proportional to the area of the curved band. This result is an approximation, because $n_x$ and $n_y$ are discrete and there are fluctuations, but we will see that this is a good approximation nevertheless. The number of states is the “volume” of this shell but by definition it is also $g(\epsilon) d\epsilon$, so in 2-D we have $g(\epsilon) d\epsilon = (1/2)\pi n \, dn$. If $n(\epsilon)$ is a smooth function we can write $g(\epsilon) = (1/2)\pi n(\epsilon) \, dn/d\epsilon$. Using $n(\epsilon) = \sqrt{\epsilon}$ and $dn/d\epsilon = 1/(2\sqrt{\epsilon})$ we see that the DOS is constant: $g(\epsilon) = \pi/4$. Since the DOS is the slope of $N(\epsilon)$, the function $N(\epsilon)$ should be well approximated by the straight line $N(\epsilon) = (\pi/4)\epsilon$, as shown in Fig. 3. The numerical results are convincing, particularly where the energy range increases and the fluctuations about the smooth functions get smaller (see Fig. 4).

For a particle in a 3-D rigid box with sides $L_x$, $L_y$, and $L_z$, we will be working with a 3-D $n$-space and again each point $(n_x, n_y, n_z)$ corresponds to an allowed value of energy where $\epsilon = (\pi^2\hbar^2)/(2M)[(n_x/L_x)^2 + (n_y/L_y)^2 + (n_z/L_z)^2]$. For a cube of side length $L$ we have $\epsilon = (\pi^2\hbar^2)/(2ML^2)n^2 = \epsilon_0 n^2$ with $n^2 = (n_x^2 + n_y^2 + n_z^2)$. Now the appropriate construction to get the DOS is a shell of thickness $dn$ and radius $n$ in the positive octant of a sphere, which leads to $g(\epsilon) = (1/2)\pi n^2 \, dn/d\epsilon$. Again, using $n(\epsilon) = \sqrt{\epsilon}$ and $dn/d\epsilon = 1/(2\sqrt{\epsilon})$, we see that the DOS now has the form $g(\epsilon) = (\pi/4)\sqrt{\epsilon}$ and $N(\epsilon) = (\pi/6)\epsilon^{3/2}$. In Figs. 5 and 6 we compare the numerical results with these smooth functions for different energy ranges. Again as the energy increases, the numerical fluctuations get smaller.

We remark here that if we had $N$ non-interacting independent particles in a rigid cube, then the total energy would be the sum of the individual energies, and this sum could be related to the surface [xx do you mean volume? xx] of a $D = 3N$-dimensional hypersphere. This problem is similar to the case of a single particle in a rigid box in a $D$-dimensional space. We would need to discuss the volume of a sphere of radius $R$ in $D$-dimensions, denoted by $V_D$ and given by

$$V_D = \frac{\pi^{D/2}}{\Gamma(D/2 + 1)} R^D = C_D R^D. \tag{3}$$
Here, $\Gamma(D + 1) = D!$, giving $C_2 = \pi$ and $C_3 = \frac{4\pi}{3}$ as expected. The surface area of this $D$-sphere is given by $S_D = D C_D R^{D-1}$. Where before we were concerned with the length of a quarter circle of radius $n$ ($D = 2$) and the area of an octant of a sphere of radius $n$ ($D = 3$), we now have the area of the positive portion of the $D$-dimensional sphere, given by $(1/2^D)S_D$ (the need for $n_x, n_y \ldots$ to be positive gives a factor of $1/2$ for each dimension). The cumulative state number is given by the volume of phase space enclosed by the boundary $n = \sqrt{\epsilon}$,

$$N(\epsilon) = \frac{1}{2D} \frac{\pi^{D/2}}{\Gamma(D/2 + 1)} \epsilon^{D/2},$$

and differentiation gives

$$g(\epsilon) = \frac{1}{2^{D+1}} D \frac{\pi^{D/2}}{\Gamma(D/2 + 1)} \epsilon^{(D/2)-1}.$$  

The forms of $N(\epsilon)$ and $g(\epsilon)$ for some representative $D$ are given in Table II. Later we will see that the DOS for one particle in $D$ dimensions is proportional to the DOS of $D$ particles in one dimension, so long as the particles do not interact.

III. PROCEDURE FOR CALCULATING AND VISUALIZING THE DENSITY OF STATES

For any quantum-mechanical system we can determine the cumulative state number and the corresponding density of states using the following procedure:

1. Solve the relevant quantum-mechanical problem to get a list of the energies of the system. (This can be an analytical expression or a list of energies obtained numerically.)
2. Sort the list of energies to get a set $\{\epsilon_1, \epsilon_2, \epsilon_3, \ldots, \epsilon_n\}$ up to some maximum energy $\epsilon_{\text{max}}$.
3. Create the cumulative state number $N(\epsilon)$ by making the set $\{\epsilon_1, 1\}, \{\epsilon_2, 2\}, \{\epsilon_3, 3\}, \ldots, \{\epsilon_n, n\}$.
4. Find the DOS by taking the numerical derivative of the cumulative state number, as in Eq. (2). Choose a window size and locate the window so that its center is at $\epsilon$. The value of $g(\epsilon)$ is the number of energies that are within that window divided by the window size. Evaluate this for all locations of the window, and you now have a list of ordered pairs $\{\epsilon, g(\epsilon)\}$. 

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As supplementary materials we include a MATLAB program used to obtain Figs. 5 and 6 with appropriate modifications the program can be used to produce Figs. 3 and 4.

We will apply this procedure to calculate and visualize the DOS for particles in rigid boxes with various geometries.

### A. Cubical box

We first will consider a cube of side length $L$.

**Step 1:** The energies are $e = (\pi^2\hbar^2)(n_x^2 + n_y^2 + n_z^2)/(2MV^{2/3})$, where we have used $L^2 = V^{2/3}$ with $V$ the volume of the box. If we set $(\pi^2\hbar^2)/(2M) = 1$ and $V = 1$, then the energies are all integers.

**Step 2:** Using Mathematica we determined the lowest 15,954 energy levels. To calculate the energies we need all the triplets $\{n_x, n_y, n_z\}$ within the sphere of radius $n_{\text{max}}$ in $n$-space. We made a list of $n_x^2 + n_y^2 + n_z^2$ with $1 \leq n_x \leq n_{\text{max}}$, $1 \leq n_y \leq \sqrt{n_{\text{max}}^2 - n_x^2}$, and $1 \leq n_z \leq \sqrt{n_{\text{max}}^2 - n_x^2 - n_y^2}$; this list had all the energies $e \leq n_{\text{max}}^2$ (we chose $n_{\text{max}} = 32$). This is a very degenerate system—of the 15,954 energy levels only 818 are distinct and the average degeneracy is 19.50. As seen in Fig. 6 for $e \sim 1000$ we have $d_e \sim 60$. Specifically, the energies from 933–954, along with their degeneracies, are given by: $\{e, g(e)\} = \{933, 24\}, \{934, 39\}, \{936, 24\}, \{937, 27\}, \{938, 24\}, \{940, 6\}, \{941, 66\}, \{942, 18\}, \{944, 9\}, \{945, 48\}, \{946, 24\}, \{947, 15\}, \{948, 18\}, \{949, 12\}, \{950, 63\}, \{952, 12\}, \{953, 45\}, \{954, 42\}.

**Step 3:** Plot $N(e)$. It is instructive to construct the set of points for the plot explicitly using the list of energies. There are only 818 steps, one for each value of $e$. The height of the step at some energy $e$ is $d_e$, the degeneracy, so this staircase has steps that get higher with energy (e.g., the step at $e = 950$ has a height of 63).

**Step 4:** While calculating the DOS, the window size needs to be adjusted to give a reasonable-looking graph. If the window is too small, the graph will look noisy; if it is too big, the graph may appear too coarse. We use trial and error to select an appropriate window size. We have included code in the online supplement in which the reader can select the maximum energy and window size and generate plots like Figs. 5 and 6.

Figures 5 and 6 display $d(e)$, $N(e)$, and $g(e)$ for this system. Again, it is evident that the agreement between the analytic result and the explicit counting of energies improves as the energy interval increases.
B. Rectangular box

The rigid rectangular box is a straightforward adjustment to the cubical case and gives us a look at a non-degenerate spectrum. In order to remove the degeneracies from the single-particle spectrum that exist in the cubical case, we will make the sides of the box have incommensurate lengths. The choice $L_x \neq L_y \neq L_z$ with $L_x = 1$, $L_y = 2/e$, and $L_z = e/2$ gives us a box of unit volume and a non-degenerate spectrum.

Step 1: The energies are $\epsilon = (\pi^2 \hbar^2)[(n_x/L_x)^2 + (n_y/L_y)^2 + (n_z/L_z)^2]/(2M)$. Again, the obvious choice for our energy scale is to set $\pi^2 \hbar^2/(2M) = 1$.

Step 2: This time we use a different method than in the cubical case. The sphere in $n$-space corresponds to an ellipse in phase space. This is a nice illustration of the difference between these abstract spaces. The method used was an exhaustive calculation of all the energies corresponding to the points $1 \leq n_x \leq n_{\text{max}}$, $1 \leq n_y \leq n_{\text{max}}$, and $1 \leq n_z \leq n_{\text{max}}$, after which we selected $\epsilon \leq (2n_{\text{max}}/e)^2$. The fact that $n_y$ and $n_z$ are multiplied by a factor of 0.74 and 1.36 respectively ensured that the sphere radius of $\sqrt{2/e}n_{\text{max}}$ was enclosed in the ellipse in phase space, and we had a complete set of energies. Although the method is inefficient, it has the advantage of transparency.

All the energies in this system are unique. In order to have degeneracies we would need two sets of integers, $\{n_x, n_y, n_z\}$ and $\{m_x, m_y, m_z\}$, such that $n_x^2 + e^2n_y^2/4 + 4n_z^2/e^2 = m_x^2 + e^2m_y^2/4 + 4m_z^2/e^2$, which is impossible as $e$ is transcendental. The lowest 62,440 energies of the system were calculated.

Step 3: The cumulative state number $\mathcal{N}(\epsilon)$ consists of steps of unit height, though the widths of the steps (level spacings) vary. For our rectangular box there are 41,435 steps, one for each energy. A plot of $d\epsilon$ vs $\epsilon$ is a series of horizontal spikes of height 1.

Step 4: In Fig. 7 we show $g(\epsilon)$ and $\mathcal{N}(\epsilon)$ for this system. [xx Fig. 7 has a label of $\rho$ which has not been defined. xx]

[xx LEFT OFF HERE xx]

C. Spherical box

The energies for a rigid sphere of radius $R$ are $\epsilon_{\text{ln}} = \hbar^2 k_{\text{ln}}^2/(2MR^2)$, where $k_{\text{ln}}$ is the $n$th zero of $j_l(r)$, the $l$th spherical Bessel function. Each $\epsilon_{\text{ln}}$ has a degeneracy of
2l + 1. It is easy to confuse $j_l(r)$ with $J_l(r)$, the ordinary Bessel function, also known as the Bessel function of the first kind; the two are related by $j_l(r) = \sqrt{\pi/(2r)}J_{l+1/2}(r)$. Note that the $n$th zero of $J_l(r)$ is written $K_{ln}$. Mathematica has a useful add-on called NumericalMath\textbackslash{}BesselZeros\textbackslash{} that lists the zeros of the various Bessel functions. In Sec. VII we define the problem of the rigid cylindrical box, where the energies are proportional to $K_{ln}^2$, so to avoid confusion we provide the following check: the first three zeros of $J_0(r)$ are \{2.4048, 5.5201, 8.6537\}, and the first three zeros of $j_0(r)$ are \{3.9374, 7.8748, 11.8122\}. Actually, the distinction between $K_{ln}$ and $k_{ln}$ is not important as far as $g(\epsilon)$ goes for the sphere and the cylinder, as the two sets of zeros are interspersed.

Step 1: The role of $\pi$ in the energies of the rectangular wells is taken over by the $k_{ln}$. In the rectangular box the zeros of the sine function are multiples of $\pi$. This allowed us to factor it out and choose the energy scale to be in units of $\hbar^2\pi^2/(2M)$ for the rectangular boxes. Now we have $\epsilon = \hbar^2(k_{ln}/R)^2/(2M)$. To compare with the square wells we use an energy scale with $\hbar^2\pi^2/(2M) = 1$; in these units, $\epsilon_{ln} = [k_{ln}/(\pi R)]^2$. Also, if the volume of the box is to be unity, then $R = [3/(4\pi)]^{1/3}$, so finally we have $\epsilon_{ln} = k_{ln}^2/(3\pi^2/4)^{2/3}$. This is the spectrum we will compare to those of the rectangular and cubical boxes.

Step 2: We calculated all energies with $k_{ln} < 95$. To ensure a complete set, we used the brute force method and calculated all the triplets \{k_{ln}, l, n\} with $0 \leq l \leq 95$ and $1 \leq n \leq 95$, sorted these 9,120 numbers, and selected the first 95. Making the triplets as opposed to just the list of $k_{ln}$ made it easy to accommodate the $2l + 1$ degeneracy when making the final spectrum.

Steps 3 & 4: See Fig. 7

D. Weyl’s theorem

It is clear from Sec. II and Fig. 7 that the general trend for the three boxes we examined is $N(\epsilon) = \alpha \epsilon^\beta$. The energy exponent does not vary much with the shape of the box. A plot of $\ln N(\epsilon)$ vs $\ln \epsilon$ illustrates this nicely, as shown in Fig. 8. The deviation from the straight line occurs only at low energies, where the shape of the box matters. Using Mathematica we performed linear fits to the log-log plots and obtained the results shown in Table II.

If the box is sufficiently large, a particle in a rigid box should not be aware of the particular shape of the box, so long as $\lambda^D \ll V$, where $V$ is the volume of the box. Here, $\lambda = 2\pi/|\vec{k}|$ is
the deBroglie wavelength ($|\vec{p}| = \hbar|\vec{k}|$) and $D$ is the dimension of the space. A slow particle will know about the edge, as it has a long wavelength, and a fast particle or high-energy state will not be sensitive to the shape because its wavelength is small. This is the content of Weyl’s theorem, which can be paraphrased as “high energy eigenvalues of the wave equation are insensitive to the shape of the boundary.” A nice account of the origin of the theorem is given by Kac, and an explicit proof at the level of this paper for the case of the cylinder and sphere is given by Lambert.

IV. $N$ PARTICLES: STATISTICAL MECHANICS

Statistical mechanics can be introduced by analyzing a model system of $N$ non-interacting particles on a single-particle spectrum, often chosen as a set of equally-spaced levels. This is a valuable pedagogical tool for exploring the statistical distributions for classical particles, identical bosons, and identical fermions. This type of model is rich with subtleties: the particles not only don’t see each other beyond obeying the Pauli exclusion principle if they are identical fermions, but their presence has no influence on the energies of the levels they fill. Real particles, on the other hand, have interactions, so how does this model give useful results? One can think of the effect of all the other particles as being a smooth mean field that can be modeled as a potential for that single particle. Another subtlety is the robustness of the spectra of these $N$-body systems: they are very insensitive to the details of the single-particle spectrum upon which they are built, depending only on its DOS.

We made a simple model of the the $N$-particle system to serve as a starting point for students to explore what happens to the DOS as $N$ increases, and to illustrate that the DOS of many-body systems like this are insensitive to the details of the single-particle spectra they are based on. In this section $E$ is used for the total energy of the system, reserving $\epsilon$ for the single-particle energy. Subscripts will be used on $g$ and $N$ to indicate the number of particles in the system, so $g_7(E)$ is the DOS for a system of seven particles. We compared $N$-particle systems built on four distinct single-particle spectra: the square, rectangular, and spherical 3-D boxes, and a spectrum with a specified DOS but random levels. A simple analytical model for the DOS is presented and compared with the numerical results. The focus is on the relationship between the original single-particle energies that the $N$ particles populate and the resulting $g_N(E)$. The model demonstrates that $g_N(E)$ depends on the
density of the single-particle spectrum, as opposed to the details of the energies themselves. This is why we can replace the exact single-particle energies (zeros of Bessel functions, etc.) with any set of numbers as long as they have the same range and density.

Using a simple algorithm, the spectrum of \( N \) identical bosons on a set of single-particle energies \( \{\epsilon_i\} \) was calculated. The range of energies was \( 0 \to E_{\text{max}} \), with \( E_{\text{max}} \) limited only by computational power and user patience. The choice of bosons avoided the subtleties of Fermi statistics. The algorithm is best illustrated with an example. Let’s look at identical bosons on the single-particle energies of the rigid cube in three dimensions. First we make a list of the single-particle-state energies: \( \{\epsilon_i\} = \{3, 6, 6, 6, 9, 9, 9, 11, 11, 11, 12, 14, 14, \ldots \} \). We choose \( E_{\text{max}} = 53 \) so the list includes the first 140 states. This means that we are guaranteed to have a complete list of energies up to \( E = 53 \). For our purposes an \( N \)-particle state is a list of occupied single-particle states, so \((4, 5, 5, 27)\) is a four-particle state with a particle in state 4, two particles in state 5, and a particle in state 27. Now list the indices of all possible one-particle states: \( \{(i)\} = \{(1), (2), (3), \ldots, (140)\} \); the energy of state \((i)\) is \( \epsilon_i \). Next list the index pairs of all possible two-particle states: \( \{(i, j)\} = \{(1, 1), (1, 2), (1, 3), \ldots, (140, 140)\} \), sort them and drop duplicates; the energy of the state \((i, j)\) is \( \epsilon_i + \epsilon_j \). Drop all states with \( E > 53 \) as you are only guaranteed a complete set of energies for \( E \leq 53 \). In general, list all possible \( N \)-particle states, sort them, drop duplicates, and sum the corresponding single-particle energies. Once you have these spectra you can use the procedure in Sec. III to get \( g_N(E) \) and \( \mathcal{N}_N(E) \).

Systems based on a random single-particle spectrum were included for comparison with those based on the rigid boxes because this removed the role of geometry. The distribution of the random numbers was such that the DOS was \( g(\epsilon) = (\pi/4)\epsilon^{1/2} \); this was accomplished by taking a set \( \{x_i\} \) of 500 random numbers uniformly distributed on the interval \([0, 1]\), sorting them, raising them to the power of \( 2/3 \), and multiplying them by \([(6/\pi)500]^{2/3} \). The logic behind this is worth mentioning. Given a set of numbers \( \{x\} \) with a distribution \( f(x) \), we can make a function \( y(x) \) such that the set \( \{y(x)\} \) has a distribution \( \alpha y^\beta \) by noting that \( f(x) \, dx = \alpha y^\beta \, dy \). In our case \( f(x) = 1 \), and we have \( dy/dx = (1/\alpha)y^{-\beta} \) so that \( y(x) = [(\beta + 1)/\alpha]^{1/(\beta+1)} x^{1/(\beta+1)} \).

All of these systems had a cumulative state number of the form \( \mathcal{N}_N(E) = \alpha E^\beta \), with both \( \beta \) and \( \ln \alpha \) being linear in \( N \). In Fig. [9 we show \( \mathcal{N}_N(E) \) vs \( E \) [xx Fig. 9 actually plots vs \( \epsilon \) instead of \( E \). Please correct wording as necessary. xx] for \( N \) particles on the single-particle
energies of a spherical well, while Figs. 10 and 11 show graphs of $\beta$ and $\ln \alpha$ as functions of $N$ for the various systems we examined. The values of $\alpha$ and $\beta$ for the random spectra were based on 100 separate single-particle spectra.

To compare with the theory, we used $g_1(\epsilon) = 0.40\epsilon^{1/2}$. [xx I don’t understand why this sentence is here. Should it be part of the next paragraph? xx]

Given a single-particle spectrum with a one-particle DOS $g_1(E)$, we can obtain a naive expression for the $N$-body density of states $g_N(E)$ iteratively. The density of $N$-body states with energy $E$ is a product of the density of $(N-1)$-body states with energy $E'$ and one-body states with energy $E - E'$, or

$$g_N(E) = \int_0^E g_{N-1}(E')g_1(E - E') dE'.$$

This expression double-counts some states. Suppose we add to the three-particle state $\{n_1, n_2, n_3\} = \{3, 17, 17\}$ a fourth particle in state 24; then $E = \epsilon_3 + 2\epsilon_{17} + \epsilon_{24}$, and there is a contribution to the integral in Eq. (6) from $g_1(\epsilon_{24})g_3(\epsilon_3 + 2\epsilon_{17})$. However, we can get to the same state by adding a particle in state 17 to the three-particle state $\{n_1, n_2, n_3\} = \{3, 17, 24\}$, and this gives a contribution to the integral in Eq. (6) from $g_1(\epsilon_{17})g_3(\epsilon_3 + \epsilon_{17} + \epsilon_{24})$. This is the origin of the double counting and its effect is to increase the number of states by a number close to $N$ at high energies, where the occupancies of the single-particle states are low. We did not fix this problem. When iterating Eq. (6) we need the following result for integer $n$ and $m$:

$$\int_0^E (E')^n (E - E')^m dE' = \frac{n!m!}{(n + m + 1)!}E^{n+m+1}.$$  

Table III gives several examples of the DOS for $N$ bosons based on single-particle spectra with level density $g_1(E) = E^b$, for $b = -1/2, 0, 1/2, 1$, corresponding to a box in 1, 2, 3, and 4 dimensions.

Immediately we see some trends. The DOS for one boson in a $p$-dimensional rigid box, Eq. (5), is the same as that of $p$ bosons in a one-dimensional rigid box [xx You see this by comparing what to what? xx]. This result is a by-product of separation of variables in the Cartesian case. However, if we put the particles into a spherical box, we also have separation of variables, but they [xx What is “they” referring to? xx] are not equivalent. The $a$ in $g_1(E) = aE^b$ changes, but the powers of $g_N(E)$ do not [xx It is not clear where this result comes from. xx]. In general, upon iterating Eq. (6), for $N$ bosons on a single-particle
spectrum with \( g_1(E) = aE^b \), we get

\[
g_N(E) = \frac{b^N}{(Nb+N-1)!} a^N E^{Nb+N-1}, \tag{8}
\]

\[
\mathcal{N}_N(E) = \frac{b^N}{(Nb+N)!} a^N E^{Nb+N} = \alpha E^\beta. \tag{9}
\]

This simple treatment exhibits the properties of the systems we have examined [xx Exhibits what properties? This sentence seems incomplete. xx]. The results in Table III and Figs. 9–11 illustrate this [xx Illustrate what perfectly? xx] perfectly. In Figs. 10 and 11 we used the values \( a = 0.4 \) and \( b = 1/2 \) in Eq. (9) for comparison. In Eq. (9) we see that \( \ln(\alpha) \) is the sum of \( N \ln(a) \) and a term that depends on \( b \), so it is not very sensitive to the value of \( a \). The theoretical value of \( \alpha \) is higher than for any of the systems examined. This is partially due to the double counting discussed above, which makes \( \mathcal{N}_N(E) \) larger, but that may not be the whole story. In the case of \( \ln(\alpha) \) and \( \beta \) the random system was closest to the theory, but we will not speculate as to why.

[xx I found this last section, and in particular the last few paragraphs to be very confusing overall. I really lost sight of what you are trying to show. Please consider revising some of this section to try to clarify things as much as possible. xx]

V. CONCLUSIONS

We have provided a graphical approach to introduce students to the density of states (DOS) for simple quantum systems. In Sec. I we introduced the concepts of degeneracy, cumulative state number \( \mathcal{N}(\epsilon) \), and DOS \( g(\epsilon) \) for these systems. In Sec. III we gave a procedure for visualizing the DOS and used it to get the DOS for a particle in rigid boxes of various shapes. We found that the shape of the box had little effect on the DOS, a demonstration of Weyl’s theorem. We then built \( N \)-particle systems on the single-particle spectra of Sec. III and found that the DOS was insensitive to the specific energies of the single-particle spectra, the single-particle DOS \( (g_1(\epsilon)) \) being the important factor. Finally, we compared our numerical results for \( \mathcal{N}_N(E) \) with an expression based on iterating the single-particle density of states and saw how the DOS for \( N \)-particle systems was simply related to \( g_1(\epsilon) \).
VI. ADDITIONAL PROBLEMS

The following problems provide additional practice with the procedure used in Section III. The programs available in Ref. 10 may be a helpful starting point.

1. Examine changes to the density of states if we continuously change one of the dimensions of the rigid rectangular box. We expect the density of states to exhibit different behavior as we change continuously from a "2-D" system ($L_z \ll L_x, L_y$), to a "3-D" system ($L_z \approx L_x, L_y$) to a "1-D" system ($L_z \gg L_x, L_y$). Let $L_x = L_y = L_0 = 1$, and then let $L_z$ vary over the range $0.01L_0 \leq L_z \leq 100L_0$.

2. The energy levels for a particle in a rigid cylindrical box of height $H$ and radius $R$ are given by
\begin{equation}
\epsilon_{qln} = \hbar^2 (q^2 \pi^2 / H^2 + K_{ln}^2 / R^2) / (2M),
\end{equation}
where the $K_{ln}$ are zeroes of the (regular) Bessel functions. Vary the height-to-radius ratio for the cylindrical box. As $H/R$ goes from near 0 to 1, you should expect a transition from "2-D" behavior to "3-D" behavior. What does this look like in terms of $g(\epsilon)$?

3. Redo the treatment of Sec. II for a relativistic particle in the 2-D rigid square box. The important difference is that relativistically $\epsilon = pc = \hbar kc$, where $k$ is the wave number and $c$ is the speed of light.

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Sample programs demonstrating how our calculations are carried out are available as supplementary material at [AIP.to.insert.URL].

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Anecdotally, one of the authors (D. M.) has been surprised by the persistent student misconception that “fermions don’t interact.” This false notion can be traced to the commonly used “system of noninteracting fermions” that introduces statistical mechanics in the intermediate course. The equidistant single-particle spectrum is a common starting point when looking at the spectra of many-body systems. It is confusing that after all the work invested in solving the single-particle Schrödinger equation, we just throw away our hard won zeros-of-Bessel-functions-based energies, and replace them with the integers.

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Tables

TABLE I: The DOS for a particle in a rigid box of $D$ dimensions. The energy $\epsilon$ is in units of the lowest single particle energy $\epsilon_0$.

| $D$ | $N(\epsilon)$ | $g(\epsilon) = dN/d\epsilon$ |
|-----|----------------|-----------------------------|
| 1   | $\epsilon^{1/2}$ | $\frac{1}{2} \epsilon^{-1/2}$ |
| 2   | $\frac{\pi}{4} \epsilon$ | $\frac{\pi}{4}$ |
| 3   | $\frac{\pi}{6} \epsilon^{3/2}$ | $\frac{\pi}{4} \epsilon^{1/2}$ |
| 4   | $\frac{\pi^2}{32} \epsilon^2$ | $\frac{\pi^2}{16} \epsilon$ |
| 5   | $\frac{\pi^2}{60} \epsilon^{5/2}$ | $\frac{\pi^2}{24} \epsilon^{3/2}$ |
| 6   | $\frac{\pi^3}{384} \epsilon^3$ | $\frac{\pi^3}{128} \epsilon^2$ |

TABLE II: Parameters for $N(\epsilon) = \alpha \epsilon^\beta$ for the three different 3-D “boxes.” The theory gives $\alpha = \pi/6 \approx 0.524$ and $\beta = 3/2$; see Table I.

|                | $\alpha$   | $\beta$  |
|----------------|------------|----------|
| Cube (theory)  | $\pi/6 \approx 0.524$ | $3/2 = 1.5$ |
| Cube (numerical)| 0.29       | 1.58     |
| Rectangular box| 0.32       | 1.56     |
| Spherical box  | 0.46       | 1.51     |
TABLE III: The DOS for $N$-particle systems built on single-particle spectra with a DOS $g_1(E) = a \, E^b$. We set $a = 1$ for simplicity but $g_N(E)$ includes a factor of $a^N$.

|   | $b = -1/2$ | $b = 0$ | $b = 1/2$ | $b = 1$ |
|---|------------|---------|------------|---------|
| $g_1(E)$ | $E^{-1/2}$ | 1       | $E^{1/2}$  | $E$     |
| $g_2(E)$ | $\pi$      | $E$     | $\frac{\pi}{2} \, E^2$ | $\frac{1}{3} \, E^3$ |
| $g_3(E)$ | $2\pi \, E^{1/2}$ | $\frac{1}{\pi} \, E^2$ | $\frac{2\pi}{105} \, E^{7/2}$ | $\frac{1}{5} \, E^5$ |
| $g_4(E)$ | $\pi^2 \, E$ | $\frac{1}{3\pi} \, E^3$ | $\frac{\pi^2}{1920} \, E^5$ | $\frac{1}{7} \, E^7$ |
| $g_5(E)$ | $\frac{4}{3} \pi^2 \, E^{3/2}$ | $\frac{1}{4\pi} \, E^4$ | $\frac{4\pi^2}{130135} \, E^{13/2}$ | $\frac{1}{9\pi} \, E^9$ |
| $g_6(E)$ | $\frac{1}{2} \pi^3 \, E^2$ | $\frac{1}{3\pi} \, E^5$ | $\frac{\pi^3}{2580450} \, E^8$ | $\frac{1}{11!} \, E^{11}$ |
| $g_7(E)$ | $\frac{8}{15} \, \pi^3 \, E^{5/2}$ | $\frac{1}{60} \, E^6$ | $\frac{8\pi^3}{654729075} \, E^{19/2}$ | $\frac{1}{13!} \, E^{13}$ |
| $g_8(E)$ | $\frac{1}{6} \, \pi^4 \, E^3$ | $\frac{1}{7\pi} \, E^7$ | $\frac{\pi^4}{10218700800} \, E^{11}$ | $\frac{1}{15!} \, E^{15}$ |

$g_N(E) = \frac{\pi^{N/2}}{(N/2-1)!} \, E^{N/2-1} \, \frac{1}{(N-1)!} \, E^{N-1} \, \frac{\pi^{N/2}}{2^N (3N/2-1)!} \, E^{3N/2-1} \, \frac{1}{(2N-1)!} \, E^{2N-1}$
Figure captions

FIG. 1: The energies for different combinations of $n_x$ and $n_y$ for a particle in a 2-D square box. The numbers at the grid sites are $n_x^2 + n_y^2$. The quarter circles represent constant $n = \sqrt{n_x^2 + n_y^2}$; here we show $n = \sqrt{36}$ and $n = \sqrt{65}$. Certain values of $n$ give circles that intersect with the grid points. These correspond to the allowed energies $\epsilon = n^2 \epsilon_0$. Notice that $n = 6$ does not intersect any grid point, while $n = \sqrt{65} \approx 8$ (dashed line) intersects four grid points, corresponding to the degeneracy of that energy level.
FIG. 2: The degeneracy $d_\varepsilon$ (upper panels) and corresponding cumulative state number $N(\varepsilon)$ (lower panels) for the lowest nine levels of a simple, discrete system. On the left, the degeneracy of the system is intact while on the right, the degeneracy has been lifted. The effect on $d_\varepsilon$ is dramatic; less so for $N(\varepsilon)$.

FIG. 3: Top: Degeneracy $d_\varepsilon$ of the allowed energies $\varepsilon$ (in units of $\varepsilon_0$) of a single particle in a 2-D square box, up to $n_x = n_y = 10$. Middle: The corresponding $N(\varepsilon)$. Theory (smooth line) gives $N(\varepsilon) = (\pi/4)\varepsilon$. Bottom: A plot of $g(\varepsilon)$ obtained using the derivative scheme in Eq. (2) with a window width of 10. Theory (smooth line) gives $g(\varepsilon) = \pi/4$. 
FIG. 4: Top: Degeneracy $d_\epsilon$ of the allowed energies $\epsilon$ (in units of $\epsilon_0$) of a single particle in a 2-D square box, up to $n_x = n_y = 40$. Middle: The corresponding $N(\epsilon)$. Theory (smooth line) gives $N(\epsilon) = (\pi/4)\epsilon$. Bottom: A plot of $g(\epsilon)$ obtained using the derivative scheme in Eq. (2) with a window width of 60. Theory (smooth line) gives $g(\epsilon) = \pi/4$.

FIG. 5: Top: Degeneracy $d_\epsilon$ of the allowed energies $\epsilon$ (in units of $\epsilon_0$) of a single particle in a 3-D rigid cubic box, up to $n_x = n_y = n_z = 10$. Middle: The corresponding $N(\epsilon)$ is compared to the theoretical result (smooth line) $N(\epsilon) = (\pi/6)\epsilon^{3/2}$. Bottom: A plot of $g(\epsilon)$ obtained using the derivative scheme in Eq. (2) with a window width of 10. Theory (smooth line) gives $g(\epsilon) = (\pi/4)\epsilon^{1/2}$.
FIG. 6: Top: Degeneracy $d_\epsilon$ of the allowed energies $\epsilon$ (in units of $\epsilon_0$) of a single particle in a 3-D cubical box, up to $n_x = n_y = n_z = 40$. Middle: The corresponding $N(\epsilon)$ (lower curve) is compared to the theoretical result (smooth line, upper) $N(\epsilon) = (\pi/6)\epsilon^{3/2}$. Bottom: A plot of $g(\epsilon)$ obtained using the derivative scheme in Eq. (2) with a window width of 50. Theory (smooth line) gives $g(\epsilon) = (\pi/4)\epsilon^{1/2}$. 
FIG. 7: The upper panel shows the cumulative state number for the spectra for a single particle in cubical, rectangular, and spherical boxes. The spectra have been normalized so that $\frac{\hbar^2 \pi^2}{2M} = 1$ and the volume of each box is 1. The three curves are essentially indistinguishable. The lower panel is a histogram of the energies for each box. The bins are 40 units wide.

FIG. 8: A log-log plot of the cumulative state number for the single-particle spectra of cubical, rectangular, and spherical boxes. The energies are in units of $\frac{\hbar^2 \pi^2}{2M}$ and the volume of each box is 1.
FIG. 9: A log-log plot of the cumulative state number for $N$-particle systems ($N = 1, 2, \ldots, 5$) on the single-particle spectrum of the sphere. The steeper lines correspond to higher values of $N$, and different line types have been used for clarity. The slopes follow $N(\beta + 1)$.

FIG. 10: The exponent of $E$ in $\mathcal{N}(E) = \alpha E^\beta$ for systems of various particle number. Each system is made by putting non-interacting particles on the corresponding single-particle spectrum described in the text. The dashed line is a theoretical value derived using the values $a = 0.4$ and $b = 1/2$ in Eq. (8). These results were obtained using a linear fit to the log $\mathcal{N}(E)$ data. (The line is a guide for the eye.) The error bars represent the standard deviation of the average values from the 100 random spectra.
FIG. 11: A graph of $\ln \alpha$ vs $N$ for the same systems as in Fig. 10. Again, these results were obtained using a linear fit to the $\ln \mathcal{N}(E)$ data. The error bars represent the standard deviations of the average values from the 100 random spectra.