

Physics Through Problem Solving XXVIII: Density of States

M. S. Santhanam

Indian Institute of Science Education and Research

Dr. Homi Bhabha Road

Pune 410008, India.

santh@iiserpune.ac.in

(Submitted 30-06-2014)

Abstract

Density of states is a quantity of fundamental interest in quantum physics. We will introduce this quantity and work out some examples using simple systems studied in introductory quantum mechanics classes such as harmonic oscillator and hydrogen atom problem.

1 Introduction

In the standard text books on quantum mechanics, the idea of density of states is not given much importance though it is one of the characteristics of a given quantum system. Knowledge of density of states will allow us to calculate the occupation probability of eigenstates, level spacing statistics, density of carriers in a semiconductor, number of conducting electrons in a free electron gas and

in general gives us information about how crowded is a given spectral regime. In this piece, we will mainly discuss about the density of states of quantum systems with discrete energies using simple examples.

Let us consider a quantum system which has discrete set of states with energy eigenvalues $E_i, i = 1, 2, 3, \dots$. We denote by $\Omega(E)$, the total number of states less than the energy E . Then, the density of states, which is the number of states in unit interval of en-

ergy, is given by,

$$\rho(E) = \frac{d\Omega(E)}{dE}. \quad (1)$$

This is a function of energy E indicating that number of discrete states in any interval depends on the which energy scale we are looking at.

2 Examples

Harmonic oscillator : Consider the simple case of harmonic oscillator whose energy is given by,

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

where ω is the angular frequency of the oscillator and n is the quantum number. In this case, it is easy to see that the total number of states below energy E is

$$\Omega(E) = \left(\frac{E}{\hbar\omega} - \frac{1}{2} \right).$$

Then, using Eq 1, we get the density of states to be,

$$\rho(E) = \frac{1}{\hbar\omega}.$$

This tells us that for harmonic oscillator density of states is a constant and is not dependent on the energy E . This result should not surprise us since we know from Eq. 1 that the energy eigenvalues are equi-spaced. Thus, in general, whenever quantum systems have energy dependence of the form $E_n \propto n$, density of states will be a constant.

Anharmonic oscillators : Consider one-dimensional quantum system whose energy is of the form, $E_n = C (n + 1/2)^\alpha$ with C being a constant and $1 \leq \alpha \leq 2$. Quantum systems whose potential is of the form $V(x) = x^m$, where $m > 0$ is an integer, will have such energies in the semiclassical limit, *i.e.*, in the limit where WKB approximation would hold good [1]. This is generally the limit of large energies or high quantum numbers. In such case, the total number of states below energy E is given by,

$$\Omega(E) = \left(\frac{E^{1/\alpha}}{\hbar\omega} - \frac{1}{2} \right).$$

Then the density of states can be easily obtained by using Eq. 1 and we get,

$$\rho(E) = \frac{E^{\frac{1}{\alpha}-1}}{\alpha\hbar\omega} \quad (2)$$

For an anharmonic oscillator with the potential $V(x) = x^4$, it is easy to use the above results to show that $\rho(E) = KE^{-1/3}$ and I will leave this as an exercise for the reader. It is clear from Eq. 2 that in the entire class of anharmonic oscillators the density of states decreases with energy. For identical interval of energy, there are more eigenstates near the ground states than at higher energies.

Infinite potential well : In this case, the energies are given by, $E_n = C_1 n^2$, where C_1 is a constant that depends on system parameters and Planck's constant. The total number of states below an energy E is,

$$\Omega(E) = \left(\frac{E}{C_1} \right)^{1/2}.$$

The density of states is given by,

$$\rho(E) = \frac{1}{2C_1\sqrt{E}}.$$

Thus, in the case of infinite potential well, the density of states goes as $E^{-1/2}$. Note that this result we could have obtained by taking $\alpha = 2$ in Eq. 2. I leave as an exercise for the reader to figure out why $\alpha = 2$ should correspond to the infinite square well potential.

Hydrogen atom : This is another useful illustrative example. The discrete energy levels are hydrogen atom problem are given by,

$$E_n = -\frac{C_2}{n^2}, \quad n = 1, 2, 3...$$

where n is the principal quantum number. Using our recipe, we get for the total density of states,

$$\Omega(E) = \sqrt{C_2} E^{-1/2}$$

and the density of states turns out to be

$$\rho(E) = \frac{\sqrt{C_2}}{2E^{3/2}}.$$

Typically, in the hydrogen atom case, $E_n = -13.6/n^2 eV$. Thus, the magnitude of energy tends to zero as n increases. In this problem, higher values of principal quantum number n corresponds to $E \ll 1$. Hence, as $n \rightarrow \infty$, the energy tends to zero, and as a result $\rho(E) \rightarrow \infty$. This explains the crowding of energy levels near $E = 0$. For $E > 0$, there is a continuum of energies.

Black body radiation : Even though the arguments above were motivated primarily from quantum physics perspective, there would be

many occasions to compute density of states in classical systems as well. One such example is the enumeration of the number of modes in a black body which is used in the calculation of Rayleigh-Jeans formula and the Planck's radiation law. We will only briefly recount the steps involved and refer the reader to text books for details [2].

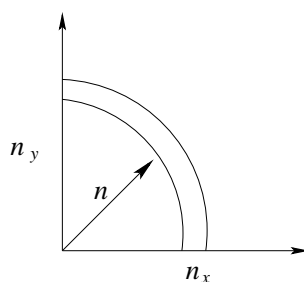


Figure 1: *Number of standing waves in the frequency range $[\nu, \nu + d\nu]$. We should determine the number of points in the shell of radius n . However, if the points are close enough we can simply assume them to be continuous and calculate the area of the shell.*

In principle, in a black body, standing waves of all possible wavelengths should be present. However, the boundary condition that waves should have a node at the walls of the cavity allows only modes of certain wavelengths to be present inside the cavity. The allowed wavelengths are obtained from the condition for standing waves in a cavity in one dimension to be $n = 2L/\lambda$, where λ is the wavelength of the standing wave and n is the number of half-wavelengths. In a 3D cavity, this condition is generalised to,

$$n_x = 2L/\lambda, \quad n_x = 1, 2, 3, \dots$$

$$\begin{aligned} n_y &= 2L/\lambda, & n_y &= 1, 2, 3, \dots \\ n_z &= 2L/\lambda, & n_z &= 1, 2, 3, \dots \end{aligned}$$

In 3D, each triplet of integers (n_x, n_y, n_z) correspond to a possible mode of standing wave inside the cavity. In a cube of side L , evidently the largest allowed standing wave will have a wavelength L . This sets the upper limit for the allowed wavelengths or equivalently frequencies in the cavity. The number of standing waves above a given value of wavelength, say $\bar{\lambda}$, is the number of such triplets (or modes) which have wavelengths above $\bar{\lambda}$. There is an easier and approximate way to calculate this quantity. Consider a 3D space of integers (n_x, n_y, n_z) and every point in this space corresponds to one possible mode of standing wave. Since there are large number of modes, we can regard this space as being essentially continuous and ask how many independent modes lie in the range of wavelengths λ and $\lambda + d\lambda$. This is given by the surface area of a shell in one octant of sphere (see figure 2) as,

$$2 \left(\frac{1}{8} \right) 4\pi n^2 dn \quad (3)$$

The factor 2 comes from two possible states of polarisation for each standing wave. We want the result in terms of frequency and so we write n in terms of frequency as,

$$n = 2L/\lambda = \frac{2L\nu}{c} \quad dn = \frac{2L}{c} d\nu. \quad (4)$$

In this, c is the velocity of light. Substituting for n from Eq. 4 in Eq. 3 we get the result for number of standing waves in the cavity in $[\nu, \nu + d\nu]$ to be,

$$\rho(\nu) d\nu = \frac{8\pi L^3}{c^3} \nu^2 d\nu \quad (5)$$

This is essentially the density of states for standing waves in black body. As frequency increases, number of modes is proportional to the square of the frequency. This application should not be surprising at all if we recognise that the eigenstates of quantum systems are essentially 'standing waves' or stationary states as we would properly call them in quantum physics.

Thus, the problem finding the density of states, at some level, boils down to the problem of enumerating all the states below a certain energy. It is essentially a counting problem. I leave it as a problem to the reader to plot these functions $\rho(E)$ for various systems. I must put in a word of caution that we have barely scratched the surface in dealing with density of states. There are other advanced methods of computing density of states, that does not a priori require the knowledge of how the energy is dependent on quantum numbers. So, in principle, given any Hamiltonian system, it may be possible to calculate the density of states without actually solving the full quantum system.

References

- [1] Uday Sukhatme, Am. J. Phys. **41**, 1015 (1973).
- [2] Arthur Beiser, The Concepts of Modern Physics, (Tata McGraw Hill Education, 2003)