# Geometry and Topology in Statistical Mechanics

Hao-Yang Yen (https://kikiyenhaoyang.github.io/kikiyen/Web/index.html)

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## 1 Lagrangian Mechanics

Lagrangian mechanics, an elegant framework in classical mechanics introduced by Joseph-Louis Lagrange, offers a concise method for describing the dynamics of physical systems. Unlike Newtonian mechanics, which relies on forces, Lagrangian mechanics employs only one function called Lagrangian with dimension energy, providing a versatile approach to analyzing motion. By expressing dynamics in terms of generalized coordinates and velocities, Lagrangian mechanics offers a unified framework applicable to a wide range of phenomena, from celestial motion to mechanical systems. In this overview, we will explore the key principles and applications of Lagrangian mechanics, illuminating its importance in understanding the behavior of physical systems.

### 1.1 Lagrangian and Action

The main objects we want to study in Lagrangian mechanics are *Lagrangian* and *action*.

**Definition. Lagrangian and generalized coordinate**
*Lagrangian* $\mathcal{L}$ is a function of *generalized coordinate* $\mathbf{q} \in \mathbb{R}^N$ and its derivative of time $\dot{\mathbf{q}}$ and is defined as

$$\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}; t) = \mathcal{T} - \mathcal{V},$$

where $\mathcal{T}$ is the kinetic energy, $\mathcal{V}$ is the potential energy and $N$ is called the *degree of freedom*. Note that $\mathbf{q}$ and $\dot{\mathbf{q}}$ are functions of time, this is why the Lagrangian is denoted by $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}; t)$.

**Definition. Action**
*Action* $\mathcal{S}$ is a functional of the $q$ and $\dot{q}$, defined as

$$\mathcal{S}[\mathbf{q}, \dot{\mathbf{q}}; t] = \int_{t_i}^{t_f} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}; t) dt.$$

These two physical quantities are the most basic concepts in Lagrangian mechanics.

### 1.2 The Least Action Principle (Hamiltonian Principle)

The path in the configuration space for a motion always has the least action.
This can be written as a variational problem, that is,

$$\left.\frac{\delta \mathcal{S}}{\delta \mathbf{q}}\right|_{classical\ path} = 0,$$

or equivalently

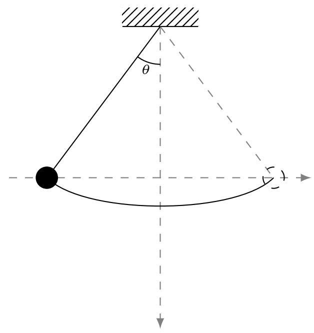
$$\delta \int_{t_i}^{t_f} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}; t) dt \bigg|_{path} = 0.$$

This principle is called *the least action principle*. One might ponder the origin of this curious principle, which remained unexplained for centuries. It wasn't until the advent of the Feynman path integral, hundreds of years later, that a satisfactory explanation was finally provided.

### 1.3 Euler-Lagrangian Equation

With the least action principle, we can derive the *Euler-Lagrangian Equation*.

**Example 1.1. Pendulum**
Consider the pendulum with the length of the rope $L$ and the mass of the particle $m$.



**solution:**
Write down the Lagrangian

$$\mathcal{L}(\theta, \dot{\theta}; t) = \frac{1}{2} m L^2 \dot{\theta}^2 - mgL(1 - \cos\theta).$$

The Euler-Lagrange equation gives

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\theta}} - \frac{\partial \mathcal{L}}{\partial \theta} = 0 \implies \boxed{\ddot{\theta} = -\frac{g}{L}\sin\theta}.$$

# 2 Hamiltonian Mechanics

Hamiltonian mechanics, pioneered by William Rowan Hamilton, offers a powerful framework for describing the dynamics of classical systems. It focuses on energy principles, expressed through the Hamiltonian function, and introduces generalized coordinates and momenta. Hamilton's equations, derived from the principle of least action, govern the system's evolution over time. This formalism provides a concise and elegant approach to analyzing complex systems, with applications spanning classical mechanics to quantum physics.

## 2.1 Legendre Transformation

In thermodynamics, we have the relations

$$dE = TdS - PdV,$$

, where $E$, $T$, $S$, $P$, and $V$ are internal energy, temperature, entropy, pressure, and volume respectively. The internal energy $E$ is a function of $S$ and $V$.
The definition of enthalpy $H$ is

$$E + PV,$$

so that

$$dH = TdS + VdP,$$

where $H$ is a function of $S$ and $P$. This method to change $E(S, V)$ into $H(S, P)$ is called *Legendre transformation.* We can do the Legendre transformation on the Lagrangian to get a new function.

## 2.2 Hamiltonian

**Definition. Hamiltonian and generalized momentum**
The *Hamiltonian* $\mathcal{H}$ is the Legendre transformation of Lagrangian. That is,

$$\mathcal{H} = -\mathcal{L} + \dot{\mathbf{q}}\mathbf{p}.$$

It is a function of generalized coordinate $q$ and *generalized momentum* $p$ and can be written as

$$\mathcal{H}(\mathbf{q}, \mathbf{p}; t) = \mathcal{T} + \mathcal{V},$$

where the generalized momentum is defined as

$$\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}}.$$

## 2.3 Hamiltonian Equations (Canonical Equations)

By the relation of Legendre transformation

$$\mathcal{H} = -\mathcal{L} + \dot{\mathbf{q}}\mathbf{p}.$$

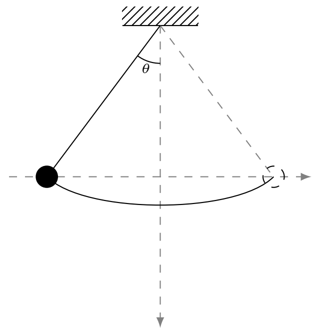
We have

$$\begin{aligned} d\mathcal{H} &= \dot{\mathbf{q}}d\mathbf{p} + \mathbf{p}d\dot{\mathbf{q}} - d\mathcal{L} \\ &= \dot{\mathbf{q}}d\mathbf{p} + \mathbf{p}d\dot{\mathbf{q}} - \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}}d\dot{\mathbf{q}} - \frac{\partial \mathcal{L}}{\partial \mathbf{q}}d\mathbf{q} \\ &= \dot{\mathbf{q}}d\mathbf{p} - \dot{\mathbf{p}}d\mathbf{q}. \end{aligned}$$

Hence we have the Hamiltonian equations (or Canonical equations)

$$\begin{cases} \dfrac{\partial \mathcal{H}}{\partial \mathbf{q}} = -\dot{\mathbf{p}}, \\ \dfrac{\partial \mathcal{H}}{\partial \mathbf{p}} = \dot{\mathbf{q}}. \end{cases}$$

**Example 2.1. Pendulum**
Consider the pendulum with the length of the rope $L$ and the mass of the particle $m$.




**solution:**
Write down the Hamiltonian

$$\mathcal{H}(\theta, p; t) = \frac{p^2}{2mL^2} + mgL(1 - \cos\theta).$$

The Hamiltonian equations give

$$\begin{cases} \dfrac{\partial \mathcal{H}}{\partial \theta} = mgL\sin\theta = -\dot{p}, \\ \dfrac{\partial \mathcal{H}}{\partial p} = \dfrac{p}{2mL^2} = \dot{\theta}. \end{cases} \implies \ddot{\theta} = -\frac{g}{L}\sin\theta.$$

## 2.4 Geometry in Hamiltonian Mechanics

The Hamiltonian equations can be rewritten in a matrix form

$$\mathbb{J}\frac{\partial \mathcal{H}}{\partial x} = \dot{\mathbf{x}}, \quad \text{where } \mathbb{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \text{ and } \mathbf{x} = (\mathbf{q}, \mathbf{p})^T$$

is called the symplectic form. This reminds the mathematician the Hamiltonian is highly related to symplectic geometry (symplectic geometry was introduced by the Hamiltonian mechanics actually). The $2N$ dimensional space composed by the generalized position and momentum is called *phase space*, and can be described by geometry.

**Definition. Phase space**
The phase space is a smooth manifold $M$ equipped with a symplectic form $\omega$. As a result, a *Hamiltonian system* is denoted by a smooth manifold $M$, a symplectic form $\omega$, and a Hamiltonian $H$ $(M, \omega, H)$. The Lagrangian is the *symplectic potential* of the manifold.

The geometric framework underlying Hamiltonian and Lagrangian mechanics is both elegant and intricate. Recognizing that the phase space can be characterized as a symplectic manifold suffices for our present discussion, and we won't delve deeply into it here. Instead, let's shift our focus to *canonical transformations*, another pivotal theory within classical mechanics.

# 3 Classical Statistical Mechanics

Classical statistical mechanics bridges the gap between microscopic particle behavior and macroscopic properties. It utilizes statistical methods to analyze ensembles of particles, predicting collective behavior based on individual interactions. Key concepts include ensembles, Boltzmann distribution, and entropy, providing insights into phase transitions and thermodynamics. This framework is essential for understanding various phenomena in physics, chemistry, and engineering.

## 3.1 Canonical Transformations

Consider a transformation that maps the original coordinate $\mathbf{x}$ in the phase space to another $\vec{\xi}$

$$\mathbf{x} \mapsto \vec{\xi},$$

then the Hamiltonian equations becomes the following form

$$\frac{\partial \mathcal{H}}{\partial \mathbf{x}} = \frac{\partial \vec{\xi}}{\partial \mathbf{x}}^T \frac{\partial \mathcal{H}}{\partial \vec{\xi}}.$$

Therefore, we can derive the equation in transformed coordinate

$$\dot{\vec{\xi}} = \frac{\partial \vec{\xi}}{\partial \mathbf{x}} \mathbb{J} \frac{\partial \vec{\xi}}{\partial \mathbf{x}}^T \frac{\partial \mathcal{H}}{\partial \vec{\xi}}.$$

The form of the Hamiltonian equations is preserved if

$$\frac{\partial \vec{\xi}}{\partial \mathbf{x}} \mathbb{J} \frac{\partial \vec{\xi}}{\partial \mathbf{x}}^T = \mathbb{J}.$$

**Definition. Canonical transformation**
The transformations $\mathbf{x} \mapsto \vec{\xi}$ preserve the form of Hamiltonian equations, that is, satisfies the condition

$$\frac{\partial \vec{\xi}}{\partial \mathbf{x}} \mathbb{J} \frac{\partial \vec{\xi}}{\partial \mathbf{x}}^T = \mathbb{J}$$

are called *canonical transformations*.

**Remark.** The Hamiltonian with the transformed coordinate may have a different form but still satisfies the Hamiltonian equations.

An essential characteristic of canonical transformations is that the collection of them constitutes a *Lie group*. Moreover, the Hamiltonian equations being preserved means that the *symplectic structure* is preserved. This is the meaning of the word ”canonical”. Therefore, one can state that the *symplectic structure* is preserved by the action of a Lie group.

## 3.2 Liouville’s Theorem

Liouville’s theorem in statistical mechanics, named after Joseph Liouville, states that the phase space volume and density of a Hamiltonian system remain constant under canonical transformations. This principle is pivotal for understanding the dynamics of complex systems and plays a crucial role in modeling macroscopic behavior. Before discussing Liville’s theorem, we discuss another critical theorem in physics.

### 3.2.1 Noether’s Theorem

**Theorem 3.1. Noether’s theorem**
All continuous symmetries of the action of a conservative physical system have a corresponding conservation law. Mathematically, if the action is invariant under the transformation of a Lie group, then it has a corresponding conservative current $J$ so that $\partial_\mu J^\mu = 0$ on the corresponding manifold.

**Remark.** The conservation of momentum, angle momentum, and energy are the results of Noether’s theorem.

As mentioned above, the collection of canonical transformations is a Lie group and the Hamiltonian and the action have a continuous symmetry as a result. This is the *Liouvill's theorem*.

**Theorem 3.2. Liouville's theorem**
The distribution (or mathematically saying, measurement, physically saying, the density), of the phase space, is invariant under the canonical transformation. Concisely,

$$\int d^{2N}\mathbf{x} = \int d^{2N}\vec{\xi}.$$

Moreover, the measurement is uniform in the phase space.

Liouville's theorem asserts that the density of phase space remains unchanged through canonical transformations. Conceptually, phase space behaves akin to a *incompressible fluid* undergoing these transformations, as shown in Figure 1. This is not only an important consequence in statistical mechanics but also an important

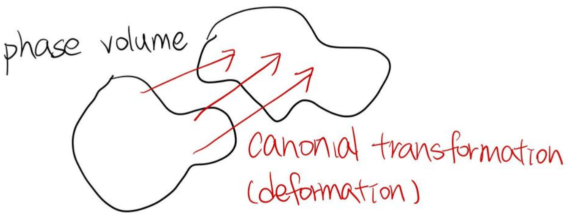



Figure 1: Phase volume behaves like the incompressible fluid.

result of symplectic geometry. The significance of this theorem is that **the density of the phase space is uniform even if the dimension (因次) of each degree of freedom may be different**. An important result of Liouville's theorem is *equipartition Theorem*.

### 3.2.2 Equipartition theorem

The equipartition theorem is a principle in statistical mechanics that describes the distribution of energy among the different degrees of freedom of a system in thermal equilibrium. Specifically, it states that, on average, each quadratic degree of freedom of a system will have an equal share of the total energy available, regardless of the specific form of the energy (kinetic or potential). In other words, for systems in equilibrium at a given temperature, the energy is equally distributed among all available modes of motion or storage.

**Theorem 3.3. Equipartition theorem**
Energy is partitioned equally amongst all energetically accessible degrees of freedom of a system.

The most intuitive example of the equipartition theorem is the *ideal gas*.

**Example 3.1. Ideal gas**
The energy of the *ideal gas* $E = \mathcal{H}$ is

$$E = \frac{3}{2}Nk_bT.$$

However, this statement is not precise. The precise statement is *the energy for three-dimensional ideal gas*. The precise expression of the energy of ideal gas is

$$E = \frac{d}{2}Nk_BT,$$

where $d$ is the dimension. The energy distributed in each degree of freedom is

$$\frac{1}{2}Nk_BT.$$

The degree of freedom can have an *arbitrary dimension*, angle (dimensionless), for instance.

# 4 Statistical Field Theory

Following our exploration of particle statistical mechanics, we now transition to a more sophisticated subject: statistical field theory. This advanced framework is employed to tackle systems featuring interactions and provides insights into phenomena like phase transitions.

## 4.1 Landau-Ginzburg Theory

The Landau-Ginzburg theory stands as a cornerstone in the realm of condensed matter physics and statistical mechanics, providing a powerful framework for understanding phase transitions and critical phenomena in various physical systems. Named after Lev Landau and Vitaly Ginzburg, who laid its foundations, this theory offers profound insights into the behavior of complex systems near critical points. At its core, the Landau-Ginzburg theory employs concepts from both classical field theory and statistical mechanics to describe the collective behavior of order parameters and fluctuations near phase transitions. By characterizing the free energy of a system in terms of an order parameter, it allows for the analysis of phase transitions in terms of symmetry-breaking phenomena. The Landau-Ginzburg theory has found wide-ranging applications across disciplines, from condensed matter physics to cosmology, and continues to be a fertile ground for theoretical exploration and experimental validation.

### 4.1.1 Partition Function

The partition function is a fundamental concept in statistical mechanics, serving as a central tool for describing the thermodynamic properties of a physical system. It encapsulates a wealth of information about the system's microscopic states and their corresponding energies, enabling the calculation of macroscopic observables such as temperature, pressure, and entropy. At its essence, the partition function represents the sum of the probabilities of all possible states accessible to the system, weighted by their corresponding energies. This sum effectively accounts for the multiplicity of states and their contributions to the system's overall behavior. In statistical mechanics, the partition function plays a pivotal role in connecting the microscopic world of individual particles or degrees of freedom to the macroscopic properties observed in thermodynamics. Through various mathematical manipulations and techniques, such as the canonical ensemble or the grand canonical ensemble, physicists can extract valuable insights into the thermodynamic behavior of complex systems from the partition function. The partition function concept finds wide-ranging applications across physics, chemistry, and engineering, providing a versatile and powerful tool for analyzing and predicting the behavior of diverse physical systems, from simple gases to complex materials and beyond. The mathematical details of the partition will be skipped here.

### 4.1.2 Symmetry and Phase

As mentioned above, we can use a partition to define a system. I denote the partition function as $\mathcal{Z}$ in this note. The partition function in Landau-Ginzburg theory can be written as the *functional integral of the mean fields*, the mean fields are fields that approximate a system's behavior by considering a large number of degrees of freedom

$$\mathcal{Z} = \int \mathcal{D}\phi \exp\left[ - N\beta \int F[\phi(x)]dx\right] = \int \mathcal{D}\phi \; e^{-N\beta L[\phi]},$$

where $L$ is a functional of the mean fields.
The functional integral is very difficult to compute, so we use the *saddle point approximation* to approximate the partition function, that is, use the relation

$$\mathcal{Z} \approx \sum_i \; e^{-N\beta L[\phi_i]},$$

where $\phi_i$ are the mean fields so that

$$\left.\frac{\delta L}{\delta\phi}\right|_{\phi_i} = 0.$$

A simple non-trivial example is *fourth order Landau theory.*

**Example 4.1. Fourth order Landau theory**
The partition function is

$$\mathcal{Z} = A\int dy \; e^{-N\beta L[y]},$$

where $L$ is the Landau free energy and can be expressed as

$$L = a_1 m + \frac{1}{2}a_2 m^2 + \frac{1}{4}a_4 m^4.$$

The saddle point approximation is

$$\mathcal{Z} \approx \sum_i e^{-N\beta L[m_i]},$$

where $\partial L/\partial m|_{m_i} = 0$. The partition function is almost determined by the extreme value points. First, consider $a_1 = 0$, that is, no external field. The extreme value can have two ways to change from one global extreme value point to two global extreme value points when the coefficients $a_2$ and $a_4$ are modified, as shown in Figure 2. The first way is changing continuously and gradually and another one is changing discretely and directly. When the global extreme value point changes from one point (or conversely) to two points, the *phase transition* happens. These two changing ways correspond to two kinds of phase transition, *first order* and second order.

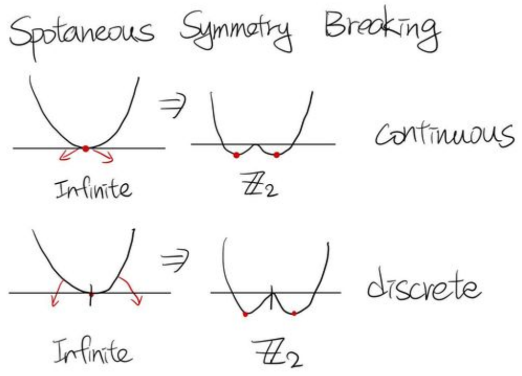



Figure 2: Spontaneous symmetry breaking.

The mathematical description of phase transition here is "symmetry breaking", we can see that the symmetry of the global extreme points changes from infinite symmetry to $\mathbb{Z}_2$. Since there is no external field, this kind of symmetry breaking is called *spontaneous symmetry breaking*.
When $a_1 \neq 0$, that is, there exists an external field. The principle is the same and is shown in Figure 3. But the symmetry breaks from $\mathbb{Z}_2$ to no symmetry. The symmetry breaking led to by the external field is called *explicit symmetry breaking*.

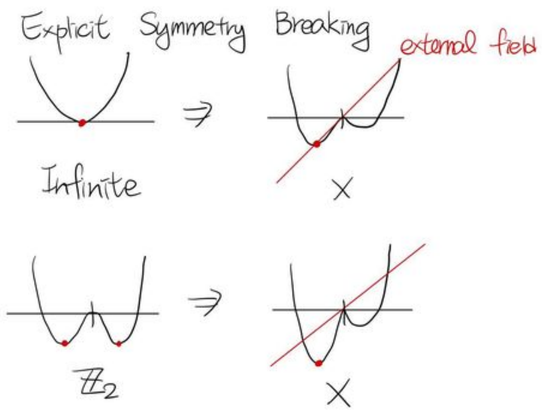



Figure 3: Explicit symmetry breaking.

## 4.2 Topological Order

*Topological order* represents a departure from Landau's theory of phase transitions. While Landau's theory categorizes phases based on symmetry and describes phase transitions as symmetry breaking, scientists have observed that certain materials exhibit distinct phases despite lacking symmetry or symmetry breaking. In response to this discovery, a new framework emerged to explain such phenomena, known as *topological order*. When the field structure becomes complex the symmetry may be hard to characterize.

**Example 4.2. Topological Defect**
The partition function is

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]/\hbar},$$

where $S$ is the action and can be expressed as

$$S = \int (|\nabla\phi|^2 - \lambda|\phi|^2 + \Delta)dx.$$

This is very hard to use the saddle point approximation and there is no symmetry in this model.

In this field, defining symmetry is not straightforward; rather, phase transitions are characterized by changes in the topological invariants of the manifold where the field is defined. These transitions are intricately tied to alterations in topological invariants, reflecting shifts in the system's underlying structure. Here, topology assumes the role of elucidating the macroscopic state of matter, capturing its global properties that transcend local details. The notion of topological order provides a comprehensive framework, employing geometry and homotopy to classify vector bundles of the *moduli space*. Through this lens, the complex interplay between spatial arrangements and intrinsic properties becomes apparent, offering profound insights into the collective behavior of matter. The applications of topological order are diverse and profound, ranging from the exotic phenomena of the Quantum Hall effect to the elusive properties of spin liquids. These phenomena underscore the fundamental role played by topological order in understanding and predicting the behavior of diverse systems. Despite its elegance and utility, topological order continues to be an active and vibrant research field, attracting the attention of physicists and mathematicians alike. Its ability to reveal deep connections between seemingly disparate systems and phenomena ensures its enduring relevance in the pursuit of understanding the fundamental nature of matter.

## References

[1] Landau, Lev Davidovich, Evgeniĭ Mikhaĭlovich Lifshits, and Evgeniĭ Mikhaĭlovich Lifshits. Mechanics. Vol. 1. CUP Archive, 1960.

[2] Goldstein, Herbert. Classical mechanics. Pearson Education India, 2011.

[3] Altland, Alexander, and Ben D. Simons. Condensed matter field theory. Cambridge university press, 2010.

[4] Wen, Xiao-Gang. Quantum field theory of many-body systems: From the origin of sound to an origin of light and electrons. OUP Oxford, 2004.

[5] Goldenfeld, Nigel. Lectures on phase transitions and the renormalization group. CRC Press, 2018.