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Thermodynamic Equilibrium, Nambu Brackets and Induced Hessians

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In this work we present a brief introduction to the concepts of classical global and local thermodynamic stability from thermodynamic information geometry perspective. We state the necessary and sufficient conditions for stable global thermodynamic equilibrium. Novel relations between Hessians, defined on different thermodynamic manifolds, have been derived, which lead to new expressions for the Weinhold and Ruppeiner thermodynamic metrics. We show that our approach is equivalent to the Nambu bracket formalism traditionally used in the calculation of the heat capacities of the system. Finally, we make our remarks on the concept of local thermodynamic stability and its relation to the global one.

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1. Introduction

In thermodynamics it is conventional to start with the energy potential E in its natural parametrization $(S, Y^1, Y^2, ..., Y^{n-1})$. The latter define the energy representation through the fundamental relation $E = E(S, Y^1, Y^2, ..., Y^{n-1})$ and first law of thermodynamics written by

$$dE = TdS + \sum_{i=1}^{n-1} X_i dY^i = \sum_{a=1}^{n} I_a E^a. \tag{1}$$

Here the intensive parameters X_i are thermodynamically conjugate to the extensive ones Y^i and generally X_i are known as chemical potentials. It is useful to encode the full set of energy natural extensive parameters in a single vector $\vec{E} = (E^1, E^2, ..., E^n)$ with their conjugate intensive parameters given by $\vec{I} = (I_1, I_2, ..., I_n)$. Consequently, the equations of state can be written in the following concise form

$$I_a = \left.\frac{\partial E(\vec{E})}{\partial E^a}\right|_{E_1,...,\hat{E}^a,...,E^n}, \tag{2}$$

where the parameters in the subscript are kept fixed except for $\hat{E}^a$.

By applying a Legendre transformation $\mathcal{L}$ along one or several natural parameters of the energy potential one can obtain all of the standard free energy potentials. In this case the one parameter Legendre family of energy derived potentials Φ_a are given by

$$\Phi_1 = \mathcal{L}_{E^1} E = E - I_1 E^1, \quad \Phi_2 = \mathcal{L}_{E^2} E = E - I_2 E^2, \quad \cdots \quad \Phi_n = \mathcal{L}_{E^n} E = E - I_n E^n. \tag{3}$$

The two parameter Legendre family of energy derived potentials Φ_{ab}, $a \neq b$, are given by

$$\Phi_{12} = \mathcal{L}_{E^1,E^2} E = E - I_1 E^1 - I_2 E^2, \tag{4}$$

$$\Phi_{13} = \mathcal{L}_{E^1,E^3} E = E - I_1 E^1 - I_3 E^3, \tag{5}$$

$$\vdots \tag{6}$$

$$\Phi_{n-1,n} = \mathcal{L}_{E^{n-1},E^n} E = E - I_{n-1} E^{n-1} - I_n E^n. \tag{7}$$

Of course, one can continue further by defining more potentials along three or more variables. At the end the Legendre transformation along all the extensive variable simultaneously leads to the trivial potential $\Phi_{1,2,...,n} = 0$, which is due to the Euler homogeneity relation

$$E = \sum_{a=1}^{n} I_a E^a. \tag{8}$$

However, the potential $\Phi_{1,2,...,n}$ may not be trivial if the energy of the system is a quasi-homogeneous function of degree r and type $(r_1, ..., r_n)$ under dilatations by a scale factor $\lambda > 0$, i.e.

$$rE = \sum_{a=1}^{n} r_a I_a E^a. \tag{9}$$

This relation reflects the Euler theorem for quasi-homogeneous functions, where I_a are given by the equations of state (2).

The situation is similar if one works in the entropy representation. In this case, choosing the entropy S as a thermodynamic potential depending on its natural parameters $(S^1, S^2, ..., S^n)$ one can write the first law of thermodynamics in the form

$$dS = \frac{1}{T} dE - \sum_{i=1}^{n-1} \frac{X_i}{T} dY^i = \sum_{a=1}^{n} \lambda_a S^a, \tag{10}$$

where $\vec{\lambda} = (\lambda_1, \lambda_2, ..., \lambda_n)$ are the thermodynamically conjugated parameters of $\vec{S} = (S^1, S^2, ..., S^n)^T$. The equations of state follow naturally by

$$\lambda_a = \frac{\partial S(\vec{S})}{\partial S^a}\bigg|_{S_1,...,\hat{S}^a,...,S^n}, \tag{11}$$

A Legendre transformation of the entropy potential along one or several of its natural parameters is used to obtain the entropy derived family of potentials. The latter are known by several names: Massieu-Planck potentials, free entropies or free information. It is important to note that entropy is not a Legendre transformation of the energy and thus entropy representation and its derived potentials are in general different from the energy representation and its derived potentials.

It is a fact that different potentials (representations) correspond to different constraints to which the system may be subjected. The thermodynamic properties of the system can be fully described once the fundamental relation in the chosen representation has been established. Therefore, one has to be able to transfer all the relevant properties between representations. This is, however, a non-trivial task. An example is given in thermodynamic information geometry [1–11], where Legendre non-invariant thermodynamic metrics lead to radically different physics when changing the potentials, while Legendre invariant ones have infinitely many conformal factors to choose from.

An important related problem is how to transfer thermodynamic information on the level of the Hessians of thermodynamic potentials either between Legendre related potentials or the same potential defined on different manifolds. The latter is due to the fact that any change of variables in a given potential induces a curved thermodynamic manifold and the new induced Hessian is radically different from the original one. Later in this paper we show that the relation between the original and the induced Hessian is given by a generalized pullback/pushforward formula including the Jacobians of the transformation and also terms involving the components of the induced metric on the new manifold. This relation can be used to transfer the conditions for global thermodynamic stability from one representation to another. Furthermore, because Hessians can be used to define thermodynamic metrics, we can relate the generalized pullback/pushforward by the components of the Weinhold metric [1] in energy representation and the Ruppeiner metric [2]in entropy representation.

The goal of this work is to present the theory of thermodynamic stability from information-theoretic perspective, while keeping it as simple as possible due to its practical importance. The structure of the paper is the following. In Section 2 we present the necessary and sufficient conditions for global thermodynamic stability in energy and entropy representations. In Section 3 we find novel relations between Hessians and Hessian metrics defined on different thermodynamic manifolds. We also show the equivalence of our approach to the Nambu bracket formalism. In Section 4 we present our remarks on the concept of local thermodynamic stability and its relation to global one. Finally, in Section 5 we give a brief summary of our results.

2. Necessary and sufficient conditions for global thermodynamic equilibrium

A given system is in thermodynamic equilibrium if its state variables do not spontaneously change over considerably long period of time. According to thermodynamics [13–16] the necessary, but not sufficient, conditions for establishing thermodynamic equilibrium between the system and its surroundings in the energy representation are given by the equalities of the intensive parameters $I_a = I^*_a$, where I^*_a are the intensive parameters of the surroundings. These parameters include temperature, pressure, chemical potentials etc. The conditions can easily be derived by the condition on the first variation of the internal energy of the system during a virtual process:

$$\delta^{(1)}E(\vec{E}) - \sum_a I^*_a \delta E^a = \sum_a \left[\left(\frac{\partial E}{\partial E^a}\bigg|_{E^1,\dots,\hat{E}^a,\dots,E^n} - I^*_a \right) \delta E^a \right] = 0. \tag{12}$$

The space of possible states of equilibrium (compatible with constraints and initial conditions) is called the space of virtual states. Due to the first law in equilibrium one has $(\partial E/\partial E^a) = I_a$ and the necessary conditions for equilibrium become

$$I_a = I^*_a = conts, \tag{13}$$

Equivalently one can work with the variation of the entropy $\delta^{(1)}S(\vec{S})$.

On the other hand, the sufficient conditions for global thermodynamic equilibrium, and thus global thermodynamic stability, can be derived by the sign of the second variation of the energy or the entropy consistent with the second law of thermodynamics.

Considering the energy as a potential the second variation $\delta^{(2)}E = \delta\vec{E}^T.\hat{\mathcal{H}}^{(E)}(\vec{E}).\delta\vec{E} > 0$ should be positive due to the fact that in equilibrium the energy of the system assumes its minimum. Here $\hat{\mathcal{H}}^{(E)}$ is the symmetric $n \times n$ Hessian matrix of the energy given by

$$\mathcal{H}^{(E)}_{ab}(\vec{E}) = \frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b}\bigg|_{E^1,\dots,\hat{E}^a,\dots,\hat{E}^b,\dots,E^n}, \quad a,b = 1,2,\dots,n. \tag{14}$$

The inequality $\delta^{(2)}E > 0$ defines $\hat{\mathcal{H}}^{(E)}$ as a positive definite quadratic form. This means that for global equilibrium it is sufficient that all eigenvalues $\varepsilon_a > 0$, $a = 1,\dots,n$, of the Hessian of the energy be strictly positive.

On the other hand, the second variation $\delta^{(2)}S = \delta\vec{S}^T.\hat{\mathcal{H}}^{(S)}(\vec{S}).\delta\vec{S} < 0$ should be negative due to the fact that in equilibrium the entropy of the system settles at its maximum. The inequality $\delta^{(2)}S < 0$ defines $\delta^{(2)}S$ as a negative definite quadratic form. This means that for global equilibrium it is sufficient that all eigenvalues $s_a < 0$, $a = 1,\dots,n$, of the Hessian of the entropy be strictly negative.

For many-parametric systems the eigenvalues of the corresponding Hessians may become too complicated for analytical treatment. In this situation one can use the Sylvester criterion for positive/negative definiteness of the Hessians to study thermodynamic stability. In energy representation the energy is strictly global convex, thus the Hessian of the energy is positive definite quadratic form. In this case Sylvester's criterion states that all the principal minors $\Delta_k > 0$ of the Hessian of the energy must be strictly positive. In entropy representation this criterion has alternating signs $(-1)^k\Delta_k > 0$ due to the fact that entropy is globally concave function.

Let us show what this means for $n = 3$ parametric thermodynamics in the energy representation. In this case the energy E is a function of its natural parameters $(E^1, E^2, ..., E^n)$ and its Hessian $\hat{\mathcal{H}}^{(E)}$ is the following 3×3 symmetric matrix

$$\hat{\mathcal{H}}^{(E)}(\vec{E}) = \begin{pmatrix} \frac{\partial^2 E}{(\partial E^1)^2}\Big|_{E^2,E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} \\ \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} & \frac{\partial^2 E}{(\partial E^2)^2}\Big|_{E^1,E^3} & \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} \\ \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} & \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} & \frac{\partial^2 E}{(\partial E^3)^2}\Big|_{E^1,E^2} \end{pmatrix}. \tag{15}$$

According to Sylvester's criterion for thermodynamic stability the first level principal minors of $\hat{\mathcal{H}}^{(E)}$ must be strictly positive:

$$\Delta_1^{(2,3)} = \frac{\partial^2 E}{(\partial E^1)^2}\Big|_{E^2,E^3} > 0, \quad \Delta_1^{(1,3)} = \frac{\partial^2 E}{(\partial E^2)^2}\Big|_{E^1,E^3} > 0, \quad \Delta_1^{(1,2)} = \frac{\partial^2 E}{(\partial E^3)^2}\Big|_{E^1,E^2} > 0. \tag{16}$$

These conditions correspond to the fact that energy is a convex function along its natural parameters. The upper indices in $\Delta_1^{(i,j)}$ indicate that the i^{th} row and column and the j^{th} row and column of the Hessian have been deleted. These condition have to be accompanied with the positiveness of the determinants of the second level principal minors:

$$\Delta_2^{(3)} = \begin{vmatrix} \frac{\partial^2 E}{(\partial E^1)^2}\Big|_{E^2,E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} \\ \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} & \frac{\partial^2 E}{(\partial E^2)^2}\Big|_{E^1,E^3} \end{vmatrix} > 0, \tag{17}$$

$$\Delta_2^{(2)} = \begin{vmatrix} \frac{\partial^2 E}{(\partial E^1)^2}\Big|_{E^2,E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} \\ \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} & \frac{\partial^2 E}{(\partial E^3)^2}\Big|_{E^1,E^2} \end{vmatrix} > 0, \tag{18}$$

$$\Delta_2^{(1)} = \begin{vmatrix} \frac{\partial^2 E}{(\partial E^2)^2}\Big|_{E^1,E^3} & \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} \\ \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} & \frac{\partial^2 E}{(\partial E^3)^2}\Big|_{E^2,E^3} \end{vmatrix} > 0. \tag{19}$$

The upper index in $\Delta_2^{(i)}$ indicates that the i^{th} row and column of the Hessian have been removed. The final part of the Sylvester criterion is a condition on the determinant of the Hessian itself:

$$\Delta_3 = \det(\hat{\mathcal{H}}^{(E)}) = \begin{vmatrix} \frac{\partial^2 E}{(\partial E^1)^2}\Big|_{E^2,E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} & \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} \\ \frac{\partial^2 E}{\partial E^1 \partial E^2}\Big|_{E^3} & \frac{\partial^2 E}{(\partial E^2)^2}\Big|_{E^1,E^3} & \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} \\ \frac{\partial^2 E}{\partial E^1 \partial E^3}\Big|_{E^2} & \frac{\partial^2 E}{\partial E^2 \partial E^3}\Big|_{E^1} & \frac{\partial^2 E}{(\partial E^3)^2}\Big|_{E^1,E^2} \end{vmatrix} > 0. \tag{20}$$

For $n = 3$ system in the entropy representation the Sylvester criterion yields:

$$\Delta_1^{(2,3)} = \frac{\partial^2 S}{(\partial S^1)^2}\Big|_{S^2,S^3} < 0, \quad \Delta_1^{(1,3)} = \frac{\partial^2 S}{(\partial S^2)^2}\Big|_{S^1,S^3} < 0, \quad \Delta_1^{(1,2)} = \frac{\partial^2 S}{(\partial S^3)^2}\Big|_{S^1,S^2} < 0, \tag{21}$$

which just reflects the fact that entropy is a concave function along its natural parameters. The other two parts of the Sylvester criterion can be written for short in the following way:

$$\Delta_2^{(3)} > 0, \quad \Delta_2^{(2)} > 0, \quad \Delta_2^{(1)} > 0, \quad \Delta_3 = \det(\hat{\mathcal{H}}^{(S)}) < 0. \tag{22}$$

If one considers different thermodynamic potentials (representations) one has to know how to transfer these conditions to the new energy or entropy derived potentials. This is a non trivial task involving several ingredients such as the properties of the Legendre transformation, the induced metric on the new curved thermodynamic manifold and the use of Maxwell relations for the particular system under consideration. In the following section we show how to construct the second ingredient, while the full construction we leave for a future work.

3. Change of variables, Nambu brackets and induced Hessians

Let us recall that $\vec{E} = (E^1, E^2, ..., E^n)$ define the natural parameters of the energy and we can think of them as coordinates in an n-dimensional flat thermodynamic space – the E-space. The Hessian of the energy in this space is directly related to the Weinhold metric [1]

$$g_{ab}^{(W)}(\vec{E}) \equiv \mathcal{H}_{ab}^{(E)}(\vec{E}) = \left.\frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b}\right|_{E^1,...,\hat{E}^a,...,\hat{E}^b,...,E^n}, \quad a, b = 1, 2, ..., n. \tag{23}$$

We can make a change of the coordinates to a new set of coordinates $\vec{e} = (e^1, e^2, ..., e^n)$. The new coordinates may not all be extensive and most certainly are not all energy natural. They span a new induced curved space – the e-space, where the induced Hessian of the energy is given by

$$g_{\alpha\beta}^{(W)}(\vec{e}) \equiv \mathcal{H}_{\alpha\beta}^{(E)}(\vec{e}) = \left.\frac{\partial^2 E(\vec{e})}{\partial e^\alpha \partial e^\beta}\right|_{e^1,...,\hat{e}^\alpha,...,\hat{e}^\beta,...,e^n}, \quad \alpha, \beta = 1, 2, ..., n. \tag{24}$$

One can check that the relation between the two Hessians is given by the following generalized pushforward from e-space to E-space:

$$g_{ab}^{(W)}(\vec{E}) = \frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b} = \sum_{\alpha,\beta} \frac{\partial e^\alpha}{\partial E^a} \left(\frac{\partial^2 E(\vec{e})}{\partial e^\alpha \partial e^\beta} - \Gamma_{\alpha\beta}^{\gamma}(\vec{e}) \frac{\partial E(\vec{e})}{\partial e^\gamma} \right) \frac{\partial e^\beta}{\partial E^b}. \tag{25}$$

The inverse of this formula is given by the generalized pullback from E-space to e-space:

$$g_{\alpha\beta}^{(W)}(\vec{e}) = \frac{\partial^2 E(\vec{e})}{\partial e^\alpha \partial e^\beta} = \sum_{a,b} \left(\frac{\partial e^\alpha}{\partial E^a} \right)^{-1} \left(\frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b} \right) \left(\frac{\partial e^\beta}{\partial E^b} \right)^{-1} + \Gamma_{\alpha\beta}^{\gamma}(\vec{e}) \frac{\partial E(\vec{e})}{\partial e^\gamma}, \tag{26}$$

where $\Gamma_{\alpha\beta}^{\gamma}(\vec{e})$ are the Christoffel symbols on the e-manifold:

$$\Gamma_{\alpha\beta}^{\gamma}(\vec{e}) = \sum_{\delta} \frac{1}{2} h^{\gamma\delta} (\partial_\beta h_{\delta\alpha} + \partial_\alpha h_{\delta\beta} - \partial_\delta h_{\alpha\beta}), \tag{27}$$

and $h_{\alpha\beta}(\vec{e})$ is the actual induced metric on the e-manifold,

$$h_{\alpha\beta}(\vec{e}) = \sum_{a,b} \delta_{ab} \frac{\partial E^a}{\partial e^\alpha} \frac{\partial E^b}{\partial e^\beta}. \tag{28}$$

Here δ_{ab} is the n-dimensional flat Euclidean metric. For simplicity in the expressions above we have suppressed the lower subscripts of the partial derivatives showing the fixed parameters.

One can think of Eq. (25) as a direct way to calculate components of the Hessian of the energy (the Weinhold metric) in E-space if one knows the components of the Hessian in e-space, while Eq. (26) does the opposite. These expressions give a new representation of the Weinhold metric in any thermodynamic coordinates.

Furthermore, one can use Legendre transformation of the energy to express Eq. (25) in terms of the Hessians of other energy derived potentials. For example, for the Φ_k potential, one finds

$$\frac{\partial^2}{\partial E^a \partial E^b}\left(\Phi_k(\vec{E}) + I_k E^k\right) = \sum_{\alpha,\beta} \frac{\partial e^\alpha}{\partial E^a}\left(\frac{\partial^2}{\partial e^\alpha \partial e^\beta}\left(\Phi_k(\vec{e}) + I_k E^k\right) - \Gamma^\gamma_{\alpha\beta}(\vec{e})\frac{\partial E(\vec{e})}{\partial e^\gamma}\right)\frac{\partial e^\beta}{\partial E^b}. \tag{29}$$

What is the relation of (25) and (26) to the Nambu bracket formalism? To answer this question one has to refer to the first law of thermodynamics in E-space. Let us recall that the equations of state in the energy representation looks like

$$I_a = \left.\frac{\partial E}{\partial E^a}\right|_{E_1,\ldots,\hat{E}^a,\ldots,E^n}. \tag{30}$$

Using this relation one can turn the components of the Hessian into first order partial derivatives over the intensive parameters:

$$\left.\frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b}\right|_{E^1,\ldots,\hat{E}^a,\ldots,\hat{E}^b,\ldots,E^n} = \begin{cases} \left.\frac{\partial I_b(\vec{E})}{\partial E^a}\right|_{E^1,\ldots,\hat{E}^a,\ldots,E^n}, \\ \left.\frac{\partial I_a(\vec{E})}{\partial E^b}\right|_{E^1,\ldots,\hat{E}^b,\ldots,E^n}. \end{cases} \tag{31}$$

The two first order derivative expressions above are different but equivalent representation of the components of the Hessian in equilibrium. The calculations of these derivatives in e-space is achieved by the appropriate Nambu brackets, i.e.

$$\left.\frac{\partial I_b(\vec{E})}{\partial E^a}\right|_{E^1,\ldots,\hat{E}^a,\ldots,E^n} = \frac{\{I_b, E^1, \ldots, \hat{E}^a, \ldots, E^n\}_{e^1,e^2,\ldots,e^n}}{\{E^a, E^1, \ldots, \hat{E}^a, \ldots, E^n\}_{e^1,e^2,\ldots,e^n}}, \tag{32}$$

$$\left.\frac{\partial I_a(\vec{E})}{\partial E^b}\right|_{E^1,\ldots,\hat{E}^b,\ldots,E^n} = \frac{\{I_a, E^1, \ldots, \hat{E}^b, \ldots, E^n\}_{e^1,e^2,\ldots,e^n}}{\{E^b, E^1, \ldots, \hat{E}^b, \ldots, E^n\}_{e^1,e^2,\ldots,e^n}}. \tag{33}$$

Nambu brackets are the generalization of the Poisson brackets for three or more variables, i.e.

$$\{f, x^1, \ldots, x^{n-1}\}_{y^1,y^2,\ldots,y^n} = \begin{vmatrix} \left.\frac{\partial f}{\partial y^1}\right|_{y^2,y^3,\ldots,y^n} & \left.\frac{\partial f}{\partial y^2}\right|_{y^1,y^3,\ldots,y^n} & \cdots & \left.\frac{\partial f}{\partial y^n}\right|_{y^1,y^2,\ldots,\hat{y}^n} \\ \left.\frac{\partial x^1}{\partial y^1}\right|_{y^2,y^3,\ldots,y^n} & \left.\frac{\partial x^1}{\partial y^2}\right|_{y^1,y^3,\ldots,y^n} & \cdots & \left.\frac{\partial x^1}{\partial y^n}\right|_{y^1,y^2,\ldots,\hat{y}^n} \\ \vdots & \vdots & & \vdots \\ \left.\frac{\partial x^{n-1}}{\partial y^1}\right|_{y^2,y^3,\ldots,y^n} & \left.\frac{\partial x^{n-1}}{\partial y^2}\right|_{y^1,y^3,\ldots,y^n} & \cdots & \left.\frac{\partial x^{n-1}}{\partial y^n}\right|_{y^1,y^2,\ldots,\hat{y}^n} \end{vmatrix}. \tag{34}$$

Equations (31), (32) and (32) allow us to relate the generalized pushforward for the Weinhold metric to the Nambu brackets in the following way

$$\begin{aligned} g^{(W)}_{ab}(\vec{E}) &= \frac{\partial^2 E(\vec{E})}{\partial E^a \partial E^b} = \sum_{\alpha,\beta} \frac{\partial e^\alpha}{\partial E^a}\left(\frac{\partial^2 E(\vec{e})}{\partial e^\alpha \partial e^\beta} - \Gamma^\gamma_{\alpha\beta}(\vec{e})\frac{\partial E(\vec{e})}{\partial e^\gamma}\right)\frac{\partial e^\beta}{\partial E^b} \\ &= \begin{cases} \left.\frac{\partial I_b(\vec{E})}{\partial E^a}\right|_{E^1,\ldots,\hat{E}^a,\ldots,E^n} = \frac{\{I_b,E^1,\ldots,\hat{E}^a,\ldots,E^n\}_{e^1,e^2,\ldots,e^n}}{\{E^a,E^1,\ldots,\hat{E}^a,\ldots,E^n\}_{e^1,e^2,\ldots,e^n}}, \\ \left.\frac{\partial I_a(\vec{E})}{\partial E^b}\right|_{E^1,\ldots,\hat{E}^b,\ldots,E^n} = \frac{\{I_a,E^1,\ldots,\hat{E}^b,\ldots,E^n\}_{e^1,e^2,\ldots,e^n}}{\{E^b,E^1,\ldots,\hat{E}^b,\ldots,E^n\}_{e^1,e^2,\ldots,e^n}}. \end{cases} \end{aligned} \tag{35}$$

All the properties we have investigated above are also valid for the Ruppeiner metric and the Hessian of the entropy:

$$g^{(R)}_{ab}(\vec{S}) \equiv \mathcal{H}^{(S)}_{ab}(\vec{S}) = \frac{\partial^2 S(\vec{S})}{\partial S^a \partial S^b}\bigg|_{S^1,\dots,\hat{S}^a,\dots,\hat{S}^b,\dots,S^n}, \quad a,b = 1,2,\dots,n. \tag{36}$$

Therefore, one has two different ways of relating thermodynamic Hessian metric data between arbitrary thermodynamic manifolds[1] (representations).

4. Heat capacities and local thermodynamic equilibrium

The physical interpretation of the components of the Hessian is related to the thermal and caloric thermodynamic coefficients of the system. For example, for three parametric system, there are in total of 12 such coefficients but only three of them are sufficient to fully describe the system. One traditionally chooses the heat capacities, which consequently can be used to define the local thermodynamic stability of the system.

The general definition of a given heat capacity $C_{x^1,x^2,\dots,x^{n-1}}$, at fixed set of thermodynamic parameters $(x^1, x^2, \dots, x^{n-1})$, is given by the derivative of the entropy in a given thermodynamic space $(y^1, y^2, \dots, y^n)$ of equilibrium states, namely

$$C_{x^1,x^2,\dots,x^{n-1}}(y^1, y^2, \dots, y^n) = T\frac{\partial S}{\partial T}\bigg|_{x^1,x^2,\dots,x^{n-1}} = T\frac{\{S, x^1, x^2, \dots, x^{n-1}\}_{y^1,y^2,\dots,y^n}}{\{T, x^1, x^2, \dots, x^{n-1}\}_{y^1,y^2,\dots,y^n}}. \tag{37}$$

The set of constant parameters $x^1, x^2, \dots, x^{n-1}$ could be a mix of all kinds of intensive and extensive variables. Additionally, all the relevant state quantities become functions of the independent parameters $y^1, y^2, \dots, y^n$. In this case we say that $(y^1, \dots, y^n)$ define the coordinates in our space of equilibrium states.

In thermodynamics local equilibrium can be defined by quasi equilibrium between different parts of the system, where some small gradients of the parameters are still allowed. If one has global equilibrium one also has a local one. The reverse is not true. Even if one of the local heat capacities fails to be positive there cannot be a global equilibrium, but local one can still exists with respect to the other heat capacities.

The identification of local stability with the positivity of the heat capacity is related again to the components of the Hessian, which is most evident for simple systems such as the ideal gas or Van der Waals gas (see for example [13–16]). Therefore, one can insist that the conditions for local thermodynamic stability is $C_{x^1,x^2,\dots,x^{n-1}} > 0$.

Heat capacities are also important for identifying the critical points of phase transitions in the system. Specifically, if a given heat capacity diverges or changes sign this would signal the presence of a phase transition and the breakdown of the equilibrium thermodynamic description of the system. In this case, as pointed out by Ruppeiner [2, 12], an alternative way of identifying such critical behaviour of the system is given by the divergences of the thermodynamic curvature

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[1] Although the change of variables is arbitrary we choose the original embedding space (the E-space) to be flat Euclidean space. This is the simplest choice for the energy potential depending on its natural coordinates. However, there is no obvious reason why this should be true and one can choose an arbitrary initial metric.

induced by the Hessian metrics. This result in thermodynamic geometry is more robust than heat capacity's method, because it relies on invariant geometric structures and does not refer to any ordering parameters.

5. Epilogue

The theory of thermodynamic stability is one of the central subjects in thermodynamics with great practical importance. Hence it is imperative that the correct generic necessary and sufficient conditions for local and global thermodynamic stability be identified.

Here we have done this in a manner suitable for the framework of thermodynamic information geometry. In our pursue of generalizing these conditions to an arbitrary thermodynamic potential and arbitrary thermodynamic space we have uncovered novel relations involving thermodynamic information metrics such as the Weinhold and Ruppeiner metrics. These relations are one of the three key ingredients to describe the information transfer of thermodynamic data, including stability conditions, between different representations. The full analysis would also require the properties of the Legendre transformation and the set of Maxwell relations in a given representation. We leave this for a future investigation.

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References

[1] F. Weinhold, *Metric geometry of equilibrium thermodynamics,*, *J. Chem. Phys.* **63** no. 6, (1975) 2479–2483.

[2] G. Ruppeiner, *Riemannian geometry in thermodynamic fluctuation theory, Rev. Mod. Phys.* **67** (1995) 605–659.

[3] J. E. Åman, I. Bengtsson and N. Pidokrajt, *Geometry of black hole thermodynamics, Gen. Rel. Grav.* **35** (2003), 1733, [arXiv:gr-qc/0304015 [gr-qc]].

[4] J. E. Åman and N. Pidokrajt, *Ruppeiner Geometry of Black Hole Thermodynamics, EAS Publ. Ser.* **30** (2008), 269-273, [arXiv:0801.0016 [gr-qc]].

[5] S. A. H. Mansoori and B. Mirza, *Correspondence of phase transition points and singularities of thermodynamic geometry of black holes,* *Eur. Phys. J. C* **74** no. 99, (2014) 2681, [arXiv:1308.1543 [gr-qc]].

[6] S. A. H. Mansoori, B. Mirza and M. Fazel, *Hessian matrix, specific heats, Nambu brackets, and thermodynamic geometry,* *JHEP* **04** (2015), 115, [arXiv:1411.2582 [gr-qc]].

[7] S. H. Hendi, S. Panahiyan, B. Eslam Panah, and M. Momennia, *A new approach toward geometrical concept of black hole thermodynamics,* *Eur. Phys. J. C* **75** no. 10, (2015) 507, [arXiv:1506.08092 [gr-qc]].

[8] H. Quevedo, M. N. Quevedo, and A. Sanchez, *Homogeneity and thermodynamic identities in geometrothermodynamics,* *Eur. Phys. J. C* **77** no. 3, (2017) 158, [arXiv:1701.06702 [gr-qc]].

[9] S. A. Hosseini Mansoori and B. Mirza, *Geometrothermodynamics as a singular conformal thermodynamic geometry,* *Phys. Lett. B* **799** (2019), 135040, [arXiv:1905.01733 [gr-qc]].

[10] T. Vetsov, *Information Geometry on the Space of Equilibrium States of Black Holes in Higher Derivative Theories,* *Eur. Phys. J. C* **79** (2019) no.1, 71, [arXiv:1806.05011 [gr-qc]].

[11] H. Dimov, R. C. Rashkov and T. Vetsov, *Thermodynamic information geometry and complexity growth of a warped AdS black hole and the warped AdS_3/CFT_2 correspondence,* *Phys. Rev. D* **99** (2019) no.12, 126007, [arXiv:1902.02433 [hep-th]].

[12] G. Ruppeiner, *Thermodynamic curvature measures interactions,* *American Journal of Physics* **78** no. 11, (2010) 1170–1180, [arXiv:1007.2160 [cond-mat.stat-mech]].

[13] I. P. Bazarov. *Thermodynamics*. A Pergamon Press Book, New York, 1964.

[14] H. B. Callen. *Thermodynamics and an Introduction to Thermostatistics.* Wiley, 1985.

[15] W. Greiner et al. *Thermodynamics and Statistical Mechanics*. Classical Theoretical Physics. Springer New York, 2012.

[16] R. H. Swendsen. *An Introduction to Statistical Mechanics and Thermodynamics.* Oxford Graduate Texts. OUP Oxford, 2020.