

# Problems of the Modern Mathematical Physics

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## Geometry of Thermodynamic Processes

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# Today

## What is

Transition from one (equilibrium) state to another?

- Stability?
- Reversibility?
- Duration?
- Reaction speed?
- Optimality?

**Keywords:** **Thermal-geometric optimization**

## Classical part

- Step 1: Thermodynamic representation  
Control parameters and restrictions on the system
- Step 2: Thermodynamic equilibrium  
Stability against perturbations

# Thermodynamic information geometry

- Step 3: Thermodynamic metric  
Interactions and phase transitions
- Step 4: Thermodynamic length  
Quantifying fluctuation probabilities
- Step 5: Optimal protocols  
Max/min thermodynamic transformations and Control theory

## Step 1: Energy representation

- **The first law of thermodynamics:**

$$dU = TdS - pdV + \mu dN + \dots = \sum_{a=1}^n I_a dE^a = \vec{I} \cdot d\vec{E}. \quad (1)$$

- **Fundamental relation:**

$$U = U(S, V, N, \dots). \quad (2)$$

- **Equations of state (EoS):**

$$I_a = \left. \frac{\partial U(\vec{E})}{\partial E^a} \right|_{\dots, \hat{E}^a, \dots}. \quad (3)$$

## Step 1: Entropy representation

- **The first law of thermodynamics:**

$$dS = \frac{1}{T}dU - \frac{p}{T}dV + \frac{\mu}{T}dN + \dots = \sum_{a=1}^n J_a dS^a = \vec{J} \cdot d\vec{S}. \quad (4)$$

- **Fundamental relation:**

$$S = S(U, V, N, \dots). \quad (5)$$

- **Equations of state (EoS):**

$$J_a = \left. \frac{\partial S(\vec{S})}{\partial S^a} \right|_{\dots, \hat{S}^a, \dots} \quad (6)$$

# Legendre transformation

## Energy derived potentials:

$$\Phi_{(a)} = \mathcal{L}_{E^a} U = U - I_a E^a, \quad (7)$$

$$\Phi_{(ab)} = \mathcal{L}_{E^a, E^b} U = U - I_a E^a - I_b E^b, \quad a \neq b. \quad (8)$$

⋮

## Entropy derived potentials:

$$\Psi_{(a)} = \mathcal{L}_{S^a} S = S - J_a S^a, \quad (9)$$

$$\Psi_{(ab)} = \mathcal{L}_{S^a, S^b} S = S - J_a S^a - J_b S^b, \quad a \neq b. \quad (10)$$

⋮

## Energy derived potentials:

$$\begin{aligned}\mathcal{L}_S U &= U - TS = F && \text{Helmholtz potential,} \\ \mathcal{L}_V U &= U + pV = H && \text{Enthalpy,} \\ \mathcal{L}_{S,V} U &= U - TS + pV = G && \text{Gibbs potential,} \\ \mathcal{L}_{S,N} U &= U - TS - \mu N = \Phi && \text{Grand potential,} \\ \mathcal{L}_{S,V,N} U &= U - TS + pV - \mu N = 0 && \text{Euler's identity.}\end{aligned}$$

## Entropy derived potentials:

$$\begin{aligned}\mathcal{L}_U S &= S - \frac{U}{T} = \Phi && \text{Massieu potential,} \\ \mathcal{L}_{U,V} S &= S - \frac{U}{T} - \frac{pV}{T} = \Xi && \text{Planck potential,} \\ \mathcal{L}_{U,V,N} S &= S - \frac{U}{T} - \frac{pV}{T} + \frac{\mu N}{T} = 0 && \text{Euler's identity.}\end{aligned}$$



## Step 2: Thermodynamic stability

Energy is strictly **convex** function:

$$U(S + \Delta S, V + \Delta V, \dots) + U(S - \Delta S, V - \Delta V, \dots) > 2U(S, V, \dots). \quad (11)$$

Entropy is strictly **concave** function:

$$S(U + \Delta U, V + \Delta V, \dots) + S(U - \Delta U, V - \Delta V, \dots) < 2S(U, V, \dots). \quad (12)$$

## Necessary conditions for equilibrium

Energy variations  $\delta U = \delta^{(1)}U + \delta^{(2)}U + \dots$ :

$$\delta^{(1)}U = 0 \quad \Rightarrow \quad T = T^*, \quad p = p^*, \quad \mu = \mu^*, \dots \quad (13)$$

$$\delta^{(2)}U \propto \sum_{a,b} \frac{\partial^2 U}{\partial E^a \partial E^b} \delta E^a \delta E^b > 0. \quad (14)$$

Entropy variations  $\delta S = \delta^{(1)}S + \delta^{(2)}S + \dots$ :

$$\delta^{(1)}S = 0 \quad \Rightarrow \quad T = T^*, \quad p = p^*, \quad \mu = \mu^*, \dots \quad (15)$$

$$\delta^{(2)}S \propto \sum_{a,b} \frac{\partial^2 S}{\partial S^a \partial S^b} \delta S^a \delta S^b < 0. \quad (16)$$

## Sufficient conditions for stability

### Sylvester criterion

All principal minors of the Hessian should be strictly:

$$\text{Energy: } \Delta_k > 0, \quad k = 1, \dots, n, \quad (17)$$

$$\text{Entropy: } (-1)^k \Delta_k > 0, \quad k = 1, \dots, n. \quad (18)$$

### Eigenvalue criterion

All eigenvalues of the Hessian should be strictly:

$$\text{Energy: } \epsilon_k > 0, \quad k = 1, \dots, n, \quad (19)$$

$$\text{Entropy: } s_k < 0, \quad k = 1, \dots, n. \quad (20)$$

## Stability under change of coordinates

### **P1: How stability changes under change of coordinates?**

Change of variables from  $\vec{E}$  space to  $\vec{e}$  space:

$$g_{ab}^{(W)}(\vec{E}) = \frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b} = \sum_{\alpha, \beta} \frac{\partial e^\alpha}{\partial E^a} \left( g_{\alpha\beta}^{(W)}(\vec{e}) - \Gamma_{\alpha\beta}^\gamma(\vec{e}) \frac{\partial E(\vec{e})}{\partial e^\gamma} \right) \frac{\partial e^\beta}{\partial E^b}.$$

Induced metric on the  $e$ -manifold:

$$h_{\alpha\beta}(\vec{e}) = \sum_{a,b} \delta_{ab} \frac{\partial E^a}{\partial e^\alpha} \frac{\partial E^b}{\partial e^\beta}, \quad (21)$$

Standard affine connection:

$$\Gamma_{\alpha\beta}^\gamma(\vec{e}) = \frac{1}{2} h^{\gamma\delta} (\partial_\beta h_{\delta\alpha} + \partial_\alpha h_{\delta\beta} - \partial_\delta h_{\alpha\beta}). \quad (22)$$

# Stability under change of potential

## **P2: How stability changes under change of the potential?**

- Solved by the eigenvalue criterion for arbitrary  $n$ .
- Solved for Sylvester:  $n \leq 3$  based on eigenvalue method.
- **Unsolved for Sylvester:** for  $n > 3$  (as far as I know!).

Energy Hessian eigenvalue equation:

$$\lambda^2 - \left( \frac{\partial^2 U}{\partial S^2} + \frac{\partial^2 U}{\partial V^2} \right) \lambda + \frac{\partial^2 U}{\partial S^2} \frac{\partial^2 U}{\partial V^2} - \left( \frac{\partial^2 U}{\partial S \partial V} \right)^2 = 0 \quad (23)$$

Energy  $U = U(S, V)$  (**strictly** convex):

$$\frac{\partial^2 U}{\partial S^2} > 0, \quad \frac{\partial^2 U}{\partial V^2} > 0, \quad \left| \begin{array}{cc} \frac{\partial^2 U}{\partial S^2} & \frac{\partial^2 U}{\partial S \partial V} \\ \frac{\partial^2 U}{\partial S \partial V} & \frac{\partial^2 U}{\partial V^2} \end{array} \right| > 0. \quad (24)$$

Change to Helmholtz potential  $F(T, V) = \mathcal{L}_S U = U - TS$   
(saddle function):

$$\frac{\partial^2 F}{\partial T^2} < 0, \quad \frac{\partial^2 F}{\partial V^2} > 0, \quad \left| \begin{array}{cc} \frac{\partial^2 F}{\partial T^2} & \frac{\partial^2 F}{\partial T \partial V} \\ \frac{\partial^2 F}{\partial T \partial V} & \frac{\partial^2 F}{\partial V^2} \end{array} \right| > 0. \quad (25)$$

# The space of equilibrium states

## The space of equilibrium states

The relation  $U = U(\vec{E})$  defines an  $n$ -dimensional surface  $\mathcal{E}^n$  embedded in  $\mathbb{E}^{n+1}$  with coordinates  $(E^1, \dots, E^n, U)$ .

## Equilibrium manifold

$\mathcal{E}^n$  becomes an **equilibrium manifold** if equipped with a proper  $n$ -dimensional Riemannian metric.

## Step 3: Choosing a metric

❶ **Hessian thermodynamic metrics**

(F. Weinhold 1975, G. Ruppeiner 1979)

❷ **Legendre invariant thermodynamic metrics**

(H. Quevedo 2016)

❸ **Covariant thermodynamic metrics**

(L. Velazquez 2012)

**P3: Choosing the metric is unclear!**



- **G. Ruppeiner 1979** ( $\epsilon = \pm 1$ ):

$$d_S^{(R)} = \epsilon \frac{\partial^2 S(\vec{S})}{\partial S^a \partial S^b} dS^a dS^b. \quad (26)$$

- **F. Weinhold 1975:**

$$d_S^{(W)} = \epsilon \frac{\partial^2 U(\vec{E})}{\partial E^a \partial E^b} dE^a dE^b. \quad (27)$$

- **Covariant metric** (L. Velazquez 2012):

$$d_S^{(Cov)} = \epsilon (\nabla_a \nabla_b S) dS^a dS^b = \epsilon \left( \frac{\partial^2 S}{\partial S^a \partial S^b} - \Gamma_{ab}^c(g) \frac{\partial S}{\partial S^c} \right) dS^a dS^b. \quad (28)$$

- **Legendre invariant metrics** (H. Quevedo 2016),  $L \in \mathbb{R}$ ,  $k \in \mathbb{Z}$ :

$$d_S^{(Q,III)} = L \sum_a \left( S^a \frac{\partial S}{\partial S^a} \right)^{2k+1} \left( \frac{\partial^2 S}{\partial S^a \partial S^b} dS^a dS^b \right). \quad (29)$$

## Step 4: Thermodynamic length and irreversibility

- **Thermodynamic length** quantifies the **distance** between two **equilibrium states**. It is the **number of fluctuations** associated with the **change of the state** of the system. In entropy natural coordinates:

$$\mathcal{L}[\gamma] = \int_{\gamma} \sqrt{g_{ab}(\vec{S})} dS^a dS^b. \quad (30)$$

In affine parametrization with parameter  $t$ :

$$\mathcal{L}(\tau) = \int_0^{\tau} \sqrt{g_{ab}(\vec{S})} \dot{S}^a \dot{S}^b dt. \quad (31)$$

- **Thermodynamic divergence** of the path (Cauchy-Schwarz),

$$\mathcal{J} = \tau \int_0^{\tau} g_{ab}(\vec{S}) \dot{S}^a \dot{S}^b dt \geq \mathcal{L}^2, \quad (32)$$

measures the **efficiency** of the quasi-static protocols.

- **$\mathcal{L}$  sets lower bounds on dissipation!**

## Step 5: Optimal finite-time thermodynamic protocols

### Thermodynamic length

$\mathcal{L}$  is a measure of the distance between two macro states on the equilibrium manifold  $\mathcal{E}^n$ .

### Optimal finite-time processes

$\mathcal{L}$  defines optimal quasistatic protocols on  $\mathcal{E}^n$ .

### Efficiency of a process

$\mathcal{L}$  is a measure of the energy required to transform the system from one state to another. It characterizes the geometric path that minimizes the dissipation (or maximizes the efficiency) of a thermodynamic process.

**P4: Generalization to nonequilibrium case?**

## An Example: Ideal Gas vs Van der Waals gas

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## Characteristics of the ideal gas

**The partition function:**

$$Z_N(\beta, V) = \frac{V^N}{N!} \left( \frac{2\pi mkT}{h^2} \right)^{\frac{3N}{2}} = \frac{V^N}{N! \lambda_T^{3N}}, \quad \beta = \frac{1}{kT}. \quad (33)$$

**Helmholtz free energy:**

$$F(T, V, N) = -kT \ln Z_N(T, V) = -kTN \left[ 1 + \ln \frac{V}{N \lambda_T^3} \right]. \quad (34)$$

**Entropy and internal energy:**

$$S = - \left. \frac{\partial F}{\partial T} \right|_{V, N} = kN \left[ \frac{5}{2} + \ln \frac{V}{N \lambda_T^3} \right], \quad U = F + TS = \frac{3}{2} NkT. \quad (35)$$

**Equation of state:**

$$p = - \left. \frac{\partial F}{\partial V} \right|_{T, N} = \frac{NkT}{V} \Rightarrow pV = NkT. \quad (36)$$

## Ruppeiner geometry and thermodynamic stability

**Entropy in natural parameters:**

$$S(U, V, N) = \frac{1}{2}kN \left( 5 + \ln \frac{64\pi^3 m^3 U^3 V^2}{27h^6 N^5} \right). \quad (37)$$

**Ruppeiner's metric** for  $N = \text{const}$ :

$$\hat{g}^{(R)} = \epsilon \hat{H}_S = \epsilon \begin{pmatrix} \frac{\partial^2 S}{\partial U^2} & \frac{\partial^2 S}{\partial U \partial V} \\ \frac{\partial^2 S}{\partial U \partial V} & \frac{\partial^2 S}{\partial V^2} \end{pmatrix} = \epsilon \begin{pmatrix} -\frac{3kN}{2U^2} & 0 \\ 0 & -\frac{kN}{V^2} \end{pmatrix}. \quad (38)$$

**Level 2 thermodynamic stability** of the ideal gas:

$$\frac{\partial^2 S}{\partial U^2} < 0, \quad \frac{\partial^2 S}{\partial V^2} < 0, \quad \det \hat{H}_S > 0 \Rightarrow U \neq 0. \quad (39)$$

**Positive definiteness** of the metric:

$$g_{UU}^{(R)} > 0, \quad g_{VV}^{(R)} > 0, \quad \det \hat{g}^{(R)} > 0 \Rightarrow \epsilon = -1 \text{ and } U \neq 0. \quad (40)$$

## Optimal process at constant volume

**Thermodynamic length:**

$$\mathcal{L}[\gamma] = \int_{\gamma} \sqrt{g_{ab}(\vec{S}) dS^a dS^b} = \int_{\gamma} \sqrt{\frac{3kN}{2U^2} dU^2 + \frac{kN}{V^2} dV^2}. \quad (41)$$

For an **isochoric process**  $V = \text{const}$ , hence

$$\mathcal{L}_V(1, 2) = \pm \int_1^2 \sqrt{\frac{3kN}{2}} \frac{|dU|}{U} = \pm \sqrt{\frac{3kN}{2}} \ln \frac{U_2}{U_1} [JK^{-1}]^{1/2}. \quad (42)$$

The **geodesic equation** on a curved manifold is given by

$$\ddot{S}^a(t) + \Gamma_{bc}^a \dot{S}^b \dot{S}^c = 0. \quad (43)$$

In  $(U, V)$  space:

$$\ddot{U}(t) - \frac{\dot{U}(t)^2}{U(t)} = 0, \quad \ddot{V}(t) - \frac{\dot{V}(t)^2}{V(t)} = 0. \quad (44)$$

At  $V = \text{const}$  one has two possibilities for i.c. and b.c.:

$$U(t) = U_0 e^{\lambda t}, \quad \lambda = \frac{\dot{U}_0}{U_0}, \quad U(0) = U_0, \quad \dot{U}(0) = \dot{U}_0 = \pm |\dot{U}_0|, \quad (45)$$

$$U(t) = U_0 \left( \frac{U}{U_0} \right)^{t/\tau}, \quad U(0) = U_0, \quad U(\tau) = U, \quad (46)$$

Therefore, one has two possibilities for the length:

$$\mathcal{L}(\tau) = \int_0^\tau \sqrt{g_{ab}(\vec{S}) \dot{S}^a \dot{S}^b} dt = \begin{cases} \sqrt{\frac{3kN}{2}} \lambda \tau = v\tau, \\ \sqrt{\frac{3kN}{2}} \ln \frac{U}{U_0}. \end{cases} \quad (47)$$

Hence the TD speed and the TD time of the process:

$$v = \sqrt{\frac{3kN}{2}} \lambda [JK^{-1}s^{-2}]^{1/2}, \quad \tau = \frac{1}{\lambda} \ln \frac{U}{U_0} [s]. \quad (48)$$



Change of entropy during an isochoric process:

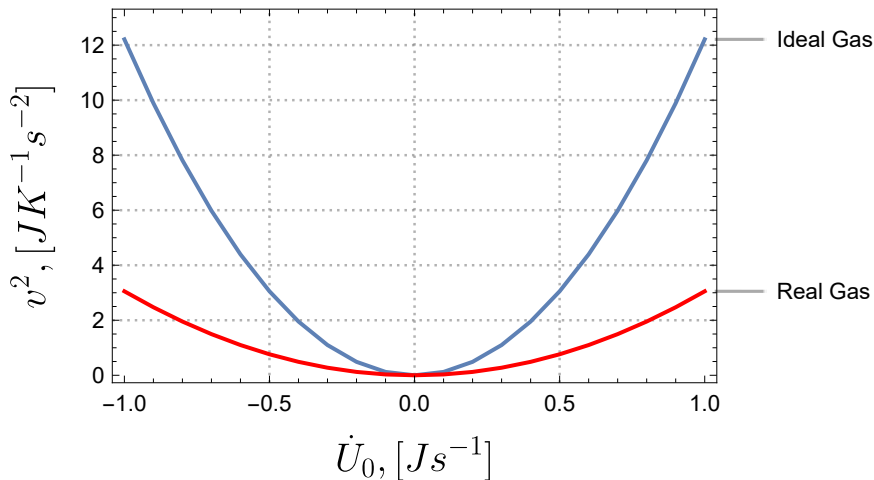
$$\Delta S = \int \frac{\delta Q}{T} = C_V \int_{T_1}^{T_2} \frac{dT}{T} = \frac{3kN}{2} \ln \frac{T_2}{T_1} = \frac{3kN}{2} \ln \frac{U_2}{U_1}. \quad (49)$$

Reversibility of the process:

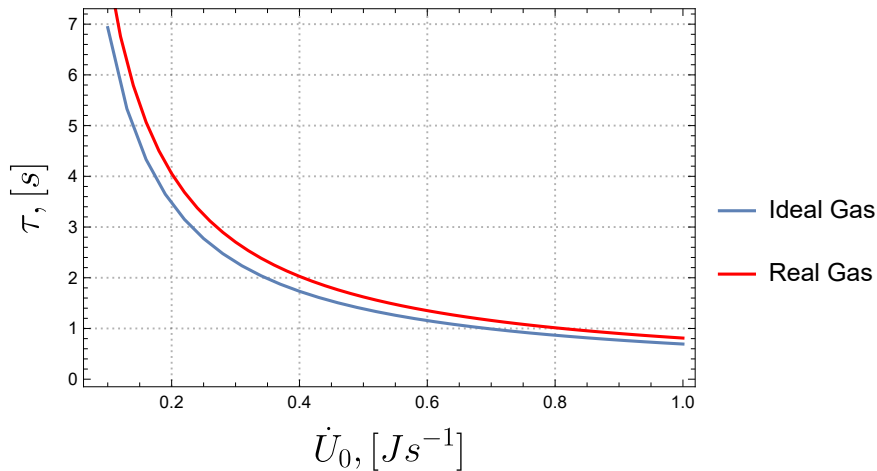
$$\mathcal{L}_V^2(1, 2) = \frac{3kN}{2} \ln^2 \frac{U_2}{U_1} = \Delta S \ln \frac{U_2}{U_1} = \mathcal{J}. \quad (50)$$

**Summary:**  $\mathcal{L}^2 \propto$  the entropy produced and  $v \propto$  the rate of entropy production.

## Isochoric process speed vs initial rates



## Isochoric process time vs initial rates



## Conclusions and future directions

- TD length sets bounds on dissipation.
- Geometric framework of system optimization and control.
- **Main problem: which metric formalism to use?**
- Generalization to nonequilibrium physics?
- Applications to quantum physics and quantum information.
- Applications to nuclear and particle physics.
- Application to black hole physics and holography.
- ...

# Applications to Black Holes and Holography

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