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HAMILTON-JACOBI FORMALISM FOR THERMODYNAMICS: A DETAILED THEORETICAL AND APPLIED STUDY

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ABSTRACT:

This study develops the Hamilton-Jacobi (HJ) formalism specifically for thermodynamics, inspired by its effectiveness in classical mechanics and optics. By recasting thermodynamic laws within a geometric context using contact manifolds and Legendre transformations, traditional equations of state emerge naturally as solutions to the HJ equation. Detailed examples for the ideal gas, van der Waals gas, and Curie-Weiss magnet demonstrate the method's capability and insight. Discussions include the concept of "thermodynamic time," the benefits of a geometric unified viewpoint, and potential avenues for future research in generalized and quantum thermodynamics.

Keywords: *Hamilton-Jacobi, thermodynamics, Legendre transform, contact geometry, equations of state, geometric thermodynamics, phase space, statistical mechanics.*

INTRODUCTION

Conjugate variables and potential functions are the fundamental building blocks of both classical mechanics and thermodynamics. Although thermodynamics is often taught through empirical laws and partial derivatives, advances have revealed that it can also be framed using the Hamilton-Jacobi approach from mechanics. This geometric perspective unifies the derivation of equations of state, thermodynamic potentials, and transformations between these potentials. The objectives of this work include: • Introducing the Hamilton-Jacobi formalism in thermodynamics incrementally. • Building the necessary geometric framework with contact manifolds and Legendre transformations. • Applying the approach to common physical systems. • Clarifying the physical insights and suggesting extensions. The present work aims to:

- Introduce the HJ formalism in thermodynamics step by step.
- Develop the geometric background using contact manifolds and Legendre transforms.
- Apply the framework to canonical physical systems.
- Clarify the physical interpretation and propose extensions.

THEORETICAL BACKGROUND

A. Conjugate Variables and Thermodynamic Potentials

In thermodynamics, state variables appear in conjugate pairs:
- (S, T) (entropy, temperature)
- (V,−P) (volume, pressure)
- (N, μ) (number, chemical potential)

These conjugate pairs are essential for the geometric analogy with mechanics, where variables like (q, p) (coordinate, momentum) play a similar role.
The first law of thermodynamics reads:

$$dU = TdS - PdV + \mu dN \qquad (1)$$

where U is internal energy, T is temperature, S is entropy, P is pressure, V is volume, N is the number of particles, and μ is the chemical potential.

Thermodynamic potentials—internal energy (U), enthalpy ($H = U + PV$), Helmholtz

free energy ($F = U - TS$), Gibbs free energy ($G = U + PV - TS$)—are related by **Legendre transforms**. The Legendre transform exchanges one variable for its conjugate.
For example:

$$F(T, V, N) = U(S, V, N) - TS \quad (2)$$

Differentiating, we obtain:

$$dF = -SdT - PdV + \mu dN \quad (3)$$

Each thermodynamic potential is useful for a different set of controlled variables.

B. Hamiltonian Mechanics and the Hamilton-Jacobi Equation

In classical mechanics, the Hamiltonian H (q, p, t) generates motion via:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad (4)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (5)$$

The Hamilton-Jacobi equation is a reformulation of mechanics in terms of a generating function S (q, t), the principal function (or action):

$$H\left(q, \frac{\partial S}{\partial q}, t\right) + \frac{\partial S}{\partial t} = 0 \quad (6)$$

Solving the HJ equation gives the action S whose derivatives yield the equations of motion. This method is particularly powerful for integrating systems analytically and for finding canonical transformations.

C. Contact Geometry and the Thermodynamic Phase Space

The geometric analogy with mechanics is deepened by the use of contact geometry, rather than symplectic geometry, because thermodynamic phase space is odd-dimensional. For a system with n degrees of freedom, there are 2n + 1 thermodynamic variables (e.g., U, S, V for a simple gas).
The contact 1-form encodes the first law:

$$\alpha = dU - TdS + PdV - \mu dN \quad (7)$$

The physical state of the system corresponds to a submanifold where $\alpha = 0$.
A Legendre submanifold is defined by a fundamental relation (e.g., $U = f(S, V, N)$).
Legendre transforms correspond to canonical transformations in this context, allowing change of variables and potentials.

HAMILTON-JACOBI FORMALISM IN THERMODYNAMICS

A. General Construction

The key idea is that for a family of substances (or systems), we can write a single relation, often called the "Hamiltonian," that connects all the relevant variables:

$$H(U, S, V, N; \alpha_i) = 0 \quad (8)$$

where α_i are material parameters (e.g., a, b for van der Waals gas). This relation is the Hamilton-Jacobi equation for thermodynamics.
Given $U = f(S, V, N; \alpha_i)$, the conjugate variables are:

$$T = \left(\frac{\partial U}{\partial S}\right)_{V,N} \quad (9)$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_{S,N} \quad (10)$$

$$\mu \equiv \left(\frac{\partial U}{\partial N}\right)_{S,V} \quad (11)$$

The equations of state for temperature, pressure, and chemical potential thus follow from partial derivatives of the fundamental relation U.

The analogy with mechanics is sharpened by realizing that the "HJ equation" in mechanics provides all the integrals of motion for a system, while in thermodynamics the analogous equation provides all equations of state.

B. Thermodynamic Time and Characteristics

In the context of the HJ formalism, the solutions to the equation define "characteristic curves" in the thermodynamic phase space. These characteristics can be parameterized by an arbitrary variable, which, although not physical time, is sometimes referred to as "thermodynamic time" due to its role in generating changes in the thermodynamic variables.

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This viewpoint is valuable for understanding irreversible processes, entropy production, and for exploring extensions to non-equilibrium thermodynamics.

APPLICATIONS: EXPLICIT HAMILTON-JACOBI EQUATIONS AND DERIVATIONS

A. The Ideal Gas

The ideal gas is described by:

$$PV = nRT \tag{12}$$

$$U = \frac{3}{2}nRT \tag{13}$$

where n is the number of moles, *R* is the gas constant, *T* is the temperature, *P* the pressure, and *V* the volume.

1. Sackur-Tetrode Entropy and Inversion

The Sackur-Tetrode equation for the entropy *S* of a monoatomic ideal gas is:

$$S = Nk\left[\ln\left(\frac{V}{N}\left(\frac{4\pi mU}{3Nh^2}\right)^{3/2}\right) + \frac{5}{2}\right] \tag{14}$$

where *N* is particle number, k Boltzmann's constant, m the particle mass, *h* Planck's constant.
To derive the Hamilton-Jacobi equation for the ideal gas, solve for *U*:

$$S - Nk\left[\ln\left(\frac{V}{N}\right) + \frac{3}{2}\ln\left(\frac{4\pi mU}{3Nh^2}\right) + \frac{5}{2}\right] = 0 \tag{15}$$

$$\ln\left(\frac{4\pi mU}{3Nh^2}\right)^{3/2} = \frac{S}{Nk} - \ln\left(\frac{V}{N}\right) - \frac{5}{2} \tag{16}$$

$$U = \frac{3Nh^2}{4\pi m} exp\left(\frac{2}{3}\left(\frac{S}{Nk} - \ln\left(\frac{V}{N}\right) - \frac{5}{2}\right)\right) \tag{17}$$

Thus, the HJ equation is:

$$U - \frac{3Nh^2}{4\pi m}\exp\frac{2}{3}\left(\frac{S}{Nk} - \ln\left(\frac{V}{N}\right) - \frac{5}{2}\right) = 0 \tag{18}$$

2. Equations of State via HJ Formalism

From the HJ equation, the thermodynamic equations of state are:
Calculating explicitly:

$$T = \left(\frac{\partial U}{\partial S}\right)_{V,N} \tag{19}$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_{S,N} \tag{20}$$

Calculating explicitly:

$$\frac{\partial U}{\partial S} = U.\frac{2}{3Nk} = \frac{2U}{3Nk} \tag{21}$$

$$T = \frac{2U}{3Nk} \tag{22}$$

Using $U = \frac{3}{2}nRT$, we recover *T* as expected.
For pressure:

$$\frac{\partial U}{\partial V} = -U.\frac{2}{3}\frac{1}{V} = \frac{-2U}{3V} \tag{23}$$

$$P = \frac{2U}{3V} \tag{24}$$

Which is equivalent to the ideal gas law $PV = nRT$.

B. The van der Waals Gas

The van der Waals equation for real gases is:

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT \tag{25}$$

where a and b are constants characterizing intermolecular interactions.

1. Entropy and HJ Equation for van der Waals Gas

Integrating the first law for a van der Waals gas, we obtain the entropy:

$$S = S_0 + Nk\ ln\left[\frac{(V-nb)\left(U+a\frac{n^2}{V}\right)^{3/2}}{N^{5/2}}\right] \tag{26}$$

To find the HJ equation, solve for U:

$$ln\left[(V-nb)\left(U+a\frac{n^2}{V}\right)^{3/2}\right]=\frac{S-S_0}{Nk}+\frac{5}{2}\,ln\,N \quad (27)$$

$$(V-nb)\left(U+a\frac{n^2}{V}\right)^{3/2}=N^{5/2}\exp\left(\frac{S-S_0}{Nk}\right) \quad (28)$$

$$U+a\frac{n^2}{V}=\left[\frac{N^{5/2}}{(V-nb)}\exp\left(\frac{S-S_0}{Nk}\right)\right]^{2/3} \quad (29)$$

$$U=\left[\frac{N^{5/2}}{(V-nb)}\exp\left(\frac{S-S_0}{Nk}\right)\right]^{2/3}-a\frac{n^2}{V} \quad (30)$$

Thus, the HJ equation is:

$$U+a\frac{n^2}{V}-\left[\frac{N^{5/2}}{(V-nb)}\exp\left(\frac{S-S_0}{Nk}\right)\right]^{2/3}=0 \quad (31)$$

2. Equations of State for van der Waals Gas

For temperature:

$$T=\left(\frac{\partial U}{\partial S}\right)_{V,N} \quad (32)$$

and for pressure:

$$P=-\left(\frac{\partial U}{\partial V}\right)_{S,N} \quad (33)$$

Explicit differentiation yields the standard van der Waals equations of state, and critical behavior can be analyzed using these derivatives.

C. The Curie-Weiss Magnet

In magnetic systems, the first law is:

$$dU=TdS+\mu_0 HdM \quad (34)$$

with H magnetic field, M magnetization.

The Curie-Weiss mean field theory gives:

$$M=N\mu\,tanh\left(\frac{\mu\mu_0(H+\lambda M)}{kT}\right) \quad (35)$$

where λ is the mean-field parameter.

1. HJ Equation for Curie-Weiss Magnet

The Helmholtz free energy (per particle) is:

$$F(M,T)=-NkT\ln\left[2\cosh\left(\frac{\mu\mu_0(H+\lambda M)}{kT}\right)\right]+\frac{1}{2}N\lambda\mu^2M^2 \quad (36)$$

The HJ equation for this system is then:

$$F+NkT\ln\left[2\cosh\left(\frac{\mu\mu_0(H+\lambda M)}{kT}\right)\right]-\frac{1}{2}N\lambda\mu^2M^2=0 \quad (37)$$

2. Equation of State and Criticality

The equation of state is recovered as:

$$H=\left(\frac{\partial F}{\partial M}\right)_T \quad (38)$$

This provides information on spontaneous magnetization, susceptibility, and phase transitions.

DISCUSSION AND EXTENSIONS

The HJ formalism in thermodynamics offers:

- A single "master equation" (HJ equation) for each physical system, from which all equations of state and thermodynamic properties can be derived.
- A geometric, contact-structure perspective connecting thermodynamics to deep mathematical frameworks.
- A bridge to statistical mechanics: many HJ equations can be directly related to entropy maximization or partition function calculations.

This formalism is not only mathematically elegant but also practically valuable for:

- Understanding transformations between different thermodynamic potentials (using Legendre transformations as canonical transformations).

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- Extending to more complex systems: mixtures, chemical reactions, or systems with additional order parameters.
- Providing a systematic way to classify thermodynamic systems, analyze critical behavior, and study phase transitions.

A. Relation to Quantum and Black Hole Thermodynamics

Recent developments in physics (see [1, 2, 9, 10]) suggest that this approach can be generalized to quantum thermodynamics and black hole thermodynamics, where entropy and energy relations become nontrivial and deeply geometric. In black hole thermodynamics, for example, the Bekenstein-Hawking entropy formula and the first law for horizons can be placed in a Hamilton-Jacobi framework, suggesting profound connections between thermodynamics, gravity, and information theory.

B. Non-Equilibrium and Statistical Thermodynamics

While the HJ formalism is most transparent for equilibrium thermodynamics, extensions to non-equilibrium settings are actively studied. The formalism has potential for analyzing:

- Irreversible thermodynamics and entropy production.
- Stochastic thermodynamics, where fluctuation theorems may be interpreted via HJ-type PDEs for large deviation functionals.
- Optimal control and thermodynamic length problems, relevant for nanotechnology and biological systems.

CONCLUSION

This study proposes a strong formalism that smoothly generates equations of state for classical physical systems by extending the Hamilton-Jacobi formalism using contact geometry. It is a reliable computing method that goes beyond theoretical elegance. Subsequent endeavors might concentrate on expanding it to non-equilibrium processes and establishing links with developing domains such as gravitational and quantum thermodynamics.

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