# Legendre Transformation under Micro Canonical Ensemble

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***Abstract*—The Legendre transformation is a crucial tool in theoretical physics, known for its symmetry, especially when applied to multivariate functions. In statistical mechanics, ensembles represent the central focus. Leveraging the dimensionless aspect of Legendre transformation, this paper explores the transformation process from the entropy characteristic function of microcanonical ensembles to the analogous definition of partition function transformation. Additionally, it derives characteristic functions, partition functions, and establishes their interrelations, along with deriving corresponding thermodynamic formulas for various ensembles. This streamlined approach sheds light on the fundamental principles of statistical mechanics and underscores the symmetry inherent in Legendre transformation.**

## I. Introduction

The Lagrange transformation, attributed to the pioneering work of Joseph-Louis Lagrange in the late 18th century[1,2,3], stands as a fundamental concept in classical mechanics, offering a powerful mathematical framework for the analysis of dynamic systems. This transformation serves as a cornerstone in the field, providing a means to elegantly describe and solve complex physical problems by converting the system's representation from Cartesian coordinates to generalized coordinates and momenta.

Introduced as part of Lagrange's efforts to reformulate classical mechanics, the Lagrange transformation offers a more streamlined approach to solving problems involving the motion of particles and rigid bodies. By expressing the system's dynamics in terms of generalized coordinates and momenta, rather than traditional position and momentum variables, the transformation enables a more comprehensive and intuitive understanding of the underlying physics[4,5,6].

Through the lens of the Lagrange transformation, Hamilton's principle becomes a central guiding principle, allowing for the derivation of Hamilton's equations of motion. These equations, in turn, provide a concise and powerful framework for describing the evolution of a system over time, offering insights into the underlying dynamics and enabling the prediction of future states.

In this paper, we explore the historical context and theoretical underpinnings of the Lagrange transformation, its mathematical formulation, and its practical applications in classical mechanics. By elucidating the principles and techniques involved, we aim to provide a comprehensive understanding of this fundamental concept and its significance in the broader context of theoretical physics[7,8,9,10]. The Lagrange transformation originates from the following partial differential equation:

$$R\frac{\partial^2 z}{\partial x^2}+S\frac{\partial^2 z}{\partial x\partial y}+T\frac{\partial^2 z}{\partial y}=0 \quad (1.1)$$

Where, if we let $p=\frac{\partial z}{\partial x}$ and $q=\frac{\partial z}{\partial y}$, and further assume that $R$, $S$, and $T$ are only functions of $p$ and $q$, then for the tangent plane of the surface $z=f(x,y)$ given by:

$$px+qy+z-v=0 \quad (1.2)$$

There should exist:

$$R\frac{\partial^2 v}{\partial q^2}-S\frac{\partial^2 v}{\partial p\partial q}+T\frac{\partial^2 v}{\partial q^2}=0 \quad (1.3)$$

Eq. (1.2) provides a transformation between the variables $x$, $y$, and their conjugate variables $p$, $q$. Specifically, the transformation can be expressed as the partial derivatives:

$$\frac{\partial z}{\partial x}=p,\quad \frac{\partial z}{\partial y}=q\quad ,\frac{\partial v}{\partial p}=x,\quad \frac{\partial v}{\partial q}=y \quad (1.4)$$

Considering the Jacobian matrices of the transformation should be mutually inverse, i.e.,

$$\begin{pmatrix}\frac{\partial p}{\partial x} & \frac{\partial p}{\partial y}\\ \frac{\partial q}{\partial x} & \frac{\partial q}{\partial y}\end{pmatrix}=\begin{pmatrix}\frac{\partial z^2}{\partial x^2} & \frac{\partial z^2}{\partial x\partial y}\\ \frac{\partial z^2}{\partial x\partial y} & \frac{\partial z^2}{\partial y^2}\end{pmatrix},\begin{pmatrix}\frac{\partial x}{\partial p} & \frac{\partial y}{\partial p}\\ \frac{\partial x}{\partial q} & \frac{\partial y}{\partial q}\end{pmatrix}=\begin{pmatrix}\frac{\partial v^2}{\partial p^2} & \frac{\partial v^2}{\partial p\partial q}\\ \frac{\partial v^2}{\partial p\partial q} & \frac{\partial v^2}{\partial q^2}\end{pmatrix}$$

We obtain:

$$\frac{\partial^2 z}{\partial x^2}=\frac{1}{\Delta}\frac{\partial^2 v}{\partial q^2}$$
$$\frac{\partial^2 z}{\partial x\partial y}=\frac{1}{\Delta}\frac{\partial^2 v}{\partial p\partial q}$$
$$\frac{\partial^2 z}{\partial y^2}=\frac{1}{\Delta}\frac{\partial^2 v}{\partial p^2}$$

and

$$\Delta=\left\|\begin{pmatrix}\frac{\partial^2 v}{\partial p^2} & \frac{\partial^2 v}{\partial p\partial q}\\ \frac{\partial^2 v}{\partial p\partial q} & \frac{\partial^2 v}{\partial q^2}\end{pmatrix}\right\|$$

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This transformation converts a quasi-linear Eq. (1.1) into a linear Eq.(1.3).

## II. LAGRANGE TRANSFORMATION

We have

$$y = y(x) \quad (2.1)$$

$$y' = t = \frac{dy}{dx} \quad (2.2)$$

$$u = u(t) \quad (2.3)$$

$$u' = \frac{du}{dt} \quad (2.4)$$

From (2.2), solve for x as a function of t and substitute into the following

$$u = xt - y \quad (2.5)$$

Differentiating the expression $u = xt - y$ with respect to $t$, we get:

$$\begin{aligned} du &= xdt + tdx - \frac{dy}{dx}dx \\ &= xdt + (t - \frac{dy}{dx})dx \\ &= xdt \end{aligned}$$

From this, it's evident that $u$ is a function of $t$, and its derivative with respect to $t$ is $x$. Eq. (2.5) determines a transformation between the variables $u$, $y$, $x$, and $t$. It maps $y = y(x)$ to

$$t = t(x), \quad u = u(t) \quad (2.6)$$

Similarly,$y = xt - u$ from Eq.(2.5), it follows that it defines another transformation that is the inverse of the one above. Hence, these two transformations are mutually inverse, and their relation is symmetric.

The Legendre transformation has a property: if two curves are tangent on the $x$-$y$ plane, then after transformation to the $u$-$t$ plane, they are also tangent, and vice versa. Transformations with this property are called contact transformations. The Legendre transformation is a special case of contact transformations.

Extending the above ideas to the case of multiple variables, consider a function $U$ of $n$ variables $q_1, q_2, \ldots, q_n$, which has continuous partial derivatives up to the second order. Let $U$ be transformed into a new set of variables $Q_1, Q_2, \ldots, Q_n$ according to the equation:

$$Q_i = \frac{\partial U}{\partial q_i}, (i = 1, 2, \ldots, n) \quad (2.7)$$

They constitute a set of transformations with respect to the original variables $q_1, q_2, \ldots, q_n$. The Jacobian determinant of these transformations with respect to the original variables $q_1, q_2, \ldots, q_n$ is given by:

$$\left\| \frac{\partial Q_i}{\partial q_j} \right\| = \left\| \frac{\partial^2 U}{\partial q_i \partial q_j} \right\|$$

From Eq.(2.7), the original variables can be solved out as

$$q_i = q_i(Q_1, Q_2, \ldots, Q_n), \quad (i = 1, 2, \ldots, n) \quad (2.8)$$

Considering the new function:

$$U^C = \sum_{i=1}^{n} Q_i \cdot q_i - U \quad (2.9)$$

Differentiating the above equation, we get:

$$dU^C = \sum_{i=1}^{n} \frac{\partial U^C}{\partial q_i} dq_i = \sum_{i=1}^{n} \partial q_i \, dQ_i$$

We have thus demonstrated:

$$q_i = \frac{\partial U^C}{\partial Q_i} \quad (i = 1, 2, \ldots, n) \quad (2.10)$$

The relationship between two functions $U$ and $U^C$ is given by Eq.(2.9). The corresponding relationships between variables and functions are respectively given by Eqs.(2.7) and (2.10). They encapsulate many duality relationships in mechanics and physics.

## III. THE SYMMETRY OF LEGENDRE TRANSFORM

Multivariable function: $\Phi = \Phi(x_1, x_2, \ldots, x_n)$, where $x_i$ $(i = 1, 2, \ldots, n)$ are independent variables. For convenience, let's assume $\Phi$ is smooth and differentiable in $N$-dimensional space, such that at each point, $s_i = \frac{\partial \Phi}{\partial x_i} = \frac{\partial \Phi}{\partial x_i}$, then

$$d\Phi = \sum_{i=1}^{n} \frac{\partial \Phi}{\partial x_i} dx_i = \sum_{i=1}^{n} s_i dx_i \quad (3.1)$$

[11,12]

If we take $m$ $(m \leq n)$ of the variables from the function $\Phi = \Phi(x_1, x_2, \ldots, x_n)$, the independent variables $x_j$ $(j = 1, 2, \ldots, m)$ are replaced by their corresponding variables $s_j$, forming a new function $\Psi$, defined by $L_j : \Phi(x_1, x_2, \ldots, x_m, x_{m+1}, \ldots, x_n) \rightarrow \Psi(s_1, s_2, \ldots, s_m, x_{m+1}, \ldots, x_n)$, where

$$\Psi = \sum_{j=1}^{m} s_j x_j - \Phi \quad (3.2).$$

Considering Eq.(3.1), we have $d\Psi = \sum_{j=1}^{m}(s_j dx_j + x_j ds_j) - \sum_{i=1}^{n} s_i dx_i$, where $j = 1, 2, \ldots, m$; $i = 1, 2, \ldots, n$; and $m \leq n$. Simplifying, we get

$$d\Psi = \sum_{j=1}^{m} x_j ds_j - \sum_{i=m+1}^{n} s_i dx_i \quad (3.3).$$

Since any given set of variables uniquely determines a function, different functions are essentially distinguished by their sets of independent variables. Therefore, the differential form of any function can be expressed as

$$d\Psi = \sum_{j=1}^{m} \frac{\partial \Psi}{\partial s_j} ds_j + \sum_{i=m+1}^{n} \frac{\partial \Psi}{\partial x_i} dx_i \quad (3.4).$$

Comparing the first half of Eq. (3.4) with Eq. (3.3), we find $x_j = \frac{\partial \Psi}{\partial s_j}$, which corresponds to $s_j = \frac{\partial \Phi}{\partial x_j}$. This shows that the two variables before and after the transformation are interrelated. Additionally, Eq. (3.2) can be rewritten as

$$\Phi + \Psi = \sum_{j=1}^{m} s_j x_j \quad (3.5)$$

The functions before and after the transformation are equivalent, demonstrating the clear symmetry of the Legendre transformation.

## IV. Legendre transformation enters statistical mechanics

The ensemble method is a core concept in the teaching of statistical mechanics, generally studying three ensembles: microcanonical ensemble, canonical ensemble, and grand canonical ensemble. For a system with $n$ independent variables, the number $N$ of equivalent characteristic functions is given by

$$N = \sum_{i=0}^{n} C_i^n = 2^n \quad (4.1)$$

For a uniform system with three independent variables, there are 8 equivalent characteristic functions, implying a total of 8 ensembles. Starting from the fundamental relationship of the microcanonical ensemble, this paper utilizes the Legendre transformation of entropy and analogously defines the transformation of the partition function, while obtaining the characteristic functions and partition functions of various ensembles.

The characteristic function of the microcanonical ensemble is entropy, with the corresponding thermodynamic formula:

$$S = k \ln \Omega(E, V, N) \quad (4.2)$$

It is often challenging to derive other functions from entropy using Legendre transformation. Due to historical reasons, the variables involved in Legendre transformation do not always appear in pairs. For example, the energy $E$ of a system is paired with the reciprocal of temperature ($\beta = 1/kT$, where $k$ is the Boltzmann constant). However, temperature is commonly used in many relationships, such as the familiar equation $F = E - TS$, which relates free energy and entropy but obscures the symmetry between $\beta$ and $E$. If we define dimensionless quantities: $S' = S/k$, $F' = \beta F$, their duality can be perfectly represented as $F'(\beta) + S'(E) = \beta E$. Therefore, we rewrite Eq. (4.2) as

$$S/k = \ln \Omega(E, V, N) \quad (4.3)$$

In differential form:

$$d \ln \Omega(E, V, N) = dS(k) = \beta dE + \gamma dV + \alpha dN \quad (4.4)$$

Starting from the dimensionless quantity $S'$, using Legendre transformation to obtain other dimensionless quantities, we have 3 pairs of corresponding variables: $\beta, E$; $\alpha, N$; $\gamma, V$. To express the dimensionless quantities as characteristic functions in statistical mechanics, we also need to know the common expressions of $\beta, \alpha, \gamma$. From the thermodynamic formula $dS = (1/T)dE + (p/T)dV - (\mu/T)dN$, we obtain

$$dS(k) = (1/kT)dE + (p/kT)dV - (\mu/kT)dN \quad (4.5)$$

Comparing Eqs. (4.4) and (4.5), we have

$$\beta = 1/kT, \quad \gamma = \beta p, \quad \alpha = -\beta\mu \quad (4.6)$$

Then Eq. (4.4) becomes

$$d \ln \Omega = dS(k) = \beta dE + \beta p dV - \beta \mu dN$$

From this equation, we derive:

$$\beta = \left.\frac{\partial \ln \Omega}{\partial E}\right|_{V,N}, \quad p = \left.\frac{1}{\beta}\frac{\partial \ln \Omega}{\partial V}\right|_{E,N}, \quad \mu = -\left.\frac{1}{\beta}\frac{\partial \ln \Omega}{\partial N}\right|_{E,V}$$

## V. The Application of Legendre Transform in Statistical Mechanics

Starting from $S_k(E, V, N)$ and performing Legendre transformations to other functions, we can analogously define the transformation of partition functions.

5.1 Transformation of characteristic functions

There are a total of 7 characteristic functions equivalent to $S_k(E, V, N)$, denoted by $x_1 = E$, $x_2 = V$, $x_3 = N$, $s_1 = \beta$, $s_2 = \gamma$, $s_3 = \alpha$.

5.1.1 Transformation of microcanonical ensemble characteristic functions

The characteristic function of the microcanonical ensemble is entropy, and there are 3 possible Legendre transformations when changing one variable of $S_k(E, V, N)$, corresponding to 3 characteristic functions and 3 ensembles.

If the variable transformation is $E \to \beta$, meaning only energy exchange between the system and the surroundings, we have from Eq. (3.5):

$$\Psi_1(\beta, V, N) + S_k(E, V, N) = \beta E \quad (5.1)$$

Rewriting this as $\Psi_1(\beta, V, N) = \beta E - S_k(E, V, N)$ and substituting $\beta = 1/kT$, we get:

$$\Psi_1(\beta, V, N) = \beta E - \beta TS = \beta(E - TS) \quad (5.2)$$

Letting $\Psi_1 = \beta F$, we obtain $F + TS = E$, which is the familiar thermodynamic equation. Here, $F(T, V, N)$ is the Helmholtz free energy, the characteristic function of the canonical ensemble. From equation (3), we get the differential equation for the function: $d\Psi_1 = Ed\beta - \gamma dV - \alpha dN$, and considering $\gamma = \beta p$, $\alpha = -\beta\mu$, we have:

$$d\Psi_1 = Ed\beta - \beta p dV + \beta \mu dN \quad (5.3)$$

If we substitute $\Psi_1 = \beta F$ into this equation, we get $dF = -SdT - pdV + \mu dN$, which is the familiar differential equation for the Helmholtz free energy.

If the variable transformation is $V \to \gamma$, meaning only force interactions between the system and the surroundings, we obtain a new ensemble characterized by:

$$\Psi_2(E, \gamma, N) + S_k(E, V, N) = \gamma V$$

If the variable transformation is $N \to \alpha$, meaning only particle number exchange between the system and the surroundings, we obtain another new ensemble characterized by:

$$\Psi_3(E, V, \alpha) + S_k(E, V, N) = \alpha N$$

5.1.2 Transformation of characteristic functions by changing two variables

If we change two variables of $S_k(E,V,N)$, there are 3 possible Legendre transformations, corresponding to 3 characteristic functions and 3 ensembles.

If the variable transformation is $E \to \beta$, $V \to \gamma$, meaning only energy exchange and force interactions between the system and the surroundings, we have from Eq. (3.5):

$$\Psi_4(\beta,\gamma,N) + S_k(E,V,N) = \beta E + \gamma V$$

Letting $\Psi_4 = \beta G$ and substituting $\beta = 1/kT$, $\gamma = \beta p$, we obtain $G + TS = E + pV$, where $G$ is the Gibbs function, a familiar thermodynamic quantity.

If the variable transformation is $E \to \beta$, $N \to \alpha$, meaning only energy exchange and particle number exchange between the system and the surroundings, we obtain another ensemble characterized by:

$$\Psi_5(\beta,V,\alpha) + S_k(E,V,N) = \beta E + \alpha N$$

Letting $\Psi_5 = \beta J$ and substituting $\beta = 1/kT$, $\alpha = -\beta\mu$, we obtain $J + TS = E - \mu N$, where $J(T,V,\mu)$ is the grand canonical potential, precisely the characteristic function of the grand canonical ensemble.

If the variable transformation is $V \to \gamma$, $N \to \alpha$, meaning only force interactions and particle number exchange between the system and the surroundings, we obtain another ensemble characterized by:

$$\Psi_6(E,\gamma,\alpha) + S_k(E,V,N) = \gamma V + \alpha N$$

5.1.3 Transformation of characteristic functions by changing three variables

If we change three variables of $S_k(E,V,N)$, there is 1 possible Legendre transformation, corresponding to 1 characteristic function and 1 ensemble.

If the variable transformation is $E \to \beta$, $V \to \gamma$, $N \to \alpha$, meaning energy exchange, force interactions, and particle number exchange between the system and the surroundings, we obtain another ensemble characterized by:

$$\Psi_7(\beta,\gamma,\alpha) + S_k(E,V,N) = \beta E + \gamma V + \alpha N$$

This last Legendre transformation changes three variables, resulting in the zero ensemble. Therefore, there are effectively 7 ensemble distributions.

5.2 Transformation of partition functions

Considering $\beta = 1/kT$, the partition function of the microcanonical ensemble is $\Omega(E,V,N) = e^{S_k} = e^{\beta TS}$.

If the variable transformation is $E \to \beta$, the characteristic function is transformed from $S_k(E,V,N)$ to $\Psi_1(\beta,V,N)$ as follows:

$$\Psi_1(\beta,V,N) = \beta E - \beta TS = \beta F \quad (5.4)$$

Correspondingly, the partition function $\Omega(E,V,N)$ is transformed to:

$$Z(\beta,V,N) = \sum_E \Omega(E,V,N)e^{-\beta E} = \sum_E e^{\beta TS}e^{-\beta E} \quad (5.5)$$

which is the partition function of the canonical ensemble.

Similarly, by analogy with Legendre transformations of characteristic functions, we can derive the partition functions of other ensembles.

If the variable transformation is $V \to \gamma$, the partition function is transformed to:

$$A(E,\gamma,N) = \sum_E \Omega(E,V,N)e^{-\gamma V}$$

If the variable transformation is $N \to \alpha$, the partition function is transformed to:

$$B(E,V,\alpha) = \sum_E \Omega(E,V,N)e^{-\alpha N}$$

If the variable transformation is $E \to \beta$, $V \to \gamma$, the partition function is transformed to:

$$C(\beta,\gamma,N) = \sum_E \Omega(E,V,N)e^{-\beta E}e^{-\gamma V}$$

If the variable transformation is $E \to \beta$, $N \to \alpha$, the partition function is transformed to:

$$\Xi(\beta,V,\alpha) = \sum_E \Omega(E,V,N)e^{-\beta E}e^{-\alpha N}$$

which is the partition function of the grand canonical ensemble.

If the variable transformation is $V \to \gamma$, $N \to \alpha$, the partition function is transformed to:

$$D(E,\gamma,\alpha) = \sum_E \Omega(E,V,N)e^{-\gamma V}e^{-\alpha N}$$

If the variable transformation is $E \to \beta$, $V \to \gamma$, $N \to \alpha$, the partition function is transformed to:

$$M(\beta,\gamma,\alpha) = \sum_E \Omega(E,V,N)e^{-\beta E}e^{-\gamma V}e^{-\alpha N}$$

5.3 Relationship between partition functions and characteristic functions

For the partition function of the canonical ensemble given in Eq. (5.5), taking the logarithm of both sides:

$$\ln Z(\beta,V,N) = \beta TS - \beta E = -\beta(E - TS)$$

Considering Eq. (5.3), we have the relationship between the partition function and the characteristic function of the canonical ensemble:

$$\ln Z(\beta,V,N) = -\Psi_1(\beta,V,N) = -\beta F \quad (5.6)$$

Therefore, the characteristic function $F = -kT\ln Z(\beta,V,N)$, which is an important expression for thermodynamic quantities in the canonical ensemble. Considering Eq.(5.2), we have the thermodynamic formulas for the canonical ensemble:

$$E = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{V,N}, \quad p = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial V}\right)_{\beta},$$

$$\mu = -\frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial N}\right)_{\beta} \quad (5.7)$$

which are consistent with what we learned in statistical mechanics.

Similarly, by analogy with Legendre transformations of characteristic functions, we can derive the relationships between partition functions and characteristic functions for other ensembles along with their corresponding thermodynamic formulas.

## VI. Conclusion

By deducing the Legendre transform and its application in multivariate functions in statistical mechanics, we can further understand the symmetry and universality of the Legendre transformation. From the above introduction, the transformation of characteristic functions unifies with the transformation of partition functions as introduced in statistical mechanics. From a mathematical perspective, transitioning from one ensemble to another in statistical mechanics is essentially a Legendre transformation involving variable transformations. Moreover, Legendre transformation does not alter the properties of the system. Therefore, from this perspective, these ensembles are equivalent.

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