

Review Paper

Concept of Macrostate and Microstate in the Classical Statistical Mechanics: A Review

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Abstract— Statistical mechanics is the branch of theoretical physics studying the microscopic properties of a system in equilibrium. When a system consists of many particles and the different methods employed are to get a macroscopic property of the system without taking individual motion into account, the probability is required. A macrostate refers to the bigger physical world whereas a microstate connects to the physical quantities in smaller dimensions. The impact of the terms has a big role in statistical mechanics to derive and explain the different physical quantities. The pressure, volume, temperature, etc. are examples of the macrostate. The different possible ways in which the system can be achieved in a particular macrostate introduce the term called microstate. A microstate of a thermodynamical system is found by defining the states of all of its constituent elements. The subject of statistical mechanics works as a bridge between quantum mechanics (micro-world) and thermodynamics (macro-world). So; the understanding of macrostate and microstate enables us to see and interpret the physical world.

Keywords— Statistical mechanics, quantum mechanics, microstate, macrostate, and thermodynamics

1. Introduction

Statistical mechanics is a subject that involves the study of the thermodynamic behavior of macroscopic systems from the available principles or laws which control the behavior of the constituent particles at the microscopic level [1-4]. For a system in equilibrium one can again try to make some very general statements based however, on the microscopic properties of the particles in the system and on the laws of the mechanics governing their behaviour. This type of study is called statistical mechanics. This gives all the results of thermodynamics plus a large number of general relations for calculating the macroscopic parameters of the system from a knowledge of microscopic constituents. The microscopic particles can be assumed to be an entity in physics like atoms, molecules, dipole moments or magnetic moments, etc. Many educators have focused on incorrect representations and alternate mental models to understand the introduction to basic thermodynamics [5-9]. The number of particles that considered to evaluate different physical properties is in the order of Avogadro's number i.e., 6.022×10^{23} atoms per mole in a macroscopic system. The molar concept is very useful to calculate the exact number of atoms that take part in chemical interaction. It is observed that each atom/particle executes translational, rotational, and vibrational motion with some internal degrees of freedom. When we consider a

macroscopic system i.e., many particles system, the particle interaction and also interaction with applied field are huge and difficult to compute different physical & thermodynamical properties of the given system. Therefore, the problem of many particles system is very complicated. To solve the issued problem, one has to introduce the concept of particle history and related interaction/heat generation. So, the thermodynamics limit must be taken into consideration before the evaluation of the final macroscopic properties of the system. In the thermodynamics limit, for N particles of volume V and density ρ obey the condition i.e., $N \rightarrow \infty, V \rightarrow \infty$ but $\rho = \frac{N}{V} = \text{finite}$. Therefore, different physical/thermodynamical properties of a macroscopic system can be evaluated using the above-mentioned thermodynamical limit condition. The role of the thermodynamic limit is to simplify the particle mutual interaction and also with the applied external field.

It has been constantly observed in the last few decades that people pay full attention to understanding the basic concepts of physics at low dimensions [10-11]. There is tremendous progress in both theory and experiments to observe and explain the small size physical quantities. In this regard, the two terms macrostate and microstate are very useful to connect the macro-world to the micro-world. The nature and properties of the macrostate relate to the system directly

including the temperature, pressure, volume, etc. Early nineteenth century, people thought that all the basic concepts of macroscopic objects and related phenomena has been understood and science has got saturation. No further research and experiments were required. But after the experimental verification of the dual nature of radiation, again people focused the research on quantum objects to search for the truth of the evolution of the earth and the creation of the universe [12]. So, there is a well-defined relation between quantum and thermodynamics; for which macrostate and microstate are to be understood correctly. In this report; we want to discuss the role of macrostate and microstate to explain the history of the universe.

2. Literature Review

To have interesting results in thermodynamics and statistical mechanics, we must perform small and simple experiments on thermal equilibrium. Statistical mechanics is the elder brother of the thermodynamics subject in which an attempt is made to apply mechanics in classical and quantum approaches to explain and predict certain phenomena related to the universe. This paper shows how the macrostate is related to microscopic properties through mechanics. It thus clarifies during the explanation to the rest of the world; how auxiliary assumptions are made to construct the microstates for the foundation of the statistical mechanics. According to the theory of classical mechanics, the microstate is a well-defined state that exists at every moment in the universe. So, each microstate is defined in the space-time coordinate. Therefore, each particle in the microstate is associated with a definite position and velocity [13]. For a given set of parameters and constraints (mass, position, energy, volume, density, etc.) of a microstate at some particular moment, the equations of motion can be used to evaluate the detailed information of the given microstates at all other moments. To calculate the different parameters of a microstate, one can use the above-mentioned method, which is called a trajectory in the system's state space coordinate. In the literature, people are using various types of notations for the microscopic system, however, in statistical mechanics, it is required to use a periodic microstate that may denote the entire mechanical system under study. For example, the immediate response of position and velocity coordinate of a particle inside the whole universe can be taken as a microstate, regardless of the truth that it is neither small nor part of whatever. Once, the position and velocity of a particle at a particular instant are known, one can calculate the position and velocity of the particle in the next instant of time. In this method, the different physical and thermodynamical properties of the studied microstate can be evaluated. Knowing the microscopic properties of a microstate, one can chase to explore other properties of the macroscopic/ macrostate. Therefore, primarily the evaluation of the position and velocity of the microstate is important and then one can go to find other information on the macroscopic systems.

3. Results and Discussion

Results should be presented in a logical sequence in the text, Here, an attempt was taken to discuss the specific role of the macrostate and microstate in the subject of statistical mechanics. The following points are discussed to understand the impotency of macrostate and microstate given the probability method of calculation for the evaluation of the thermodynamical systems. Therefore, an understandable language on microstate and macrostate is given below.

Macrostate: The specification of the macroscopic variables for a system is known as macrostate of the system. The examples of the macroscopic variable are pressure (P), temperature (T), volume (V), entropy (S) number of particles (N) and internal energy (U). When you define N, P, V & T of the system, then the given system is said to be in macrostate. The macrostate which have maximum number of microstates is called most probable macrostate. A thermodynamics system can have lot of macrostates. Let a system have 4 macrostates. The first macrostate system has 10 microstates, second macrostate has 30 microstate, third macrostate has 3 microstates and fourth macrostate has 6 microstates. Here the most probable macrostate is second system. Therefore, the most probable macrostate is the equilibrium state of the system. At equilibrium, pressure (P), volume (V), temperature (T), and internal energy (U) are the macroscopic parameters that can be used to define different measurable properties of the thermodynamical system. For instance, the macrostate of a fluid flow system can be defined by pressure (P), volume (V), and temperature (T). A thermodynamical system is said isolated system, if it does not allow to exchange both mass and energy with surrounding. For an isolated thermodynamical system, a macrostate can be defined by the number of particles (N) and volume (V), and internal energy (U). But in a closed system (exchange of energy only with the surroundings, no particle), at thermal equilibrium, a given macrostate of a thermodynamical system is defined by a number of particles (N) and volume (V), and temperature (T) [14]. Again, a thermodynamical system is said to be open system, if it allows both mass and energy to exchange with surrounding. Therefore, for an open thermodynamical system at thermal equilibrium, a macrostate can be defined by using the thermodynamical parameters such as chemical potential (μ), volume (V), and temperature (T) [15].

The equilibrium is a state of a thermodynamical system in which measured macroscopic variables such as pressure, volume, temperature, and internal energy are remaining constant with the function of time and also do not permit to flow of both energy and matter with the surrounding. The definition of an equilibrium state in an isolated system is to attain the maximum value of the entropy S (E, N, V) and not change with time. Again, the equilibrium state in a closed system can be defined as a state corresponding to the minimum value of Helmholtz free energy A (N, V, T); whereas an equilibrium state in an open system can be defined to attain a minimum of Gibb's free energy G (N, P, T) [16]. The role of the equilibrium state is very important to

define and calculate different physical properties corresponding to a thermodynamical system.

Microstate: Microstate of the system- Distinct internal arrangements of the system corresponding to a particular macrostate is known as microstate of the system. For example- if there are 40 students in the class maintain temperature 25°C. By rearranging students, one can make 10 types of the systems (internal arrangements). These various internal arrangements are called microstates corresponding to the given room. When some restrictions/constraints are imposed to a system, the microstates accessible to the system are called accessible microstates. A microstate of a thermodynamical system is found by defining the states of all of its constituent elements. Moreover, the nature of the constituent elements of the system decides the specification of the microstate. Depending upon the nature of the involved elements/particles, the microstate can be discussed in two different cases (a) classical particles and (b) quantum particles.

Microstates of the classical particles: For a complete description of the microstates of a system consisting of classical particles, one has to specify the position (q) and the conjugate momentum (p) of every constituent particle of the given system. In a classical particle system, the time evolution of position and momentum is defined by the classical Hamiltonian operator (H). The sum of the kinetic and potential energy is termed the Hamiltonian operator. Here, Hamilton's equation of motion for N particles in a 3-dimension plane can be written as $\dot{q}_i = \frac{\partial H(p,q)}{\partial p_i}$ and $\dot{p}_i = -\frac{\partial H(p,q)}{\partial q_i}$, where $i = 1, 2, 3, \dots, 3N$ [17].

The conjugate terms (q_i, p_i) can be used to define the position/state of a particle at any instant of time in phase-space coordinates. Therefore, every single particle has 3-position coordinates and 3-momentum coordinates. The sum of 6-dimensional coordinates is called phase space. Therefore, to evaluate any physical quantities related to a single particle in a thermodynamics system, the 6-dimensional coordinate systems can be used. Similarly, for N particles, the state of the system can be defined by $3N$ canonical position coordinates $q_1, q_2, q_3, \dots, q_{3N}$ and $3N$ canonical momenta coordinates such as $p_1, p_2, p_3, \dots, p_{3N}$. So, the above $6N$ variables form a $6N$ -dimensional phase space or Γ -space of the system. Any point we choose in the phase space represents a microstate of the given classical particle system. Each particle/ representative point in the Γ -space satisfying the relation; $H(q, p) = E$, where E = total energy of the system, defines the energy surface and is useful for the calculation of the conservation of the energy in statistical mechanics.

Microstates of Quantum Particles: The state of a quantum particle is represented by the wave function; $\psi(q_1, q_2, q_3 \dots)$. Mathematically, a wave function can be defined by using a complete orthonormal basis of

eigenfunctions of the Hamiltonian operator. Therefore, the final expression for a wave function can be written as; $\psi = \sum_n c_n \phi_n$; $\hat{H}\phi_n = E_n \phi_n$, where E_n the eigenvalues correspond to the eigenstate ϕ_n [18]. Using the above relations, one can calculate different physical parameters for a quantum mechanical system.

Illustration- Let us consider a magnetic system having a magnetic moment (μ) and localized magnetic ion of spin ($1/2$) at thermal equilibrium (T). The eigenstate associated with spin up (\uparrow) is (1,0) and the eigenstate associated with spin down (\downarrow) is (0,1) respectively. When an external magnetic field (H) is applied to the magnetic system, the energy responded to by the system will be $\vec{E} = -\vec{\mu} \cdot \vec{H}$. The energy will be positive ($+\mu H$) for a down spin (\downarrow) and energy will be negative ($-\mu H$) for an up spin (\uparrow). Here, the energy of two microstates associated with a macrostate (N, H, T) with $N = 1$, are $+\mu H$ and $-\mu H$, which correspond to down spin and up spin respectively. Similarly, one can write four microstates for two magnetic ions. The four microstates are $\downarrow\downarrow, \uparrow\downarrow, \downarrow\uparrow$ & $\uparrow\uparrow$. The energy corresponding to a microstate $\downarrow\downarrow$ is about $-2\mu H$, the energy corresponding to $\uparrow\downarrow$ & $\downarrow\uparrow$ are zero and the energy corresponding to a microstate $\uparrow\uparrow$ is about $+2\mu H$. If a thermodynamical system has N particles of spin $-1/2$, then there will be a 2^N number of microstates [18].

4. Conclusion and Future Scope

In the conclusion, it is observed that calculation of the macroscopic properties of a thermodynamic system became difficult because of the response of the external field by the microscopic particles and also interactions among them. So, it is wiser to use the thermodynamics limit for the measurement of the macroscopic properties i.e., pressure, temperature, volume, and internal energy of a thermodynamic system. Discuss the role of the macrostate and microstate in the evaluation of the thermodynamical properties of the system is done. Macrostate refers to the equilibrium state in connection with entropy (E, N, V) Helmholtz free energy $A(N, V, T)$, and Gibb's free energy $G(N, P, T)$ but microstate refers to the nature of the particles system (classical or quantum). In a classical particles system, any point in Γ -space (6-dimensional space, 3-position, and 3-momentum coordinates) gives the microstate whereas, in a quantum particle system, the position of each microstate is fixed by the wave function and the other physical quantities are calculated by using operator method. So, once we can calculate the microstate and its properties then go for the macroscopic properties of the system and consistently study the history of the universe.

Data Availability

Research data will provide on reasonable request.

Conflict of Interest

Authors declare that they do not have any conflict of interest.

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Authors' Contributions

S. K. Parida- researched literature and conceived the study. gaining ethical approval, draft of the manuscript, reviewed and edited the manuscript and approved the final version of the manuscript.

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