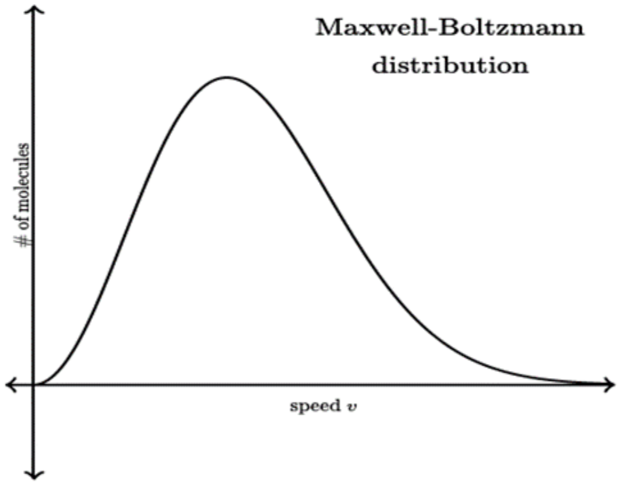

Application of Higher Mathematics in Physics

Taking the example of Thermodynamics

Research and Writing by CLC's students:

Simos Michalopoulos / Philippos Kaloudis / Philippos Tsoukis

Mentored and supervised by:

Ms. Vasileia Chatzidogiannaki BSc. Physics (EKPA), MA Applied Mathematical and Physics Science (EMP), MA Physical and Technological Applications (EMP) and CLC's Physics/Math teacher

Ms. Panagiota Tsamtsakiri BSc. Math & MSc Statistics (Aristotle of Thessaloniki), Ph.D. candidate (AUEB) and CLC's Math teacher

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Abstract

There is a profound connection between mathematics and physics. This paper delves into the relationship between higher mathematics and the field of physics, with a specific focus on the application of advanced mathematical concepts within the realm of thermodynamics.

The paper commences with a series of examples of the pivotal role of higher mathematics in formulating and solving complex problems in physics. These examples span a wide range of topics, from calculus and linear algebra to group theory and complex analysis, showcasing how these mathematical techniques are instrumental in modeling and predicting the behavior of physical systems.

Furthermore, this paper delves into the intricate alliance between advanced mathematics and the realms of thermodynamics and statistics, showcasing how mathematical rigor enriches our comprehension of complex physical systems.

The paper continues with an exploration of the foundational principles of thermodynamics, elucidating concepts such as energy conservation, entropy, and the laws of thermodynamics. Subsequently, it extends its reach to statistical mechanics, where probability theory and statistical methods provide essential tools for understanding and predicting random phenomena in the physical world.

Through the example of the application of statistical thermodynamics on chemical reactions, the paper showcases how statistical thermodynamics can help us understand how the rate of a chemical reaction and the position of the equilibrium point between the forward and backward reactions is placed.

In summary, this paper provides a comprehensive view of the multifaceted role of advanced mathematics in physics, with a focus on thermodynamics and statistics.

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Applications of Higher Mathematics in Physics

Mathematics is an abstract area of knowledge that includes the topics of numbers, formulae and related structures, shapes and the spaces in which they are contained, quantities and changes. Mathematics lies in the very heart of Physics, playing a vital role in scientific calculations, as well constituting a representation of our universe and its properties. Many different branches of Mathematics are applied in Physics for diverse purposes and goals, related to the studied phenomena and properties.

Calculus

Calculus is a branch of Mathematics that involves the study of change. Before its invention, Maths was completely static, which hinders modelling the physical universe, as it is constantly moving and changing. From subatomic particles or cells in our organism to the stars in space and entire galaxies, no objects are always at rest. This calls for the development of new mathematical tools that enable the complete description of change, helping us understand the different states of stars, particles and generally all objects.

Calculus was developed in the 17^{th} century by Gottfried Leibniz and Isaac Newton independently. Although Newton is considered the first to develop Calculus, contemporary notation is attributed to Leibniz.

Fundamentally, Calculus is divided into differential and integral calculus. Differential calculus studies rates of change of functions, whereas integral calculus allows us to primarily find a function, where the rate of change is already known.

In Physics, Calculus can be applied to study motion, as the equations of motion of a particle are functions of time. When knowing one of the functions of displacement, velocity, or acceleration with respect to time, we can use differentiation or integration to determine the rest of the functions. Additionally, through other functions, such as the function of force with respect to displacement, we can use integration to find work.

Calculus can also be applied in electricity, as both integral and differential calculus are vital for the calculation of the voltage or current through a capacitor.

Additionally, integral calculus helps us determine the exact length of a power cable necessary to connect situations that are miles apart from each other.
Another application of Calculus and more specifically Vector Calculus lie in electromagnetism, where it is widely used in calculations regarding electromagnetic phenomena. It allows us to extract information about the distribution of electromagnetic fields, the energy associated with the field, as well as electromagnetic radiation.
Calculus can be used in acoustics, in order to compute resonance and forced oscillations, as air resistance varies at different frequencies and resonates throughout an enclosed space whenever a musical instrument is played. Calculus helps us make improvements on acoustics, by improving the listener's experience.

Linear Algebra

Linear Algebra is the branch of Mathematics focused on linear equations, their solutions and many topics connected to them, such as matrices, vector spaces, inner products and more. Linear Algebra finds applications in many branches of Physics.
In Kinematics, the speed and direction of a moving particle are represented by vectors in a three-dimensional Euclidean space. This results in a vector space, where Linear Algebra can be applied to describe it.
In Statics, a subdivision of mechanics concerned with the forces that act on bodies at rest under equilibrium conditions, both rotational and translational, Linear Algebra can be applied to study the forces that act on objects, as they are represented by vectors mathematically. For instance, a static structure, such as a bridge has loads, which must be calculated at various points. Linear Algebra can assist in the mathematical representation of the system, as these are vector providing the direction and magnitude of forces at isolated points.
Initially, in the theory of electromagnetism, Maxwell's equations deal with vector fields in 3-dimensional space which can change with time. Thus, at each point of space and time, two vectors are specified, giving the electrical and the magnetic fields at that point.

In the theory of relativity, the transformation of the distances and times from one to the other is given by a linear mapping of vector spaces. The Lorentz transformations are linear and allow us to map different spaces and reference frames.
Additionally, Linear Algebra can be applied in Quantum Mechanics, where an experiment is characterized by an abstract space of complex functions. Each function is considered to constitute a vector itself. This results in a vector space of functions, whereby methods of Linear Algebra can be used to analyze the experiment.

Differential Equations

Differential equations are equations involving a function and one or more of its derivatives. They are useful in Mathematics, as they connect different rates of change and functions.
Initially, differential equations can be applied in Mechanics. The fundamental functions in Kinematics are those of displacement, velocity and acceleration with respect to time, connected through connected through differentiation and integration. Therefore, when they are involved in equations to study several types of motion, they frequently create differential equations, which can be solved by both analytical and non-analytical techniques. A primary example is the defining equation of Simple Harmonic Motion that involves both displacement and acceleration (the second derivative of displacement with respect to time), resulting in a differential equation. In Mechanics, differential equations can be applied to simplify calculations in Rectilinear Motion, Vertical Motion, Elastic Strings, Pendula, Projectile Motion and so on.
Differential equations are also very useful in electronics, which essentially deal with the emission, flow, and control of electrons in vacuum and matter. It is also fundamentally concerned with the design of circuits using transistors and microchips, and with the behaviour and motion of electrons in semiconductors, conductors, vacuum, or gas. Differential equations are useful in Electronics, as they facilitate solving problems, occurring in the analysis of electronic circuits.
Finally, differential equations can also be applied in Modern Quantum and Nuclear Physics. Nuclear Physic focus on the structure of the nuclei of atoms,

their formation, stability and decay, aiming to understand fundamental nuclear forces in nature, their symmetries, and the resulting complex interactions between protons and neutrons in nuclei and amongst quarks. One the other hand, Quantum Physics studies matter and energy at the most fundamental level, aiming to uncover the properties and behaviours of the very building blocks of nature. In Nuclear Physics, differential equations can be useful when studying fusion in stars, which is the reaction in which two light atomic nuclei combine, or fuse, to form a single heavier one, simultaneously releasing massive amounts of energy, providing power to the sun and the stars.

Group Theory

In Modern Algebra, Group Theory is the study of groups, which are systems consisting of a set of elements and a binary operation that can be applied to two elements of the set, which together satisfy certain axioms. Groups are crucial in Modern Algebra, as their structure can be found in many mathematical phenomena. For instance, they can be found in geometry, representing phenomena such as symmetry and certain types of transformations. Group theory has also many applications in Physics.

Group Theory is a powerful tool for studying symmetric physical systems, which include molecules and crystals with symmetry. Additionally, Group Theory is applied in many problems of atomic and nuclear Physics.

In Quantum Mechanics, Group Theory can be very helpful when solving practical problems using the Schrödinger equation, which is the fundamental equation of the science of submicroscopic phrnomena, having the same importance as Newton’s Laws of Motion in Classical Mechanics. One very important component of this equation is the Hamiltonian, which is an operator associated with the energy of the system. In many practical problems, the Hamiltonian may display various symmetries, enabling the application of Group Theory to facilitate solution.

Complex Analysis

Complex Analysis is the study of complex numbers along with their derivatives, manipulation and other properties. It essentially serves as an extension of fundamental concepts of real analysis, such as limits, derivatives, integrals and infinite series to complex numbers. Complex Analysis is an extremely powerful tool in Mathematics, with an unexpectedly large number of applications to the solution of physical problems.

Initially, Complex Analysis can be applied in Electronics, where complex numbers show up in circuits and signal processing. It can be used in the Hilbert Transform, which is defined as the transform in a signal, whereby the phase angle of all components is shifted by $\pm\frac{\pi}{2}$. Additionally, it can be applied to design power systems.

Complex Analysis is also very useful in advanced reactor kinetics and control theory, which essentially focuses on the control of dynamical systems in engineered processes and machines. It can also be applied in Plasma Physics. Physical applications of Complex Analysis also lie in Quantum Mechanics, where it's used in the Charge, Parity and Time Reversal Theory, which essentially states that every relativistic quantum field theory has a symmetry that simultaneously reverses charge, the orientation of space (parity) and the direction of time. It is also very useful in conformal field theory, which is a theory that remains invariant through a set of conformal transformations, meaning that it looks the same at all length scales. Complex Analysis can also be found in Wick's Theorem, which expresses a time-ordered product of fields as a sum of several terms, teach of which is a product of contractions of pairs of fields and Normal ordered products of remaining fields. Finally, Complex Numbers are essential to Quantum Mechanics, as they appear in the Wave Equation.

Topology and Geometry

Topology is a branch of Mathematics that studies the properties of spaces that are invariant under any continuous deformation. It is a relatively new branch of Mathematics, with most of the research having been done after 1900. Geometry is also a significant branch of Mathematics, concerned with the shape of individual objects, spatial relationships among various objects and the properties of surrounding space. Both Topology and Geometry have very important applications in Physics.

Firstly, Topology provides very useful insight into the Physics of materials, such as how some insulators can sneakily conduct electricity along a single-atom layer on their surfaces. Additionally, some of the fundamental properties of subatomic particles are at their heart topological, such as the spin state of an electron, which can be represented by its wave function. Finally, Topology provides a useful framework in Physics for the development of topological quantum field theories, which are unification theories that strive to attain a theory of everything.

Geometry is also very significant in Physics, as it helps us understand spacetime. In Relativity, spacetime is a concept that unites space and time, resulting in 4 dimensions: three to represent space and one to represent time. In spacetime objects of mass create curvature, the geometry of which helps us understand the characteristics of motion, such as the force of gravitation.

Mathematics in Thermodynamics

Thermodynamics is essentially a branch of Physics that examines the relationship between heat, work, temperature and energy. Broadly, it deals with the transfer of energy from one place to another and from one form to another. Its premise is that heat is a form of energy corresponds to a definite amount of mechanical work.

Several branches of Mathematics are applied in Thermodynamics. Initially, differential calculus is frequently used, since the change of thermodynamic functions is continuous in a certain range. This essentially means that calculus can be effectively introduced into chemical thermodynamic functions, as the premise of differential calculus is that a function is continuous at a specific point of its domain.

Another major branch of Mathematics that is applied in Thermodynamics are Statistics and Probability, in cooperation with concepts from Calculus. Statistical thermodynamics focuses on the behaviour of microscopic particles, to study macroscopic substances, such as gases. This can be attained by the application of several statistical methods and probability theory.

Since there are several vector quantities in Thermodynamics, vector mathematics, as well as vector calculus are also very important, in order to effectively analyse them and therefore understand the framework of a thermodynamic system, as well as the functions involved in it.

As can be deduced, Physics would not have developed without Mathematics. For Physicists it is a tool to represent the physical world and constitutes a necessary tool to answer many questions about our universe and its constituents. Mathematics is a language that helps us understand Physics and model it, providing a very good representation of our world and its fundamental properties.

Equations and principles of Statistical Mechanics and Thermodynamics

Statistical mechanics and thermodynamics are branches of physics that deal with the behavior of systems consisting of a large number of particles, such as atoms and molecules. Mathematical equations play a crucial role in describing and understanding the behavior of these systems.

Boltzmann distribution

The first one is the fundamental Boltzmann distribution that describes the probabilities of particles occupying different energy states within a system. It's based on the principle that particles tend to distribute themselves among available energy states in a way that maximizes the system's entropy while satisfying the constraints imposed by energy conservation. equation in statistical mechanics and is given by:

$$P_i = {}^{e^{-E_i/kT}}/_{Z}$$

, where:

- P_i is the probability of finding a particle in state i,
- E_i is the energy of state i,
- k is the Boltzmann constant,
- T is the temperature of the system,
- Z is the partition function, which sums over all possible states to ensure the probabilities sum up to 1.

The principles of the Boltzmann distribution are:

1. Microstates and Macrostates: In statistical mechanics, a microstate refers to a specific arrangement of particles' positions and momenta within a system. A macrostate refers to a set of macroscopic properties, such as temperature, energy, and pressure. For a given macrostate, there are typically numerous possible microstates that correspond to it.

2. Equilibrium and Maximum Entropy: The Boltzmann distribution arises when a system reaches thermal equilibrium, meaning it has no net energy exchange with its surroundings and has maximized its entropy for a given macrostate. Entropy is a measure of the system's disorder or randomness.

3. Maximization of Entropy: In thermal equilibrium, the system tends to occupy the macrostate that corresponds to the maximum number of microstates. This maximizes the entropy of the system. The reason for this preference is rooted in probability: a macrostate with more corresponding microstates is more likely to occur.

4. Energy and Temperature Influence: Higher energy states are less likely to be occupied than lower energy states due to the exponential term $e^{-E_i/kT}$. At higher temperatures, higher energy states become more probable, leading to increased thermal fluctuations.

5. Implications: The Boltzmann distribution has profound implications for various phenomena, such as:

- **Thermal Equilibrium:** When a system is in thermal equilibrium, the distribution of particles among different energy states follows the Boltzmann distribution.
- **Temperature Dependence:** The distribution depends exponentially on the inverse of temperature, emphasizing the role of temperature in determining the probabilities of different states.
- **Boltzmann's Entropy Formula:** The entropy of a system can be related to the number of particles in each energy state, leading to the famous formula $S = k\ln(W)$ where W is the number of microstates corresponding to a given macrostate.

Partition function

The second one is the central concept in statistical mechanics and is the partition function. Specifically, it's a sum of the Boltzmann factors for all possible energy states of a system:

$$\sum_i e^{-E_i/kT}$$

The partition function allows us to calculate various thermodynamic quantities, such as the free energy, entropy, and average energy of the system. Entropy S of a system is related to the number of ways it can arrange its energy among its particles. It plays a central role in understanding the behavior of energy and matter in various physical processes. The equation for entropy is: $S = k\ln(W)$ and it's principles are:

1. Statistical Interpretation: At a microscopic level, a system is composed of a large number of particles (atoms, molecules, etc.) with various possible arrangements of positions. Entropy arises from the idea that there are many possible ways (microstates) that these particles can be arranged to produce a given macroscopic state (macrostate) of the system.

2. Boltzmann's Entropy Formula: Ludwig Boltzmann formulated a relationship between entropy and the number of microstates corresponding to a macrostate.

3. Connection to Probability: Entropy is related to the likelihood of a system being in a particular state. Systems tend to be in states with higher entropy because there are more ways to arrange particles in those states. This is based on the idea that higher probability configurations are more likely to be observed due to the large number of ways they can occur.

4. Maximization of Entropy: In statistical mechanics, one of the fundamental principles is that a system in thermal equilibrium tends to evolve towards the state of maximum entropy given its constraints. This principle is known as the maximum entropy principle or the principle of equiprobability. It implies that the system explores all the available microstates with equal probability, leading to the equilibrium Boltzmann distribution.

5. Entropy and Energy Distribution: Entropy is closely related to the spreading of energy throughout a system. Systems naturally evolve towards states with more distributed energy, as this allows for a greater number of energy-sharing arrangements, resulting in higher entropy.

6. Entropy and Irreversibility: Entropy is also linked to the concept of irreversibility. Many natural processes tend to increase the entropy of a system. For example, when heat flows from a hotter object to a colder one, the overall entropy of the system increases, and this process is irreversible according to the second law of thermodynamics.

7. Change in Entropy: The change in entropy ΔS for a reversible process can be expressed as:

$$\Delta S = \frac{Q}{T}$$

, where:

- ΔS is the change in entropy,
- Q is the heat added or removed from the system,
- T is the absolute temperature of the system.

8. Entropy and Information Theory: Entropy also has connections to information theory. In the context of information theory, entropy represents the uncertainty or randomness in a set of data or information.

Thermodynamic Potentials

Another potential is thermodynamic quantities such as internal energy (**U**), Helmholtz free energy (**F**), Enthalpy (**H**), and Gibbs free energy (**G**). Those are functions that provide information about the state of a thermodynamic system. These quantities are related to each other through various mathematical equations, such as the Legendre transformations. principles and key concepts related to thermodynamic potentials:

1. Fundamental Thermodynamic Variables: Thermodynamic potentials are functions of certain fundamental variables, such as temperature (T), pressure

(P), volume (V), and particle number (N). The choice of variables depends on the nature of the system and the type of process under consideration.

2. Extensive and Intensive Quantities: Thermodynamic potentials can be classified into two types of variables: extensive and intensive. Extensive variables (e.g., internal energy U, entropy S, and volume V) depend on the amount of substance in the system. Intensive variables (e.g., temperature T, pressure P, and chemical potential μ) are independent of the system size.

3. Different Thermodynamic Potentials: There are several types of thermodynamic potentials, each suited to describe specific types of processes and constraints. The main ones are:

- **Internal Energy (U):** Represents the total energy of the system.
- **Helmholtz Free Energy (F):** Relates to the work that a system can do while at constant temperature and volume.
- **Enthalpy (H):** Pertains to the heat exchange in a system at constant pressure.
- **Gibbs Free Energy (G):** Describes the maximum non-expansion work that a system can do on its surroundings at constant temperature and pressure.

4. Legendre Transformations: Thermodynamic potentials are often related to each other through Legendre transformations, which involve changing one set of variables to another while keeping the physics unchanged. For example, the Legendre transformation of the internal energy U with respect to volume V yields the enthalpy H.

5. Minimization Principle: In thermodynamics, systems tend to evolve towards states of minimum Gibbs free energy (G) at constant temperature and pressure. This principle is used to predict the direction of chemical reactions that reach equilibrium.

6. Equilibrium Conditions: The equilibrium conditions for a system are usually expressed in terms of changes in thermodynamic potentials. For instance, in a closed system at constant temperature and pressure, a spontaneous process occurs if the Gibbs free energy decreases ($\Delta G<0$).

7. Maxwell Relations: Maxwell's relations are a set of partial derivatives that link various second derivatives of thermodynamic potentials. They provide relationships that can simplify calculations and help derive thermodynamic identities.

8. Thermodynamic Potentials and Thermodynamic Processes: Different thermodynamic potentials are useful for describing various types of processes:

- U is particularly useful for closed systems and energy transfer.
- H is used for processes at constant pressure.
- F is used for processes at constant temperature.
- G is used for processes at constant temperature and pressure, and it determines the equilibrium conditions.

Maxwell's relations

A set of mathematical relationships derived from the properties of partial derivatives of thermodynamic potentials are Maxwell's relations. These relations play a crucial role in simplifying calculations and understanding the relationships between different thermodynamic variables. Principles related to Maxwell's relations are:

1. Partial Derivatives and Cross-derivatives: In thermodynamics, various thermodynamic potentials are functions of multiple independent variables, such as temperature (T), pressure (P), volume (V), and entropy (S). Partial derivatives and cross-derivatives of these potentials provide information about how different quantities change with respect to changes in the independent variables.

2. Symmetry of Mixed Partial Derivatives: Maxwell's relations arise from the symmetry of mixed partial derivatives. If a second derivative of a thermodynamic potential with respect to two different variables is taken in both orders, the resulting expressions are often equal due to the continuity of partial derivatives.

3. Four Main Maxwell's Relations: There are four primary Maxwell's relations, each connecting derivatives of pairs of thermodynamic potentials with respect to pairs of independent variables. These relations are derived from the basic thermodynamic potentials: internal energy (U), enthalpy (H), entropy (S), and Gibbs free energy (G).

The four main Maxwell's relations are:

- $\left(\partial Q/_{\partial T}\right)_S = -\left(\partial P/_{\partial S}\right)_V \left(\partial V/_{\partial T}\right)_S = -\ \left(\partial S/_{\partial P}\right)_V$ **:** Relates the temperature change with volume at constant entropy to the negative change in pressure with respect to entropy at constant volume.
- $\left(\partial T/_{\partial P}\right)_V = -\left(\partial V/_{\partial S}\right)_P \left(\partial P/_{\partial T}\right)_S = \ \left(\partial S/_{\partial V}\right)_P$**:** Relates the temperature change with pressure at constant entropy to the change in volume with respect to entropy at constant pressure.
- $\left(\partial S/_{\partial V}\right)_T = -\left(\partial P/_{\partial T}\right)_V \left(\partial V/_{\partial S}\right)_T = \left(\partial T/_{\partial P}\right)_V$ **:** Relates the change in entropy with volume at constant temperature to the change in pressure with respect to temperature at constant volume.
- $\left(\partial S/_{\partial P}\right)_T = -\left(\partial V/_{\partial T}\right)_P \left(\partial P/_{\partial S}\right)_T = -\left(\partial T/_{\partial V}\right)_P$ **:** Relates the change in entropy with pressure at constant temperature to the negative change in volume with respect to temperature at constant pressure.

4. Practical Use and Derivations: Maxwell's relations are invaluable in simplifying calculations involving changes in thermodynamic variables. They allow researchers and engineers to relate derivatives and integrals of different thermodynamic potentials without needing to perform complex calculations directly from the first principles.

5. Role in Thermodynamics: Maxwell's relations highlight the interdependence of different thermodynamic variables and provide a deeper understanding of the relationships between them. They are used to derive important thermodynamic equations, analyze equilibrium conditions, and predict how changes in one variable affect others.

Equilibrium Conditions

Finally, equilibrium conditions are fundamental concepts in thermodynamics that describe the stable states in which a system's macroscopic properties remain constant over time. Understanding equilibrium conditions is essential for predicting the behavior of systems and analyzing their thermodynamic properties. key concepts related to equilibrium conditions:

1. Mechanical Equilibrium: In a system at mechanical equilibrium, there is no net force or torque acting on it, and the pressure is uniform throughout the system. This condition is defined by the equality of pressures within and outside the system.

2. Thermal Equilibrium: Thermal equilibrium is reached when there is no net heat flow between two objects in contact. In thermal equilibrium, their temperatures are the same, and there is no temperature gradient between them.

3. Chemical Equilibrium: Chemical equilibrium occurs when the rates of forward and reverse reactions in a chemical system are equal. At chemical equilibrium, the concentrations of reactants and products remain constant over time.

4. Phase Equilibrium: Phase equilibrium involves coexistence of multiple phases (solid, liquid, gas) in a system without any phase changes occurring. Each phase has a specific equilibrium pressure and temperature.

5. Equilibrium State and Potential Minimization: In thermodynamics, equilibrium states are characterized by the minimization of certain thermodynamic potentials. For example, a system at constant temperature and pressure tends to minimize its Gibbs free energy (G).

6. Maximum Entropy Principle: The principle of maximum entropy states that a closed system in equilibrium will evolve toward the state that maximizes its entropy while satisfying given constraints. This leads to the Boltzmann distribution in statistical mechanics.

7. Equilibrium Thermodynamics and Irreversibility: Equilibrium conditions are idealized states that often serve as reference points for real processes. Actual processes often involve deviations from equilibrium, leading to irreversibility and entropy production, as described by the second law of thermodynamics.

8. Equilibrium Diagrams: Equilibrium phase diagrams, such as the phase diagram of a substance, provide information about the stable phases and their equilibrium conditions as temperature and pressure change.

9. Le Chatelier's Principle: Le Chatelier's principle states that a system at equilibrium, when subjected to an external change (change in temperature, pressure, etc.), will adjust itself to counteract that change and restore equilibrium.

10. Equilibrium and Thermodynamic Potentials: Different thermodynamic potentials, such as enthalpy (H) and Gibbs free energy (G), provide valuable information about equilibrium conditions and the direction in which processes will spontaneously occur.

11. Dynamic Equilibrium: In some cases, systems can reach dynamic equilibrium, where certain properties (like concentration) fluctuate around an average value while remaining constant on average over time.

In conclusion, the principles of thermodynamics provide a deep understanding of the fundamental behavior of energy and matter in a wide range of physical systems. These principles have profound implications for our understanding of natural processes, energy conversion, and the behavior of substances under different conditions.

Understanding Reactions in Terms of Rate & Equilibrium

Whenever there is a chemical reaction it involves the breaking of bonds, and so, because bonded atoms are (typically) in a state of lower entropy, the breaking of these bonds increases entropy, and therefore requires energy. The energy for this comes from the kinetic energy of the particles. The average kinetic energy of particles in a large sample of those particles, if measured quantitatively, is what we call temperature, and so whenever temperature is mentioned, it is important to recognize that this is only used so far as it is one statistical tool (the mean function) that can be used in the study of the chemical reactions. It can be further added that in ideal gasses we consider that aside from the collisions, each particle experiences no forces from any other particles, thus in this unrealistic state, the potential energy is 0 so the total energy is equivalent to the kinetic energy, and therefore temperature is simplified to mean kinetic energy. If the kinetic energy of the particles (activation energy E_a) in a given collision is subsequent, and they have the proper direction/orientation, then the reaction takes place.

The applications of statistical thermodynamics are to better understand chemical reactions. In the following, it shall be examined how statistical thermodynamics can help us understand how the rate of a chemical reaction and the position of the equilibrium point between the forward and backward reactions is placed (in reactions in which backward reactions do exist).

Before anything else is developed it is necessary to note the need from which statistical thermodynamics originally arose. If one were to attempt to try to approach a chemical reaction as one approaches the collision between two balls, but with many more balls, they would find themselves unable to perform the simulation/calculation that would help them further understand the reaction. Even today, an attempt to simulate the many thousands of independent particles, with a priori different kinetic energies and orientations and directions would be practically impossible with any computer. By using statistical thermodynamics, we can use the fact that there are a great number of particles to our advantage, by recognizing that when there is a very large number of particles, each particle can be treated as any other particle, and using average information about all particles, we can understand the whole set of particles.

Maxwell-Boltzmann Distribution

By considering the set of particles to be very large, which it is as mentioned previously, we can for a given average kinetic energy approximate a distribution for the kinetic energies of the particles, which can be used for calculations that involve sums of functions for each particle.

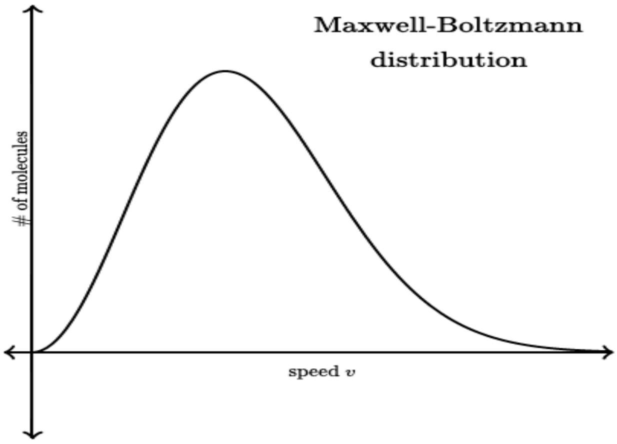

Figure 1.1[1]

It is understood that the Maxwell-Boltzmann distribution represents the likely distribution of the particles given the assumption that the behavior of a system tends towards maximum entropy. Through higher mathematics and Lagrangian mechanics it can be found that the minimum value of the entropy function is:

$$S = \frac{M}{N} \times ln\, ln\, (\Omega)$$

, where S is the entropy of a system M is the number of particles, N is Avogadro's number and Ω is the number of microscopic configurations of the

[1]https://deepai.org/machine-learning-glossary-and-terms/maxwell-boltzmann-distribution

particles. We see from this that by considering the set of particles as one collection of particles, as we do by using Ω, we can simply find a value for the entropy of a system. In this formula we can see how the Boltzmann distribution changes with temperature, as S is given JK^{-1}, as it is temperature dependent. The evaluation of the distribution previously described is done by evaluating the ways that a particle can move at a certain velocity. The probability of the given particle moving at that velocity, is proportional to the ways that the particle can do so. This affects the rate of reaction, as one of the conditions for a successful collision given is that the particles have combined an energy that surpasses the activation energy E_a. The Boltzmann distribution defines the rate of the reaction by defining how many particles are above the activation energy. In addition, by taking this distribution, and by taking a value for the activation energy of the reaction, we may determine what portion of the particles have the necessary activation energy to perform the reaction. This is useful, as the rate of reaction is affected by the kinetic energy of the particles, but it is not only affected by this, but also as mentioned previously, the orientation of the particles.

Orientation in Collisions

In order for the reaction to take place, the two particles colliding must do so in an orientation that allows for the reaction to take place. It is noted that there are always two particles involved in a collision, as if the step is unimolecular there is no collision, and it is statistically improbable that more than two particles collide with the correct orientations. It follows that, depending on the restriction on the orientation of particles from no restriction for unimolecular steps to total restriction for theoretical tri-molecular steps, there will be a certain coefficient between 0 and 1 that relates the number of collisions with sufficient energy to the number of collisions with sufficient energy that are successful. This changes from reaction to reaction and is known as the Arrhenius constant, and it is also called the pre-exponential factor (this second naming will be further explained in the next section). We should note the difference between this restriction on the rate of reaction and the one presented in the previous section. While previously temperature affected the kinetic energy of the particles, the limiting factor of orientation is not at all affected by temperature but remains constant for any reaction. Here is another example of our ignorance of the circumstances of a particular event (the orientation of the particles in one collision). However, by taking the number of collisions to be a large number, we can understand the behavior of the whole system, i.e. we do not know if a collision is in the correct orientation, but we do know approximately what the chance of it being in the correct orientation is.

The Rate Constant

In order to connect these two features of a reaction to the particular use, i.e. determining the rate of reaction, the concept of a rate expression must be introduced. For a reaction:

$$aA + bB \rightarrow cC + dD$$

the rate constant (k) for a particular temperature is:

$$k = \frac{(rate\ of\ reaction\ at\ particular\ concentration)}{[A]^a \times [B]^b}$$

, and this remains constant for all reactions with given concentrations at that temperature. As mentioned previously, the rate of the reaction is increased by increase in collisions (resultant from higher speed) and is restricted by a fixed Arrhenius constant and by a variable activation energy that affects the rate in a way that varies. These can be connected to the rate constant through the simple equation:

$$k = A \times e^{\frac{-E_a}{RT}}$$

, where A is the Arrhenius constant, E_a is the activation energy, R is the ideal gas constant and T is the absolute temperature (now we see why the Arrhenius constant is called the pre-exponential factor). In effect we notice in this equation the ‘intuitive’/expected relationship between temperature and activation energy:

by increasing the E_a, $e^{\frac{-E_a}{RT}}$ becomes closer to zero (power becomes a bigger negative number), and as T increases $e^{\frac{-E_a}{RT}}$ increases (less negative power). This is the implementation of the insight from the Maxwell-Boltzmann distribution, regarding the effect of temperature and activation energy to the rate. The previous may in turn be used to understand the systems of dynamic equilibrium in which statistical mechanics finds use.

The Equilibrium Constant

It is understood that systems 'tend towards disorder'. In other words, as time progresses the energy in a system tends to be dissipated across the system. This can be explained by the notion that there are more ways for disorder to exist than for any particular ordered structure, and so as changes occur to a system, they result in a maximum value for entropy, as the arrow of time progresses. A useful metric to have in mind is ΔG, also known as Gibbs' free energy which effectively represents how 'spontaneous' (how far the reaction is to bring the system to a state of greater energetic stability) a reaction is. As reactions tend to increase entropy, a high spontaneity (low Gibbs' free energy value) is related to a high ΔS value. Given that an equilibrium is really two simultaneous reactions which are related, we can use this relationship to find at which point ΔS and ΔG are maximized and minimized respectively (for the overall reaction).

The equilibrium constant (k) can be related to ΔG by the expression:

$$\Delta G \ = -RTln(k)$$

, where k is equilibrium constant, R is the ideal gas constant and T is the temperature in Kelvin. This equilibrium constant is expressed by:

$$k = \frac{[C]^c * [D]^d}{[A]^a * [B]^b}.$$

This can be shown (when the system is in dynamic equilibrium) to be equal to $constant * \frac{kforward}{kbackward}$, where:

$k_f = \frac{rate\ of\ forward\ reaction}{[A]^a * [B]^b}$ is the forward reaction rate constant and

$k_f = \frac{rate\ of\ backward\ \ reaction}{[C]^c * [D]^d}$ is the backward reaction k constant, and k is a different constant. Although the mathematics is simple it provides insight. So:

$$\frac{k_f}{k_b} = \frac{rate\ of\ forward\ reaction\ * [C]^c * [D]^d}{rate\ of\ backward\ reaction\ * [A]^a * [B]^b}$$

, which simplifies to $k = \frac{[C]^c * [D]^d}{[A]^a * [B]^b}$

, which is a constant away from the equilibrium constant. Thus, we see that the equation for Gibbs' free energy, and the definition of the equilibrium constant, are themselves connected to the rate expression and constants, for a given system of dynamic equilibrium (in which some information i.e rates of forward and backward reactions, is known).

Generalization

A system of dynamic equilibrium although can be generally intuitively understood, it cannot be dealt with intuitively, and what has been attempted to be shown through the above example, is that knowledge about the system may be gotten through traditional mechanics, but only after the tools in same have been adapted for use in environments in large numbers of objects. Indeed, the above is the beginning of the theory on which much of the industrial pharmaceutical processes are predicated, almost all reactions used in such being reversible, thus requiring considerations based on that which has been shown above. Understanding acids and bases and their behavior is another application of the principles described above, which themselves are only the beginning of the uses of the wider principles of thermodynamics: applying traditional mechanics to systems with a great number of 'objects', for which only information about the average of the system is known.

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