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Subject: Physics

Production of Courseware

e-Content for Post Graduate Courses

Paper No. : Statistical Mechanics

Module : Ensemble Theory(classical)-I (Concept of Phase Space and its Properties)

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Description of Module	
Subject Name	Physics
Paper Name	Statistical Mechanics
Module Name/Title	Equilibrium, Thermodynamic Parameters and Response Functions
Module Id	M10

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1. Learning Outcomes

After studying this module, you shall be able to

- Examine the relationship between an n particle system and its time evaluation in phase space
- Construct phase space trajectory and phase space volume of some interesting physical systems
- To recognize phase space as a hyperdimensional space with interesting geometrical properties.
- Appreciate the significance of phase space as a discrete space of consisting of cells each of minimum volume h^{3N} as per the Heisenberg's uncertainty principle, where N is the number of particles in the system

2. Introduction

In the microscopic description of a macroscopic system, made up of a large number of particles (~ 10^{23}), state of the system at any instant t requires specification of instantaneous position and momentum of each of the constituting particles making the system. This leads us to so called work bench of statistical mechanics, a kind of a conceptual space, where all the action in statistical mechanics happens for its statistical study. Phase space provides us the methodology for counting the number of possible states (microstates) for a given system of interest. In this module we study this idea leading to a hyper-dimensional space of momentum and position co-ordinate space called phase space. In this module we look at properties both classically and quantum mechanically of this hyperspace, which shall be useful later in statistical description of the system. The key notions are phase point, phase space trajectory and dimensionality.

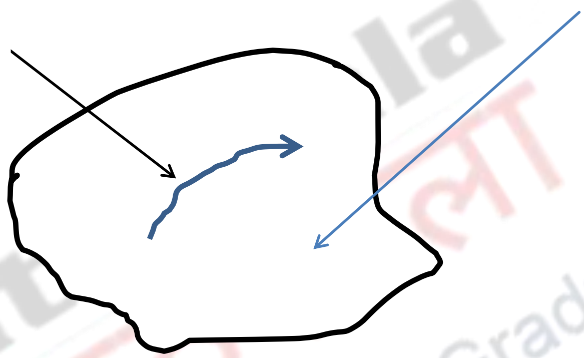
3. Degrees of Freedom

In classical mechanics degrees of freedom, f, corresponds to a number of independent parameters needed to completely define position and motion of a mechanical system. Consider a system made up of a single particle allowed to move in all three directions. The state of such a system at any instant can be described by three position co-ordinates or three momentum co-ordinates, amounting to 3 degrees of freedom. If we constrain this particle to move in a plane, only two position co-ordinates or two momentum co-ordinates are needed to describe its state, reducing the number of degrees of freedom to 2. If we further constrain to move the particle along a straight line, one position or one momentum co-ordinate are needed to describe its state, thereby system having 1 degrees of freedom.

If a system has N particles, for its complete description we require 3N position co-ordinates or 3N momentum co-ordinates a total of 6N co-ordinates, i.e. f = 3N.

4. Phase Space

At any given instant, knowledge of degrees of freedom provides us a geometrical way of visualizing state of a mechanical system by means of a space which must have the dimensionality equal to the degrees of freedom of the system. Such a geometrical construct is called a phase space. Each point of the phase space describing a state corresponds to a set of co-ordinates in $6N$ dimensions $(q_1, q_2\, q_3 \dots\dots\dots\dots q_{3N};\ p, p_2\, p_3 \dots\dots\dots\dots p_{3N})$ is called a ***phase point***. The number of position and momentum co-ordinates is two times the number of degrees of freedom for the system. As the system evolves with time, state of the system traverses a trajectory in phase space, going from one state of a system to another and so on (figure 1).



This evolution of ***phase trajectory*** with time is determined by the Hamilton's equations of motion,

$$\dot{q_i} = \frac{\partial H(q_i, p_i)}{\partial p_i}$$

$$\dot{p_i} = -\frac{\partial H(q_i, p_i)}{\partial q_i}$$

Where, $H(q_i, p_i)$ is the Hamiltonian of the system, which has no explicit dependence on time. Then H=E is the energy of the system. For a free particle system this amounts to satisfying the condition

$$\sum_{k=1}^{3N} \frac{p_k^2}{2m} = E$$

In general for a interacting system this amounts to

$$\sum_{k=1}^{3N} \left(\frac{p_k^2}{2m} + \frac{1}{2} \sum_{j=1}^{3N} V(q_{jk}) \right) = E$$

From here it is obvious that phase point shall traverse a trajectory on the surface of (3N-1) dimensions satisfying the above condition.

This space with 6N dimensionality is also referred to as hyperspace of statistical mechanics with which we have to deal with while counting the all possible microstates which a typical system can visit., indeed a very complex entity with N as large as Avogadro's number.

5. Visualisation of Phase Space

For visualization of phase space, we must try to identify the region of interest , which decides the volume of the phase space available to the system, which as we shall see later ultimately decides the calculation of entropy of the system through an interesting counting procedure. We will at the moment focus only on visualization of the phase space of some simple systems.

5.1 **Phase space of a free particle confined to move along a line**

Free particle confined to move along a straight line, say x-axis, of length L with constant Energy E. The Energy of this particle as it moves over this line is the kinetic energy which it possesses, such that we can write:

$$\frac{p^2}{2m} = E$$

This implies that for all values of q on the straight line of length L, momentum can have only two values: $p = \pm\sqrt{2mE}$. This looks like two straight lines parallel to q axis

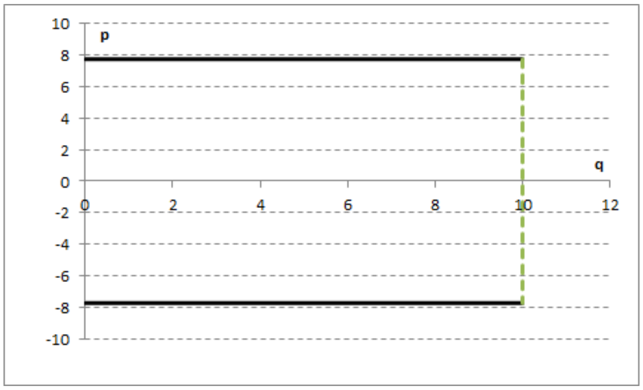


Figure 2 Phase space of a free particle confined to move on a straight line

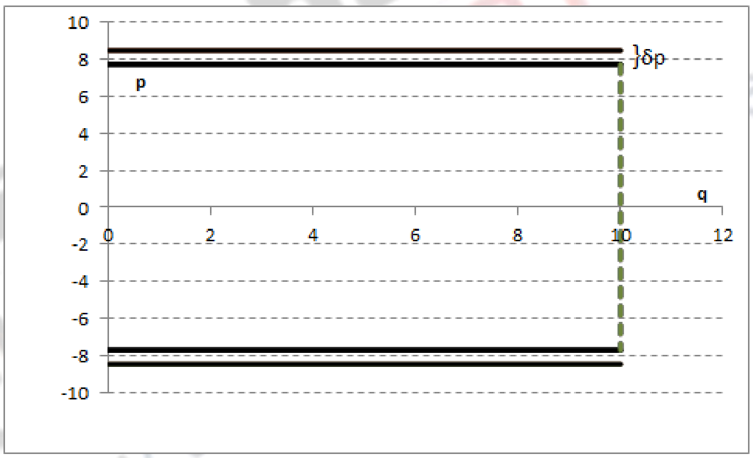


Figure 3 Motion of a particle in one dimension confined to move on a straight line of length L

Figure 2 above shows the phase space of a free particle moving with constant energy, which are two lines for two possible values of momentum ($\boldsymbol{p = \pm\sqrt{2mE}}$) which the particle can take. Figure 3 shows the two regions of phase space accessible to the free particle between the two parallel lines. Where length L in which particle is confined is a line of length L=10.

5.2 **Phase Space of a Simple Harmonic Oscillator***:*

The Energy E of a one dimensional harmonic Oscillator

$$\boldsymbol{E = \frac{p^2}{2m} + \frac{kq^2}{2}}$$

Where p is linear momentum, q is position co-ordinate, m is the mass of the body executing simple harmonic oscillation in one dimension and k is the force constant. The parametric form of this equation is given by

$$p = a\,sin\,\omega t,\, q = b\cos\omega t$$

Where $a = \sqrt{2mE}$, $b = \sqrt{\frac{2E}{k}}$ and $\omega = \sqrt{2mk}$

Following Figure shows the phase space of a linear simple harmonic oscillator whose energy lies between E and E+δE

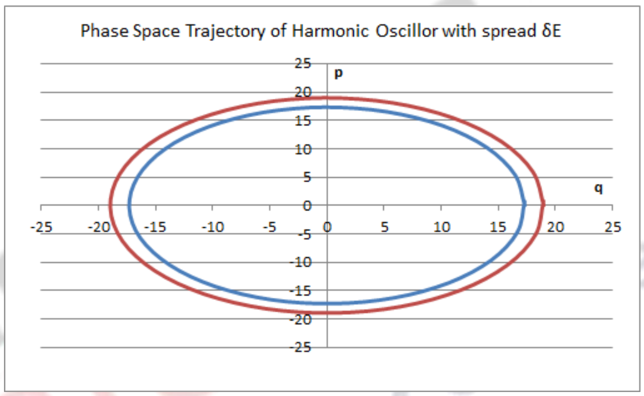


Figure 4 Phase space trajectory of a particle of mass m executing simple harmonic oscillator with energy lying between $\boldsymbol{E}$ and $\boldsymbol{E + \delta E}$

Region lying between the two ellipses is the phase space region accessible to the particle executing simple harmonic oscillations with energy lying between $\boldsymbol{E}$ and $\boldsymbol{E + \delta E}$.

6. Properties of Hyperspace

It is worth exploring some of the geometrical properties of this hyperspace , which we shall find useful at later stage, while calculating the phase space volume and counting the number of possible states.

6.1 Distance of a point in N dimensional hyperspace and Consequence of small change in position

Let there be a point $\boldsymbol{x} = (\boldsymbol{x_1}, \boldsymbol{x_1}, \dots \dots \dots \dots \dots, \boldsymbol{x_N})$. Then the distance of this point from the origin is defined as

$$|\boldsymbol{x}| = \left[\sum_{i=1}^{N} \boldsymbol{x}_i^2\right]^{\frac{1}{2}}$$

Suppose N is a very large number, say Avogadro's number. If some of x_i are not zero then $|x| \sim N^{\frac{1}{2}}$, which is indeed a large number. Furthermore, if each x_i changes by a small amount, $\delta x_i \sim \epsilon$,then $|\delta x| \sim \epsilon N^{\frac{1}{2}}$. Interestingly even if ϵ is small, $|\delta x|$ can be large, since N is very large.

6.2 **Volume of a sphere in N dimensional space**:

Let us note that volume of a sphere in 3-dimensional space is given by $V = \frac{4}{3}\pi r^3$ and surface area which is derivative of V with respect to r is given by $4\pi r^2$. Obviously, therefore, volume (V_n) of an n dimensional sphere of radius r shall be proportional to r^n and surface area $(s_n)$of this sphere is proportional to nr^{n-1}.

Thus $V_n = C_n r^n$, where C_n is the portionality constant and can be calculated easily using the value of a Gaussian integral. We know that

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$$

This implies that

$$\int_{-\infty}^{\infty} dx_1 \ldots\ldots \int_{-\infty}^{\infty} dx_n \sum_{i=1}^{N} e^{-x_i{}^2} = \prod_{i}^{N} \int_{-\infty}^{\infty} dx_i \;\; e^{-x_i{}^2} = \pi^{\frac{n}{2}}$$

Also, in spherical polar co-ordinates the above integral can be written as

$$\int_0^{\infty} s_n\, dr\, e^{-r^2} = \int_0^{\infty} nC_n r^{n-1} \;\; e^{-r^2} dr = \pi^{\frac{n}{2}}$$

Therefore,

$$nC_n \int_0^{\infty} r^{n-1} e^{-r^2} dr = \pi^{\frac{n}{2}}$$

Making a change of variable $r^2 = y$,

$$\frac{nC_n}{2} \int_0^{\infty} y^{\frac{n}{2}-1} e^{-y} dy = \pi^{\frac{n}{2}}$$

$$\frac{nC_n}{2}\Gamma(\frac{n}{2}) = \pi^{\frac{n}{2}}$$

Where

$\int_0^\infty y^{\frac{n}{2}-1}e^{-y}dy = \Gamma(\frac{n}{2})$ is the standard gamma function.

Therefore,

$$C_n = \frac{\pi^{\frac{n}{2}}}{\frac{n}{2}\Gamma\left(\frac{n}{2}\right)} = \frac{\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)}$$

Hence

$$V_n = \frac{\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)} r^n = \frac{\pi^{\frac{n}{2}}}{\frac{n}{2}!} r^n$$

And the surface area of hypersphere is which is derivative of V_n with respect to r is:

$$S_n = \frac{n\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}+1\right)} r^{n-1} = \frac{2\pi^{\frac{n}{2}}}{\left(\frac{n}{2}-1\right)!} r^{n-1}$$

7. Phase Space and Quantum Mechanics

We have seen that classically phase space is a continuum in hyperspace of 3N position c-ordinates and 3N momentum co-ordinates i.e. a total of 6N co-ordinates or degrees of freedom. Each point in the phase space or each set of points $(q_1, q_2\, q_3 \,\ldots\ldots\ldots\ldots\, q_{3N};\, p, p_2\, p_3 \,\ldots\ldots\ldots\ldots\, p_{3N})$ represents the state of a given macroscopic system. And since q's and p's form a continuum, therefore there are infinitely accessible phase points in phase space.

However, because of Heisenberg's uncertainty principle, quantum mechanics, which states that a particle cannot occupy a certain volume in co-ordinate space and a certain volume in momentum space simultaneously. This means that there is a minimum volume in phase space within which it is not possible to indicate certainly the state of the system. Such that the product of $\Delta p\Delta q$ is of the order of h i.e.

$$\Delta q_x\, \Delta p_x \geq h\ , \Delta q_y\, \Delta p_y \geq h, \Delta q_z\, \Delta p_z \geq h$$

In general this amounts to for a system of 1 particle a minimum volume of phase space equal to h^3. If there are N particles in the system, it shall amount to h^{3N} volume of phase space. This brings in quantization of the phase space, which has immediate consequence on the counting on probable states for a given state of a macroscopic system.

5. Summary

In this module we have learnt

- About the important concept of degrees of freedom for a N particle system
- About the concept of phase space, the work bench of statistical mechanics, and the meaning of dimensionality of phase space, phase point, phase trajectory and constant energy surface.
- About how phase trajectory for a system evolves and determined by Hamilton's equations of motion.
- How phase trajectory can be visualized in the case of a particle confined to move along a straight line of length L with constant energy E?
- How phase space accessible to a particle executing simple harmonic oscillator with energy lying in the interval E and $E + \delta E$?
- How to calculate volume and surface area of a hypersphere in an n dimensional space? A useful result in counting the number of probable states available for a given state of a macroscopic system
- How in going from classical mechanics to quantum mechanics we discretize the phase space into cells with each cell with a minimum volume of h^{3N} guided by Heisenberg's uncertainty principle which has an important implication of counting the number of probable states in a system?

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Appendix:

Spreadsheet to plot phase space of a free particle, of a free particle with an energy spread and of a simple harmonic oscillator.