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GEOMETRICAL APPROACH TO OPTIMIZATION PROBLEMS IN EQUILIBRIUM THERMODYNAMICS

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Abstract. Using a geometrical formalism of equilibrium thermodynamics we formulate and solve an optimal control problem for ideal gases. Thermodynamic state is given by a Legendrian manifold equipped with Riemannian structures. A problem of finding an optimal thermodynamic process maximizing the work functional leads to the integrable in Liouville's sense Hamiltonian system. We provide its exact solution by means of angle-action variables and prove a controllability of the dynamical system.

1. Introduction

Optimization problems in thermodynamics are of both theoretical and practical interest, since in many gas motions, such as filtration in porous media (see [1, 2, 3]), Euler flows (see [4]), the medium can be involved in some thermodynamic process, say, isenthalpic or isentropic, and it is natural to investigate processes along which the work of the gas reaches its maximum value. One of the first works originated the investigation in this direction is [5]. Later, in [6] methods of constructing optimal heat engines with linear heat transfer laws were developed, and in [7], methods of optimal control theory, in particular, Pontryagin's maximum principle [8, 9], were applied. In a series of works [10], the optimization problem in non-equilibrium thermodynamics was studied.

In the present work we use a geometrical formulation of thermodynamics to solve the problem of optimal control for ideal gases. The geometrical approach goes back to classical works [11, 12, 13] and in modern terms of contact and symplectic geometry is presented in [14], where, above all, a remarkable link between thermodynamics and measurement theory was observed, which is of special importance in this work. This work is a continuation of [15]. Here, we also address the controllability problem.

The paper is organized in the following way. First of all, we briefly remind all necessary geometrical constructions and their connection with measurement (see [14] for more details). Then, we formulate the optimization problem for any gas and solve it in case of ideal gases. In this case the Hamiltonian system turns out to be integrable, and using Liouville's theorem (see, for example, [16]) we

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give its exact solution in terms of angle-action variables. The trajectories of the dynamical system in the question lie on an invariant manifold that may have two or three connected components. This brings us to the question of controllability of the dynamical system, since for the existence of the optimal trajectory, for a given pair of initial and final states one has to find such an invariant manifold that initial and final states belong to the same connected component of the last. We prove that the system is controllable.

2. Geometry and thermodynamics

In this section, we briefly describe thermodynamics from measurement viewpoint and give necessary geometrical constructions following [14].

Let us assume that we have a random vector $X\colon (\Omega, \mathcal{A}, q) \to W$, where Ω is a set of elementary events, $\mathcal{A}$ is a σ-algebra on Ω, q is a probability measure, i.e. a map from the probability space $(\Omega, \mathcal{A}, q)$ to some vector space W of dimension $n < \infty$. Then, if $x \in W$ is assumed to be a result of the measurement of the random vector X, then one should choose such a probability density ρ, that

$$\int_\Omega \rho dq = 1, \qquad \int_\Omega X\rho dq = x.$$

Using the principle of minimal information gain $I = \int_\Omega \rho \ln \rho dq$ (see [14] for details) we get the following result.

Theorem 2.1. *Measurements of a random vector X are given by the Legendrian manifold $L \subset \mathbb{R} \times W \times W^*$ of the contact form*

$$\theta = du - \sum_{i=1}^{n} \lambda_i dx_i,$$

where u is a coordinate on $\mathbb{R}$, $\lambda \in W^*$, i.e. $\theta|_L = 0$ and $u|_L = I$.

Thus, given a Legendrian manifold $L \subset \mathbb{R} \times W \times W^*$ one gets measurements of a random vector X, and the value of the information gain I.

If one computes the variance $\sigma_2(X)$ of the random vector X, one observes that it coincides with the restriction of the universal quadratic form

$$\kappa = d\lambda \cdot dx = \sum_{i=1}^{n} d\lambda_i \cdot dx_i \tag{2.1}$$

to the manifold L, i.e. $\kappa|_L = \sigma_2(X)$. Here $\cdot$ means a symmetric product. This implies that the Legendrian manifold L has to be Riemannian with respect to metric $\kappa|_L$. More precisely, the Legendrian manifold L consists of *phases*, where the form $\kappa|_L$ is either positive or negative, separated from each other by a degeneration set of $\kappa|_L$.

Let us now turn to thermodynamics. It is well known that contact geometry is a natural framework for equilibrium thermodynamics (see [11, 12, 13]). Indeed, any thermodynamic system in equilibrium is described by two types of variables, extensive $W(e, v)$, where e and v are specific inner energy and volume respectively, and intensive $W^*(p, T)$ standing for pressure and temperature, and additionally specific entropy $s \in \mathbb{R}$. The corresponding contact structure θ in thermodynamic case is given by the first law of thermodynamics

$$\theta = -ds + T^{-1}de + pT^{-1}dv.$$

A thermodynamic state is therefore a Legendrian manifold $L \subset \mathbb{R} \times W \times W^*$, on which $\theta|_L = 0$. This brings us to a conclusion that thermodynamics can be viewed as a theory of measurement of extensive variables (e, v). The differential quadratic form κ in thermodynamics is

$$\kappa = d(T^{-1}) \cdot de + d(pT^{-1}) \cdot dv, \tag{2.2}$$

and the negativity of $\kappa|_L$ gives us applicable states. To see how positivity of (2.1) corresponds to negativity of (2.2) we refer to [15]. If one takes some vector field $Y \in D(L)$, then $-\kappa|_L(Y, Y)$ is a function on L that gives us the variance of measurement of energy e and volume v at the point $(e, v) \in L$.

Let us now choose (e, v) as coordinates on L, then for a given function $\sigma(e, v)$ the condition $\theta|_L$ forces

$$L = \left\{ f_1 = p - \frac{\sigma_v}{\sigma_e} = 0,\ f_2 = T - \frac{1}{\sigma_e} = 0,\ f_3 = s - \sigma(e, v) = 0 \right\}. \tag{2.3}$$

Thermodynamic processes can be understood as contact transformations $\phi\colon \mathbb{R} \times W \times W^* \to \mathbb{R} \times W \times W^*$, preserving the Legendrian manifold L. Infinitesimal version of such transformations is given by contact vector fields X. They are defined by *generating functions* (see, for example, [17]):

$$X_f = T\,(pf_p + Tf_T)\,\partial_e - Tf_p\partial_v + (f + Tf_T)\,\partial_s + T\,(f_v - pf_e)\,\partial_p - T\,(f_s + Tf_e)\,\partial_T,$$

where $f \in C^\infty(\mathbb{R} \times W \times W^*)$ is a generating function of the vector field X_f. One can easily show that X_f is tangent to a surface $\{f = 0\}$. Let us choose restrictions Y_1 and Y_2 of vector fields X_{f_1} and X_{f_2}, where f_1 and f_2 are given by (2.3), to L as a basis in the module of vector fields on L. They are of the form

$$Y_1 = \frac{\sigma_v}{\sigma_e^2}\frac{\partial}{\partial e} - \frac{1}{\sigma_e}\frac{\partial}{\partial v}, \quad Y_2 = \frac{1}{\sigma_e^2}\frac{\partial}{\partial e}. \tag{2.4}$$

Note that $Y_3 = X_{f_3}|_L = 0$.

3. Optimal control

In this section, we formulate and solve an optimal problem on an ideal gas state Legendrian manifold and discuss the controllability of our dynamical system.

3.1. Problem. Let us look for a thermodynamic process $l \in L$ as an integral curve of some vector field $Y = u_1Y_1 + u_2Y_2$, where Y_1 and Y_2 are base vector fields (2.4). We will interpret coefficients u_1 and u_2, which are the functions on L, as control parameters. The admissible domain U for control parameters $u = (u_1, u_2)$ will be defined as follows

$$U = \left\{ u \in \mathbb{R}^2 \mid -\frac{\kappa|_L(Y, Y)}{e^2} \leq \delta \right\}, \tag{3.1}$$

where $\delta > 0$ is a constant. From the physical viewpoint condition (3.1) means that the variance of e and v is limited by a constant, depending on the square of energy.

If one introduces the work 1-form $\omega = pdv$, then one can define the quality functional by the following way:

$$J = \int_0^{t_0} \omega(Y)dt \to \max_{u \in U}. \tag{3.2}$$

Condition (3.2) means that the work of the gas reaches its maximum along the process $l \subset L$.

Using the notation $x = (e, v)$ and assuming that both initial state $x^{(1)} = (e^{(1)}, v^{(1)})$ and final state $x^{(2)} = (e^{(2)}, v^{(2)})$ are fixed, as well as t_0, one gets an extremal problem in the form

$$\begin{aligned} &\dot{x} = (Y^{(1)}(x,u), Y^{(2)}(x,u)), \quad x \in \mathbb{R}^2,\, u \in U, \\ &x(0) = x^{(1)},\, x(t_0) = x^{(2)}, \\ &J = \int_0^{t_0} \omega(Y)dt \to \max_{u \in U}, \end{aligned} \tag{3.3}$$

where the $Y^{(1)}(x,u)$ and $Y^{(2)}(x,u)$ are the coefficients of the unknown vector field

$$Y = Y^{(1)}(x,u)\frac{\partial}{\partial e} + Y^{(2)}(x,u)\frac{\partial}{\partial v},$$

and they are defined by means of (2.4). Optimal problem (3.3) can be formulated for any thermodynamic state model.

3.2. Solution for ideal gases. The Legendrian manifold L for ideal gases is given by $\{f_1 = f_2 = f_3 = 0\}$, where

$$f_1 = pv - RT, \quad f_2 = e - \frac{nRT}{2}, \quad f_3 = s - R\ln\left(e^{n/2}v\right),$$

where R is the universal gas constant, n is the degree of freedom of the molecule. Therefore, vector fields Y_1 and Y_2 are

$$Y_1 = -\frac{2ev}{nR}\partial_v, \quad Y_2 = -\frac{2e^2}{nR}\partial_e. \tag{3.4}$$

The differential quadratic form $\kappa|_L$ is

$$\kappa|_L = -\frac{nR}{2e^2}de \cdot de - \frac{R}{v^2}dv \cdot dv. \tag{3.5}$$

Using (3.4), (3.5) and (3.1) we obtain the admissible domain U for control parameters as

$$U = \left\{(u_1, u_2) \in \mathbb{R}^2 \mid \frac{4}{n^2R}u_1^2 + \frac{2}{nR}u_2^2 \le \delta\right\}.$$

Let us introduce new coordinates (q_1, q_2) on L by the following way:

$$e = \frac{nR}{2q_1}, \quad v = \exp\left(-\frac{q_2}{q_1}\right).$$

In these coordinates vector fields (3.4) will take a simpler form

$$Y_1 = \partial_{q_2}, \quad Y_2 = \partial_{q_1} + \frac{q_2}{q_1}\partial_{q_2}.$$

The Pontryagin's function of problem (3.3) in coordinates $q = (q_1, q_2)$ will be

$$P(q, \lambda, u) = -\frac{Ru_1}{q_1^2} + \lambda_1 u_2 + \lambda_2 \left(\frac{q_2 u_2}{q_1} + u_1\right), \tag{3.6}$$

where $\lambda = (\lambda_1, \lambda_2)$ are Lagrangian multipliers.

Due to Pontryagin's maximum principle [8, 9] the function $P(q, \lambda, u)$ has to reach its maximum value on U. Since $P(q, \lambda, u)$ is linear with respect to (u_1, u_2), the maximum value is reached on the boundary ∂U.

Theorem 3.1 ([15])**.** *The controls (u_1, u_2) obey the following law on the extremal trajectory*

$$u_1^* = \frac{n\sqrt{R\delta}}{2}\cos\tau^*, \quad u_2^* = \sqrt{\frac{nR\delta}{2}}\sin\tau^*, \tag{3.7}$$

where

$$\tau^*(q, \lambda) = \pi(2k + 1) - \arctan\left(\frac{\sqrt{2}q_1(q_1\lambda_1 + q_2\lambda_2)}{\sqrt{n}\,(R - q_1^2\lambda_2)}\right), \quad k \in \mathbb{Z}.$$

Substituting control parameters (3.7) to the Pontryagin's function (3.6), we get the Hamiltonian $H(q, \lambda) = P(q, \lambda, u^*(q, \lambda))$:

$$H(q, \lambda) = \frac{1}{2q_1^2}\sqrt{nR\delta\,(nq_1^4\lambda_2^2 + 2q_1^4\lambda_1^2 + 4q_1^3q_2\lambda_1\lambda_2 + 2q_1^2q_2^2\lambda_2^2 - 2Rnq_1^2\lambda_2 + R^2n)}. \tag{3.8}$$

Optimal trajectories are found from the canonical equations

$$\dot{q} = \frac{\partial H}{\partial \lambda}, \quad \dot{\lambda} = -\frac{\partial H}{\partial q}, \tag{3.9}$$

with Hamiltonian (3.8).

Theorem 3.2 ([15])**.** *The function $G(q, \lambda) = q_1\lambda_2$ is the integral of Hamiltonian system (3.9), which commutes with Hamiltonian (3.8) with respect to the Poisson bracket $[G, H]$, where the bracket is uniquely determined by the equality*

$$[G, H]\Omega \wedge \Omega = dG \wedge dH \wedge \Omega, \quad \Omega = dq \wedge d\lambda.$$

Thus system (3.9) is integrable in Liouville's sense. Invariant manifold M of canonical system (3.9) is given by levels of its integrals

$$M = \left\{(q, \lambda) \in \mathbb{R}^4 \mid H(q, \lambda) = H_1,\, G(q, \lambda) = H_2\right\},$$

where H_1 and H_2 are constants. In coordinates (q_1, q_2) it is given by

$$\lambda_1 = \frac{-2H_2R\delta nq_2 \pm \sqrt{D}}{2Rn\delta q_1^2}, \quad \lambda_2 = \frac{H_2}{q_1},$$

where $D = 2R\delta n\left(4H_1^2q_1^4 - \delta Rn^2(R - H_2q_1)^2\right)$.

One can see that the manifold M only exists if $D \geq 0$. Therefore, considering D as a polynomial in q_1, we drive to a conclusion that M may have various numbers of connected components.

Theorem 3.3. *The manifold M has three connected components if levels of integrals H_1 and H_2 satisfy the inequality*

$$n\sqrt{\delta}H_2^2 - 8H_1\sqrt{R} \geq 0. \tag{3.10}$$

In other cases, the manifold M has two connected components.

Proof. Due to (3.8) one concludes that $H_1 > 0$. By means of scale transformation

$$H_1 \mapsto R^{3/2}n\sqrt{\delta}H_1, \quad H_2 \mapsto H_2 R, \quad q_1 \mapsto \frac{q_1}{\sqrt{2H_1}}. \tag{3.11}$$

we reduce all the dimensional constants in D. Then, the condition $D = 0$ is equivalent to

$$q_1^4 - (1-\mu q_1)^2 = 0, \tag{3.12}$$

where $\mu = H_2/\sqrt{2H_1}$.

From (3.12), one gets the expression for roots of the polynomial D:

$$q_{1,2}^* = -\frac{\mu}{2} \pm \frac{1}{2}\sqrt{\mu^2+4}, \quad q_{3,4}^* = \frac{\mu}{2} \pm \frac{1}{2}\sqrt{\mu^2-4}. \tag{3.13}$$

One can see that two real roots $q_{1,2}^*$ always exist, while the other two $q_{3,4}^*$ are real only if $\mu^2 \geq 4$. Therefore, if $\mu^2 \geq 4$, then the number of connected components is three, otherwise two.

By means of inverse scale transformation we get (3.10). □

To construct solution to (3.9), we introduce the so-called action-angle variables, in terms of which (3.9) takes its simplest form.

Theorem 3.4 ([15])**.** *Angle variables Ω_1 and Ω_2 are of the form*

$$\Omega_1 = \pm\int \frac{4H_1 q_1^2 dq_1}{\sqrt{D}}, \quad \Omega_2 = \frac{q_2}{q_1} \pm \int \frac{n^2 R\delta(R - H_2 q_1)dq_1}{q_1\sqrt{D}}.$$

Hamiltonian system (3.9) is equivalent to

$$\dot{\Omega}_1 = 1, \quad \dot{\Omega}_2 = 0,$$

and its solution is

$$\Omega_1 = t + \alpha_1, \quad \Omega_2 = \alpha_2, \tag{3.14}$$

where constants α_1, α_2 are found by means of conditions at the ends.

Thus we have got a solution to (3.9) in quadratures.

3.3. Controllability. Let $x^{(1)} = (x_1, x_2)$ be an initial state, and $x^{(2)} = (y_1, y_2)$ be a final state. Let us apply scale transformation (3.11) to quadratures (3.14). We obtain

$$t_0 = \int\limits_{\sqrt{2H_1}x_1}^{\sqrt{2H_1}y_1} \frac{q_1^2 dq_1}{\sqrt{q_1^4 - (1-\mu q_1)^2}}, \tag{3.15}$$

$$0 = \frac{y_2}{\sqrt{2H_1}y_1} - \frac{x_2}{\sqrt{2H_1}x_1} + \int\limits_{\sqrt{2H_1}x_1}^{\sqrt{2H_1}y_1} \frac{1-\mu q_1}{q_1\sqrt{q_1^4-(1-\mu q_1)^2}}dq_1, \tag{3.16}$$

where t_0 is given.

Note that expressions (3.15) are valid only if $\widehat{D} = q_1^4 - (1 - \mu q_1)^2 > 0$ everywhere on $[\sqrt{2H_1}x_1, \sqrt{2H_1}y_1]$, or, in other words, if x_1 and y_1 belong to the same connected component of the invariant manifold M. One may expect that for some pairs (x_1, y_1) of initial and final states we will not be able to construct such a manifold M by means of constants μ, H_1, that there exists a trajectory from x_1 to y_1, and our system is not controllable. But the following theorem claims the opposite.

Theorem 3.5. *For any initial state (x_1, x_2), where $x_1 > 0$, and any final state (y_1, y_2), where $y_1 > 0$, there exist constants μ and $H_1 > 0$, such that the state (y_1, y_2) is reachable from the state (x_1, x_2) in a finite time t_0, i.e. dynamical system (3.3) is controllable.*

Proof. It is easy to show that under condition $q_1 > 0$ (only such have physical sense) the roots of the polynomial $\widehat{D}(q_1) = q_1^4 - (1 - \mu q_1)^2$ satisfy inequalities

$$0 < q_1^*(\mu) < q_4^*(\mu) \le q_3^*(\mu),$$

while $q_2^*(\mu) < 0$ for any $\mu \in \mathbb{R}$, and roots q_3^*, q_4^* only exist if $\mu \ge 2$. For certainty and without loss of generality, we will assume that $y_1 > x_1$. For the existence of the trajectory from x_1 to y_1 one needs $\widehat{D}(q_1)$ to be positive in $[\sqrt{2H_1}x_1, \sqrt{2H_1}y_1]$. Therefore the following inequalities must be satisfied

$$\begin{gathered} \sqrt{2H_1}z_1 > q_1^*(\mu), \quad \mu \in (-\infty, 2), \\ \sqrt{2H_1}z_1 > q_3^*(\mu), \quad \text{or} \quad q_1^*(\mu) < \sqrt{2H_1}z_1 < q_4^*(\mu), \quad \mu \in [2, +\infty), \end{gathered}$$

where z_1 is either x_1, or y_1. The corresponding domains for z_1 are shown in Fig. 1.

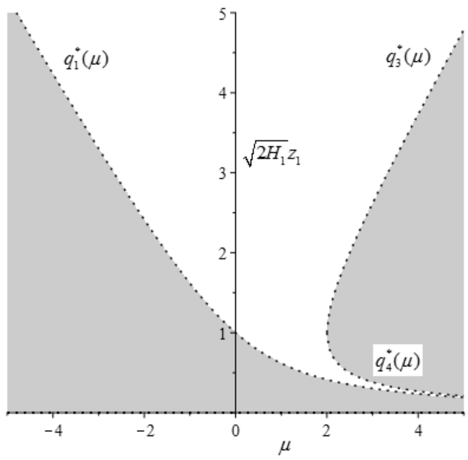

FIGURE 1. Admissible x_1 and y_1 belong to white domain

Let arbitrary $x_1 > 0$ and $y_1 > 0$ be given. One needs to choose the constant $H_1 > 0$ in such a way that solutions μ_2^* and μ_3^* of equations $\sqrt{2H_1}y_1 = q_4^*(\mu)$ and

$\sqrt{2H_1}x_1 = q_1^*(\mu)$ are related as $\mu_2^* \geq \mu_3^*$. Then, one can find such a $\mu^* \in [\mu_3^*, \mu_2^*]$, that the interval $[\sqrt{2H_1}x_1, \sqrt{2H_1}y_1]$ does not contain singularities of the integrand in (3.15). This is shown in Fig. 2.

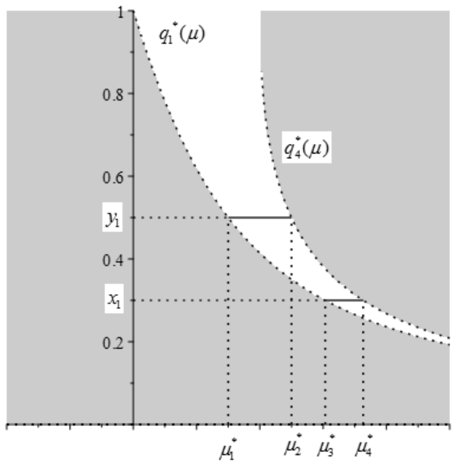

FIGURE 2. Relations between μ_2^* and μ_3^*. For given x_1, y_1 and H_1 there is no common μ since $\mu_2^* < \mu_3^*$

Let us find μ_2^* and μ_3^*.

$$\sqrt{2H_1}x_1 = q_1^*(\mu) \Longrightarrow \mu_3^* = \frac{1 - 2H_1 x_1^2}{x_1\sqrt{2H_1}},$$

$$\sqrt{2H_1}y_1 = q_4^*(\mu) \Longrightarrow \mu_2^* = \frac{1 + 2H_1 y_1^2}{y_1\sqrt{2H_1}},$$

from what it follows that for $\mu_3^* \leq \mu_2^*$ one needs to choose H_1 satisfying the condition

$$H_1 \geq \frac{y_1 - x_1}{2x_1 y_1(x_1 + y_1)} > 0.$$

One can see that for given $0 < x_1 < y_1$ such H_1 can always be found.

For the pair (x_2, y_2) the analysis is trivial.

Thus, the system is controllable. $\square$

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