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EXPLOITING THE SECOND LAW IN WEAKLY NON-LOCAL CONTINUUM PHYSICS

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Abstract

Some peculiarities of the exploitation of the entropy inequality in the case of weakly non-local continuum theories are investigated and refined. As an example, the simplest internal variable theories are investigated. It is shown that the proper application of Liu's procedure leads to the Ginzburg-Landau equation in the case of a weakly non-local extension of the constitutive space.

Keywords: weakly non-load, Liu's procedure, Ginzburg-Landau equation, non-equilibrium thermodynamics.

1. Introduction

In the last decades there has been a continuous interest in developing generalized classical continuum theories that are able to describe non-local effects. In this paper we investigate some general aspects of *weakly non-local* (gradient) theories where the material functions depend on the different derivatives of the basic state variables.

One can generalize classical theories introducing higher order space derivatives into the material functions. Weakly non-local continuum theories appear in different parts of physics. For example, the weakly non-local generalization of classical ideal Euler fluids, considering pressure that depends on the gradient of the density, has been known for more than a century. These are the so called Korteweg fluids [1]. Another example can be the weakly non-local heat conduction. Here the Guyer-Krumhansl equation of weakly non-local (and wave) heat conduction [2] is the most important example, but there are several other theories, e.g. the Cimmelli-Kosiński model [3]. One can find numerous other examples of weakly non-local theories under different names, like gradient theories, theories with coarse grained thermodynamic potentials, phase-field models, etc...

The general Korteweg fluids are not good models of any particular physical phenomena, only some restricted forms can be important. The mentioned weakly non-local heat conduction models also introduce specific constitutive functions. The Second Law restricts the form of any constitutive equation. There are different methods and principles to understand how and under what conditions the Second Law restricts the form of gradient dependent constitutive functions.

For weakly non-local equations the traditional methods of irreversible thermodynamics seemingly do not work. One cannot recognize thermodynamic forces and currents. Introducing dynamic variables, which were a great help modelling inertial (memory) effects [4, 5, 5, 6, 7, 8] does not help at all. In the case of weakly non-local thermodynamic theories, one should apply additional principles or/and special considerations; like the virtual power of Germain and Maugin [9], a microstructure theory based on the concept of microforce balance of Gurtin [10], the theory of substructural interactions initiated by Goodman and Cowin [11], etc...

The investigations toward the weakly non-local extension of extended thermodynamics by Lebon, Jou and co-workers [12, 13, 14, 15] show well the renewed attempts to build up a satisfactory theory that uses uniform methods to describe non-local and memory effects.

In this paper, all the basic ingredients and the mathematical background, to exploit the Second Law inequality in weakly non-local continuum theories, are collected and investigated. In the next section a short review of the methods to exploit the Second Law inequality is given. We collect some arguments why Liu's procedure unified with a traditional Onsagerian approach is favorable, and emphasize the most important differences between local and weakly non-local theories. In the following section the suggested method is applied in the simplest possible case, to get the gradient extension of the traditional relaxation equation of a single dynamic variable. We will arrive at the Ginzburg-Landau equation. A new, generalized formulation of Liu's theorem, suitable for our purposes, and its direct proof from Farkas' lemma are given in an Appendix.

2. Methods to Exploit the Second Law Inequality – Procedures of CIT, Coleman-Noll and Liu

In every non-equilibrium thermodynamic theory, an important theoretical problem is to formulate the correct form of the evolution equations taking into account the requirement of the entropy inequality. The most predictive methodological solution of the problem is due Coleman and Mizel. According to them one should look for the solution of the entropy inequality taking into account the evolution equations as constraints [16, 17]. In continuum physics the dynamic equations are partially determined (e.g. as balances of extensives), except some constitutive, material functions. The task is to ensure the non-negativity of the entropy production with appropriate constitutive assumptions. Therefore, one should specify the undetermined material functions in such a way that in the case of all possible solutions of the dynamic equations the form of the constitutive functions ensures the non-negativity of the entropy production. In this case, the Second Law expresses a material property, the inequality is fulfilled independently of the initial and boundary conditions. The entropy and the entropy current are both constitutive and are to be determined according to the above requirement (as it was suggested originally by Müller and applied in extended rational thermodynamics [7]). The entropy should possibly preserve its potential character in a general sense, therefore solving the above problem the practical aim is a simplification in such a way that the constitutive quantities could be calculated from the entropy function.

There are three basic methods to exploit the entropy inequality.

- *Heuristic.* This is the force-current method of classical irreversible thermodynamics (CIT). In classical problems, in the case of simple state spaces, the form of the entropy production is quadratic and the inequality can be solved. The method can be justified by Liu's procedure in the case of the traditional, simplest state spaces [18], and the method can be generalized to include non-classical entropy currents [19, 20].
- *Coleman-Noll procedure.* In the Coleman-Noll procedure one exploits the constraints (e.g. dynamic equations) directly, substituting them into the entropy inequality. The degenerate form of Liu's theorem (Theorem 5.5) is applied. One usually assumes a specific form of the entropy current. There are essentially two choices here. The entropy current can be the classical ($\mathbf{j}_s = \mathbf{j}_q/T$), or a generalized one. In weakly non-local considerations both classical (see e.g. [10, 21]) and generalized forms are applied (see e.g [22]). Generalizations of the entropy currents (or currents of other thermodynamic potentials) can be suggested on different grounds and they give good results with the procedure [23, 24].
- *Liu's procedure.* With Liu's procedure one applies Liu's theorem with Lagrange-Farkas multipliers (Theorem 5.3 in the Appendix). At first glance the application of this method seems to have only practical advantages. However, as the Lagrange multiplier method preserves the simple form of the constraints in question in constrained extremum problems, Lagrange-Farkas multipliers preserve and exploit the structure of the constraints and the entropy inequality. The question is not purely mathematical, because there are cases where the multipliers cannot be eliminated and they can get physical significance. Moreover, an inevitable advantage of Liu's method is that the structure of entropy inequality makes it possible to solve the physical problem completely.

The first two exploitation methods are frequently applied in the case of weakly non-local continuum theories beside the mentioned examples. Here we suggest that we apply Liu's procedure adapted to the specialities of the generalized weakly non-local constitutive functions.

We emphasize the following important peculiarities. The entropy current is considered as an independent constitutive quantity. With a proper choice of the constitutive space and considering the entropy as a primary constitutive quantity, we can solve the Liu equations, determine the entropy current and simplify the entropy inequality. The point of view of Onsagerian CIT is important because with a proper identification of thermodynamic currents and forces the resulted entropy inequality can be solved, determining all constitutive quantities.

In the following we will apply the following terminology. The functions in the differential equations form the *basic state space*. The basic state variables and some of their derivatives can be included in the *constitutive state space* (or simply state space [25]), in the domain of the constitutive functions. The entropy inequality with its special balance form determines the independent variables of the algebraic problem: those are the derivatives of the constitutive state, called *process directions*. The choice of the constitutive state space is crucial and determines the restricted constitutive functions after applying Liu's procedure.

In weakly non-local continuum physical calculations with Liu's procedure, one should consider some additional practical rules. Depending on the particular state space, some space derivatives of the original constraints (e.g. dynamic equations) further restrict the process direction space, therefore, they should be considered in Liu's theorem as additional constraints. One can find other examples on the application of derivative constraints in [3, 26, 27].

REMARK 2.1 *The mentioned exploitation methods of the Second Law are algebraic. Therefore, the solubility of the dynamic equations is not important, the associated problems can be well or ill posed on the applied function spaces, etc... For example the number of the equations can be less than the number of variables in the basic state space. The* wanted fields, *the functions searched in the final resulting differential equation can be different from the basic state* [28].

Let us give a simple example to illustrate the role of derivative constraints and some other aspects of the above considerations.

EXAMPLE 1 In this example the *basic state space* is formed by two times differentiable real functions $x : \mathbb{R} \mapsto \mathbb{R}$. The *constitutive space* is spanned by the basic state and its derivative (x, x'). We are looking for scalar valued differentiable functions F and S as lying in the constitutive space so that

$$S'(x, x') \geq 0$$

for all (x, x') satisfying the *constraint*

$$F(x, x') = 0. \tag{1}$$

Evidently $S'(x, x') = \partial_1 S x' + \partial_2 S x''$, where ∂_n denotes the partial derivative according to the n-th variable. Therefore, the space of the *process directions* (the space of independent variables in Liu's theorem) is spanned by x''. We are looking for conditions on S and F so that the above inequality should be true for all (x, x') solving (1), but independently of the values of x''. The degenerate case of Liu's theorem (Theorem 5.5) gives some conditions. The single Liu equation is

$$\partial_2 S = 0.$$

Therefore S is independent of x'. The dissipation inequality can be written in the following simple form

$$\partial_1 S x' = \frac{\mathrm{d}S}{\mathrm{d}x}(x) x' \geq 0. \tag{2}$$

The above inequality does not give any condition for F. However, let us observe, that one of our previous assumptions was too strong. The process direction variable x'' is not really independent of the state space, the derivative of (1) gives a further restriction

$$\partial_1 F x' + \partial_2 F x'' = 0. \tag{3}$$

Considering this condition we apply Liu's theorem (Theorem 5.3) with the multiplier method, introducing the multipliers λ_1 and λ_2 for the constraints (1) and (3) respectively

$$\begin{aligned}&\partial_1 S x' + \partial_2 S x'' - \lambda_2(\partial_1 F x' + \partial_2 F x'') - \lambda_1 F \\ &\quad = (\partial_1 S - \lambda_2 \partial_1 F)x' + (\partial_2 S - \lambda_2 \partial_2 F)x'' - \lambda_1 F \geq 0.\end{aligned}$$

Therefore, we can read the Liu equation as follows

$$\lambda_2 \partial_2 F - \partial_2 S = 0.$$

Expressing the multiplier and substituting into the dissipation inequality we get

$$\partial_1 S x' - \lambda_2 \partial_1 F x' - \lambda_1 F = (\partial_1 S - \partial_2 S (\partial_2 F)^{-1} \partial_1 F)x' - \lambda_1 F \geq 0.$$

In this example we face a partially degenerate case, hence with $\lambda_1 = 0$ we can give the general solution of the above inequality, as

$$\partial_1 S - \partial_2 S (\partial_2 F)^{-1} \partial_1 F = L(x, x')x',$$

where L is non-negative. Given a function S we can calculate F, with appropriate conditions on L. For example, if $S(x, x') = x \cdot x'$ and $L = constant$, then $F(x, x') = f(x^{L-1}x')$ is a solution of the above equation for any $f : \mathbb{R} \mapsto \mathbb{R}$.

3. Weakly Non-local Dynamic Equation for an Internal Variable – Ginzburg-Landau Equation

Ginzburg-Landau equation is one of the most important pattern forming equations of physics [29]. Its physical content and the way to obtain it is sound and transparent. The traditional derivation of the equation comprises two main ingredients (see e.g. [30])

- The static, equilibrium part is derived from a variational principle.
- The dynamic part is added by stability arguments (relaxational form).

The two parts are connected loosely and in an ad hoc manner. As a classical field equation defined on non-relativistic space-time, the Ginzburg-Landau equation should be compatible with the general balance and constitutive structure of continuum physics. Recently there have been several efforts to give a uniform reasoning of the equation on a pure thermodynamic ground, and to generalize the method of the derivation [10, 24, 31, 18]. The treatment of Ginzburg-Landau equation is a kind of test of weakly non-local (gradient) thermodynamic theories.

Let us denote a scalar internal variable (e.g. an order parameter of a second order phase transition) characterizing the material by ξ. We assume a free energy density that depends on the internal variable and also on the gradient of the internal variable $f(\xi, \nabla\xi)$. The usual form of the Ginzburg-Landau free energy density is

$$f(\xi, \nabla\xi) = f_0(\xi) + \gamma(\nabla\xi)^2/2, \tag{4}$$

where γ is a material coefficient, f_0 is the static (equilibrium) free energy and we introduce the following notation $\Gamma_\xi = \partial_\xi f(\xi, \nabla\xi) = f_0'(\xi)$. Here ∂_ξ is the partial derivative by the variable ξ.

According to the traditional reasoning, the rate of change of ξ in a given volume V is negatively proportional to the free energy changes of the material.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \xi \mathrm{d}V = -l\delta\int_V f(\xi, \nabla\xi) dV. \tag{5}$$

Here δ denotes the variation of the total free energy. If we assume that the above statement is valid in any volume then we obtain the *Ginzburg-Landau equation* as

$$\partial_t\xi = -l(\partial_\xi f - \nabla\cdot\partial_{\nabla\xi} f) = -l(\Gamma_\xi - \gamma\Delta\xi), \tag{6}$$

where ∂_t denotes the partial time derivative, l is a material coefficient. Here we assumed a fixed boundary, therefore, the change of the internal variable ξ is not related to the mechanical motion.

In the following we apply Liu's procedure [32] to derive the Ginzburg-Landau equation from different assumptions.

We are looking for a dynamic equation of ξ in the following general form

$$\partial_t\xi - \mathcal{G} = 0, \tag{7}$$

where $\mathcal{G}$ is a constitutive function, which form is to be restricted by the Second Law. Therefore, we require the following inequality for all solutions of the above equations

$$\partial_t f + \nabla\cdot\mathbf{j}_f \le 0. \tag{8}$$

Here the specific free energy f and its current density $\mathbf{j}_f$ are constitutive quantities. We called the thermodynamic potential related to our internal variable ξ as free energy because of traditional reasons based on the fact that internal energy and temperature do not play any role in the following considerations. However, it is well known that the above inequality is a consequence of the entropy inequality. The difference in the sign of the free energy and entropy productions is based on the different convexity properties. The existence of thermodynamic potential functions is connected to the expected stability properties of the material in the case of simple, homogeneous boundary conditions. If we postulate the Second Law in one system of variables for one kind of potential function, we can obtain other formulations by suitable Legendre transformations.

Let us assume that the constitutive space, the domain of the constitutive functions $\mathcal{G}$, f and $\mathbf{j}_f$ is spanned by ξ, $\nabla\xi$, $\nabla^2\xi$ and $\nabla^3\xi$. ∇^i denotes the i-th spatial derivative of the corresponding function. In this case the above inequality can be written as

$$\partial_t f + \nabla\cdot\mathbf{j}_f = \partial_1 f\,\partial_t\xi + \partial_2 f\cdot\nabla\partial_t\xi + \partial_3 f : \nabla^2\partial_t\xi + \partial_4 f\cdot:\nabla^3\partial_t\xi \\ + \partial_1\mathbf{j}_f\cdot\nabla\xi + \partial_2\mathbf{j}_f : \nabla^2\xi + \partial_3\mathbf{j}_f\cdot:\nabla^3\xi + \partial_4\mathbf{j}_f :: \nabla^4\xi \leq 0.$$

Here ∂_i denotes the partial derivative of the corresponding constitutive function according to its i-th variable, respectively. The dots always denote full contraction of the quantities of different tensorial orders.

One can see that the space of the process directions (independent variables) is spanned by $\partial_t\xi$, $\nabla\partial_t\xi$, $\nabla^2\partial_t\xi$, $\nabla^3\partial_t\xi$ and $\nabla^4\xi$. Moreover, let us observe that these variables are not really independent, the gradient of (7) connects them. Therefore, in addition to (7) one should consider the following constraint

$$\nabla\partial_t\xi - \nabla\mathcal{G} = \nabla\partial_t\xi - \partial_1\mathcal{G}\nabla\xi - \partial_2\mathcal{G}\cdot\nabla^2\xi - \partial_3\mathcal{G} : \nabla^3\xi - \partial_4\mathcal{G}\cdot:\nabla^4\xi = 0. \quad (9)$$

We can recognize a peculiarity of weakly non-local (gradient) theories. The constraints depend on the particular state space, some space derivatives of the original constraints (e.g. dynamic equations) further restrict the process direction space, therefore, they should be considered in Liu's theorem as additional constraints. One can find other examples on the application of derivative constraints with internal variables and Coleman-Noll technique [3] and also with Liu's procedure [26, 27].

Introducing Γ_1 and Γ_2 Lagrange-Farkas multipliers for the constraints (7) and (9) respectively, one can get the following Liu equations

$$\begin{aligned} \partial_1 f &= \Gamma_1, \\ \partial_2 f &= \Gamma_2, \\ \partial_3 f &= \mathbf{0}, \\ \partial_4 f &= \mathbf{0}, \\ (\partial_4\mathbf{j}_f + \Gamma_2\partial_4\mathcal{G})^s &= \mathbf{0}. \end{aligned}$$

Here the superscript ^{s} denotes the symmetric part of the corresponding fourth order tensor. The first two equations determine the multipliers. From the third and fourth equations it follows that the free energy does not depend on its third and fourth variables $s = s(\xi, \nabla\xi)$. Taking into account these requirements one can give a solution of the fifth equation and determine the free energy current as

$$\mathbf{j}_f(\xi,\nabla\xi,\nabla^2\xi,\nabla^3\xi) = -\partial_2 f(\xi,\nabla\xi)\mathcal{G}(\xi,\nabla\xi,\nabla^2\xi,\nabla^3\xi) + \mathbf{j}_0(\xi,\nabla\xi,\nabla^2\xi). \quad (10)$$

For the sake of clarity we explicitly denoted the variables of the corresponding functions. $\mathbf{j}_0$ can be an arbitrary function. With the above solution of the Liu equations the dissipation inequality can be simplified considerably

$$\nabla \cdot \mathbf{j}_0 + (\partial_\xi f - \nabla \cdot \partial_{\nabla\xi} f)\mathcal{G} \leq 0. \tag{11}$$

Now we treat two special cases.

1) Let us assume that $\mathbf{j}_0 \equiv 0$. In this case one can give the general solution of the above inequality. That solution can be interpreted by the well-known traditional method of irreversible thermodynamics, choosing appropriate forces and currents. Assuming that the free energy is the primary quantity (given by static measurements), $\mathcal{G}$ is the constitutive quantity to be determined, the *thermodynamic current* and it should be proportional to the given function, the *thermodynamic force*. Therefore, the Ginzburg-Landau equation follows as

$$\partial_t \xi = \mathcal{G} = -L(\partial_\xi f - \nabla \cdot \partial_{\nabla\xi} f), \tag{12}$$

where L is a non-negative constitutive function. (12) is the Ginzburg-Landau equation. One can get back the traditional (6) form using the specific free energy function with a form like (4) and dealing with a strictly linear theory in a thermodynamic sense, where L is a constant material coefficient.

2) Now let us investigate the case when the additional free energy current $\mathbf{j}_0$ is not zero. Our principal assumption is that any changes of the free energy should be connected to the change of ξ. In particular, the current of the free energy vanishes if ξ is constant,

$$\mathbf{j}_0 = \mathbf{A}\mathcal{G}. \tag{13}$$

In addition, we should require that $\mathcal{G}$ does not depend on the third derivative of ξ, $\mathcal{G} = \mathcal{G}(\xi, \nabla\xi, \nabla^2\xi)$. Similar assumption was introduced by Nyíri [20] and later exploited extensively in [18]. Now (11) can be written as

$$\begin{aligned}(\nabla \cdot \mathbf{A})\mathcal{G} + \mathbf{A} \cdot \nabla\mathcal{G} + (\partial_\xi f - \nabla \cdot \partial_{\nabla\xi} f)\mathcal{G} = \\ \mathcal{G}\left[\partial_\xi f + \nabla \cdot (\mathbf{A} - \partial_{\nabla\xi} f)\right] + \mathbf{A} \cdot \nabla\mathcal{G} \leq 0.\end{aligned} \tag{14}$$

Now one can recognize the functions $\mathbf{A}$ and $\mathcal{G}$ as *thermodynamic currents*, the functions to be determined in accordance with the inequality above. A general Onsagerian solution can be written as

$$\begin{aligned}\mathbf{A} &= L_{11}\nabla\mathcal{G} + L_{12}(\partial_\xi f + \nabla \cdot (\mathbf{A} - \partial_{\nabla\xi} f)),\\ \mathcal{G} &= L_{21}\nabla\mathcal{G} + L_{22}(\partial_\xi f + \nabla \cdot (\mathbf{A} - \partial_{\nabla\xi} f)),\end{aligned}$$

where L_{11}, L_{12}, L_{21} and L_{22} are constitutive functions with a suitable tensorial order, the components of the conductivity matrix $\mathbf{L}$ which is negative definite.

In isotropic materials $L_{12} = \mathbf{0}$ and $L_{21} = \mathbf{0}$ and $L_{11} = -l_1\mathbf{I}$, $L_{22} = -l_2$ where l_1 and l_2 are non-negative scalar constitutive functions. In this case $\mathbf{A}$ can be eliminated, resulting in

$$\partial_t \xi = \mathcal{G} = -l_2(\partial_1 f - \nabla \cdot \partial_2 f) + l_2\nabla \cdot (l_1\nabla\partial_t\xi). \tag{15}$$

Eq. (15) is a generalization of the Ginzburg-Landau equation with a characteristic additional term containing the second spatial derivative of the rate of ξ. The additional term does not change the equilibrium solutions of the equations. It was derived by Gurtin [10] for the Ginzburg-Landau and Cahn-Hilliard equations by the hypothesis of microforce balance. In [18] I have argued that the appearance of this kind of corrections is a natural consequence of the generalization of the entropy current in the case of dynamic internal variables. The consequences of this kind of terms were observed in different thermodynamic systems. E.g. adding this term to the Cattaneo-Vernote equation of heat conduction one obtains the Guyer-Krumhansl equation. Regarding diffusion problems see e.g. [33].

4. Conclusions and Discussion

The requirement of a non-negative entropy production is a strong form of the Second Law. It contains two independent assumptions: the existence of a thermodynamic potential function and a dynamics that makes this potential function increase. The stability of materials in isolated systems incorporates some other conditions (e.g. concave entropy function), too (see [34] in the case of discrete systems). Coleman-Mizel methodology is a kind of basic philosophical requirement of a thermodynamic theory: the acceptable theories are those, where the entropy inequality is the consequence of pure material properties and independent of other elements of the theory (e.g. initial conditions). Considering only general principles ensures a kind of universality and some stability properties to any thermodynamic theories.

It is interesting to know that the doubled variational-thermodynamic structure of the Ginzburg-Landau equation can be generalized considerably. That is the idea behind the General Equation for the Non-equilibrium Reversible-Irreversible Coupling (GENERIC) [35, 36, 37], where the variational part and a formalism from mechanics plays the leading role (different brackets, geometrical point of view, etc.), but both parts are represented. In this paper we unified the variational and the thermodynamic parts of the derivation of the Ginzburg-Landau equation on a pure thermodynamic ground, where we did not refer to any kind of variational principle. However, the derived static part turned out to have a complete Euler-Lagrange form. The dynamic part contains a first order time derivative, therefore, one cannot hope to derive it from a variational principle of the Hamiltonian type [38]. In our approach we get the ‘reversible’, ‘variational’ part as a specific case of the thermodynamic, irreversible thinking, but one cannot hope the contrary, the irreversible part cannot be derived from a variational, reversible thinking.

Understanding the compatibility of the weakly non-local theories with the Second Law it can be considered as one of the challenges of contemporary non-equilibrium thermodynamics. In this paper it was shown that one of the most important pattern forming equations, the Ginzburg-Landau equation, was a straightforward consequence of the entropy inequality in a non-locally extended constitutive space. One can consider higher order derivatives in the constitutive state space and higher order derivatives of the constraints to investigate different materials.

Weakly non-local, pattern forming equations emerge in different fields of physics independently of thermodynamic argumentation [39, 40]. Cross and Hohenberg argued that one could not expect general principles beyond free energy minimization and reviewed perturbation techniques to get the corresponding 'amplitude' or 'phase field' equations. In this paper a general thermodynamic approach to pattern forming equations is proposed. The method is fully compatible with classical 'linear irreversible thermodynamics' [41, 42] and also with the free energy minimization techniques. However, we have shown that the deeper Second Law argumentation can be more informative than the traditional variational approaches. The reviewed general concepts outline the mathematical background and the key ingredients of an efficient formalism to exploit the Second Law in weakly non-local continuum theories.

5. Appendix: Liu's Theorem as a Variant of Farkas' Lemma and Some of its Consequences

In 1972 Liu introduced a method of the exploitation of the entropy principle [32]. Liu's procedure became a basic tool to find the restrictions posed by the entropy inequality. The method is based on a linear algebraic theorem, called Liu's theorem, in the thermodynamic literature [7, 25] and on an interpretation of the entropy inequality, one of the fundamental ingredients of the Second Law. Recently, Hauser and Kirchner recognized that Liu's theorem is a consequence of the fundamental theorem of linear inequalities, a famous statement of optimization theory and linear programming, the Farkas' lemma [43]. That theorem was proved first by Farkas in 1894 [44] and independently by Minkowski in 1896 [45]. In this appendix we formulate and generalize Liu's theorem in a way that it is best adapted to our purposes and shows the whole train of thought from Farkas' lemma to Liu's theorem, giving a simple proof to every statement in question.

Farkas' lemma can be formulated in several different forms that are more or less equivalent [46, 47]. Here we start from a simple variant.

LEMMA 5.1 (FARKAS) *Let* $\mathbf{a}_i \neq \mathbf{0}$ *be independent vectors in a finite dimensional vector space* $\mathbb{V}$, $i = 1 \dots n$, *and* $S = \{\mathbf{p} \in \mathbb{V}^* \mid \mathbf{p} \cdot \mathbf{a}_i \geq 0, i = 1 \dots n\}$. *The following statements are equivalent for a* $\mathbf{b} \in \mathbb{V}$*:*

(i) $\mathbf{p} \cdot \mathbf{b} \geq 0$, *for all* $\mathbf{p} \in S$.
(ii) *There are non-negative real numbers* $\lambda_1, \dots, \lambda_n$ *such that* $\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i$.

Proof: S is not empty. In fact, for all $k, i \in \{1, \dots, n\}$ there is a $\mathbf{p}_k \in \mathbb{V}^*$ such that $\mathbf{p}_k \cdot \mathbf{a}_k = 1$ and $\mathbf{p}_k \cdot \mathbf{a}_i = 0$ if $i \neq k$. Evidently $\mathbf{p}_k \in S$ for all k.

(ii) $\Rightarrow$ (i) $\mathbf{p} \cdot \sum_{i=1}^n \lambda_i \mathbf{a}_i = \sum_{i=1}^n \lambda_i \mathbf{p} \cdot \mathbf{a}_i \geq 0$ if $\mathbf{p} \in S$.

(i) $\Rightarrow$ (ii) Let $S_0 = \{\mathbf{y} \in \mathbb{V}^* \mid \mathbf{y} \cdot \mathbf{a}_i = 0, i = 1...n\}$. Clearly $\emptyset \neq S_0 \subset S$.

If $\mathbf{y} \in S_0$ then $-\mathbf{y}$ is also in S_0, therefore $\mathbf{y} \cdot \mathbf{b} \geq 0$ and $-\mathbf{y} \cdot \mathbf{b} \geq 0$ together. Therefore for all $\mathbf{y} \in S_0$ it is true that $\mathbf{y} \cdot \mathbf{b} = 0$.

As a consequence $\mathbf{b}$ is in the set generated by $\{\mathbf{a}_i\}$, that is, there are real numbers $\lambda_1, ..., \lambda_n$ such that $\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i$. These numbers are non-negative, because with the previously defined $\mathbf{p}_k \in S$, $0 \leq \mathbf{p}_k \cdot \mathbf{b} = \mathbf{p}_k \cdot \sum_{i=1}^l \lambda_i \mathbf{a}_i = \lambda_i \mathbf{p}_k \cdot \mathbf{a}_i = \lambda_k$ is valid for all k. ■

REMARK 5.1 *In the following, the elements of* $\mathbb{V}^*$ *are called* independent variables *and* $\mathbb{V}^*$ *itself is called the* space of independent variables. *The inequality in the first statement of the lemma is called* aim inequality *and the non-negative numbers in the second statement are called* Lagrange-Farkas multipliers. *The inequalities determining* S *are the* constraints.

In the calculations an excellent reminder is to use Lagrange-Farkas' multipliers similarly to Lagrange multipliers in the case of conditional extremum problems:

$$\mathbf{p} \cdot \mathbf{b} - \sum_{i=1}^n \lambda_i \mathbf{p} \cdot \mathbf{a}_i = \mathbf{p} \cdot \left(\mathbf{b} - \sum_{i=1}^n \lambda_i \cdot \mathbf{a}_i \right) \geq 0, \quad \forall \mathbf{p} \in \mathbb{V}^*$$

From this form we can read the second statement of the lemma.

REMARK 5.2 *The original statement does not require the independency of the vectors in the constraint. We need some extra conditions and that generalization destroys the simplicity of the proof. However, we do not need this generalization in thermodynamics.*

The geometric interpretation of the theorem is important and graphic: either vector $\mathbf{b}$ *belongs to the cone generated finitely by the vectors* $\mathbf{a}_i$ *(*$Cone(\mathbf{a}_1, ..., \mathbf{a}_n) = \{\lambda_1 \mathbf{a}_1 + ... + \lambda_n \mathbf{a}_n \mid (\lambda_1, ..., \lambda_n) \in \mathbb{R}^{+n}$*), or there exists a hyperplane separating* $\mathbf{b}$ *from the cone.*

5.1. Affine Farkas' Lemma

This generalization of the previous lemma was first published simultaneously by A. Haar and J. Farkas in the same number of the same journal, with different proofs [48, 49]. Later it was reproved independently by others several times (e.g. [50, 47]). Here we give a simple version again.

THEOREM 5.2 (AFFINE FARKAS) *Let* $\mathbf{a}_i \neq \mathbf{0}$ *be independent vectors in a finite dimensional vector space* $\mathbb{V}$ *and* α_i *real numbers,* $i = 1...n$ *and* $S_A = \{\mathbf{p} \in \mathbb{V}^* \mid \mathbf{p} \cdot \mathbf{a}_i \geq \alpha_i, i = 1...n\}$. *The following statements are equivalent for a* $\mathbf{b} \in \mathbb{V}$ *and a real number* β*:*

(i) $\mathbf{p} \cdot \mathbf{b} \geq \beta$, *for all* $\mathbf{p} \in S_A$.

(ii) *There are non-negative real numbers* $\lambda_1, ..., \lambda_n$ *such that* $\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i$ *and* $\beta \leq \sum_{i=1}^n \lambda_i \alpha_i$.

Proof: S_A is not empty. In fact, $\alpha_i \mathbf{p}_k \in S_A$ for all k ($\mathbf{p}_k \cdot \mathbf{a}_k = 1$ and $\mathbf{p}_k \cdot \mathbf{a}_i = 0$ if $i \neq k$ as previously).

(ii) $\Rightarrow$ (i) $\mathbf{p} \cdot \mathbf{b} = \mathbf{p} \cdot \sum_{i=1}^n \lambda_i \mathbf{a}_i = \sum_{i=1}^n \lambda_i \mathbf{p} \cdot \mathbf{a}_i \geq \sum_{i=1}^n \lambda_i \alpha_i \geq \beta$.

(i) $\Rightarrow$ (ii) First we will show indirectly that the first condition of lemma 5.1 is a consequence of the first condition here, that is if (i) is true then $\mathbf{p} \cdot \mathbf{b} \geq 0$, for all $\mathbf{p} \in S$.

Thus, let us assume the contrary, hence there is $\mathbf{p}' \in S$, for which $\mathbf{p}' \cdot \mathbf{b} < 0$. Take an arbitrary $\mathbf{p} \in S_A$, then $\mathbf{p} + k\mathbf{p}' \in S_A$ for all real numbers k. But now $(\mathbf{p} + k\mathbf{p}') \cdot \mathbf{b} = \mathbf{p} \cdot \mathbf{b} + k\mathbf{p}' \cdot \mathbf{b} < \beta$, if $k \geq \frac{\beta - \mathbf{p} \cdot \mathbf{b}}{\mathbf{p}' \cdot \mathbf{b}}$. That is a contradiction.

Therefore, according to Farkas lemma (Lemma 5.1) there exist Lagrange-Farkas multipliers $\lambda = (\lambda_1, ..., \lambda_n) \in \mathbb{R}^{n+}$ such that $\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i$. Hence $\beta \leq \inf_{p \in S_A} \{\mathbf{p} \cdot \sum_{i=1}^n \lambda_i \mathbf{a}_i\} = \inf_{p \in S_A} \{\sum_{i=1}^n \lambda_i \mathbf{p} \cdot \mathbf{a}_i\} = \sum_{i=1}^n \lambda_i \alpha_i$. ■

REMARK 5.3 *The multiplier form is a good reminder again*

$$(\mathbf{p} \cdot \mathbf{b} - \beta) - \sum_{i=1}^n \lambda_i (\mathbf{p} \cdot \mathbf{a}_i - \alpha_i) = \mathbf{p} \cdot (\mathbf{b} - \sum_{i=1}^n \lambda_i \cdot \mathbf{a}_i) - \beta + \sum_{i=1}^n \lambda_i \alpha_i \geq 0, \quad \forall \mathbf{p} \in \mathbb{V}^*.$$

REMARK 5.4 *The geometric interpretation is similar to the previous one, but everything is affine.*

5.2. Liu's Theorem

Here the constraints are equalities instead of inequalities, therefore the multipliers are not necessarily positive.

THEOREM 5.3 (LIU) *Let $\mathbf{a}_i \neq \mathbf{0}$ be independent vectors in a finite dimensional vector space $\mathbb{V}$ and α_i real numbers, $i = 1...n$ and $S_L = \{\mathbf{p} \in \mathbb{V}^* \mid \mathbf{p} \cdot \mathbf{a}_i = \alpha_i, i = 1...n\}$. The following statements are equivalent for a $\mathbf{b} \in \mathbb{V}$ and a real number β:*

(i) $\mathbf{p} \cdot \mathbf{b} \geq \beta$, *for all* $\mathbf{p} \in S_L$,

(ii) *There are real numbers* $\lambda_1, ..., \lambda_n$ *such that*

$$\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i \tag{16}$$

and

$$\beta \leq \sum_{i=1}^n \lambda_i \alpha_i. \tag{17}$$

Proof: A straightforward consequence of the previous affine form of Farkas' lemma because S_L can be given in a form S_A with the vectors $\mathbf{a}_i$ and $-\mathbf{a}_i$, $i = 1, ..., n$: $S_L = \{\mathbf{p} \in \mathbb{V}^* \mid \mathbf{p} \cdot \mathbf{a}_i \geq \alpha_i, \quad \text{and} \quad \mathbf{p} \cdot (-\mathbf{a}_i) \geq -\alpha_i, i = 1...n\}$.

Therefore, there are non-negative real numbers $\lambda_1^+, ..., \lambda_n^+$ and $\lambda_1^-, ..., \lambda_n^-$ such, that $\mathbf{b} = \sum_{i=1}^n (\lambda_i^+ \mathbf{a}_i - \lambda_i^- \mathbf{a}_i) = \sum_{i=1}^n (\lambda_i^+ - \lambda_i^-)\mathbf{a}_i = \sum_{i=1}^n \lambda_i \mathbf{a}_i$ and $\beta \le \sum_{i=1}^n (\lambda_i^+ \alpha_i - \lambda_i^- \alpha_i)$. ■

REMARK 5.5 *The multiplier form is a help in the applications again*

$$0 \le (\mathbf{p}\cdot\mathbf{b}-\beta) - \sum_{i=1}^n \lambda_i(\mathbf{p}\cdot\mathbf{a}_i - \alpha_i) = \mathbf{p}\cdot(\mathbf{b}-\sum_{i=1}^n \lambda_i\cdot\mathbf{a}_i) - \beta + \sum_{i=1}^n \lambda_i\alpha_i, \quad \forall \mathbf{p} \in \mathbb{V}^*.$$

REMARK 5.6 *In the theorem with Lagrange multipliers for a local conditional extremum of a differentiable function we apply exactly the above theorem of linear algebra after a linearization of the corresponding functions at the extremum point.*

Considering the requirements of the applications we generalize Liu's theorem to take into account vectorial constraints. First of all let us remember some well known identifications of linear algebra: $\mathrm{Lin}(\mathbb{U}^*, \mathbb{V}) \equiv \mathrm{Bilin}(\mathbb{U}^* \times \mathbb{V}^*, \mathbb{R}) \equiv \mathbb{V} \otimes \mathbb{U}$, where Bilin denotes the bilinear mappings of the corresponding spaces (see e.g. [51]).

THEOREM 5.4 (VECTOR LIU) *Let $\mathbf{A} \neq \mathbf{0}$ in a tensor product $\mathbb{V} \otimes \mathbb{U}$ of finite dimensional vector spaces $\mathbb{V}$ and $\mathbb{U}$. Let $\boldsymbol{\alpha} \in \mathbb{U}$ and $S_{VL} = \{\mathbf{p} \in \mathbb{V}^* \mid \mathbf{p}\cdot\mathbf{A} = \alpha\}$. The following statements are equivalent for a $\mathbf{b} \in \mathbb{V}$ and a real number β:*

(i) $\mathbf{p}\cdot\mathbf{b} \ge \beta$, *for all* $\mathbf{p} \in S_{VL}$.
(ii) *There is a* $\boldsymbol{\lambda} \in \mathbb{U}^*$ *such that*

$$\mathbf{b} = \mathbf{A}\cdot\boldsymbol{\lambda}, \tag{18}$$

and

$$\beta \le \boldsymbol{\lambda}\cdot\boldsymbol{\alpha}. \tag{19}$$

Proof: Let us observe that we can get back the previous form of the theorem by introducing a linear bijection $\mathbf{K} : \mathbb{U} \to \mathbb{R}^n$, a *coordinatization* in $\mathbb{U}$. Therefore, applying it for $\mathbf{K}\cdot\mathbf{A} = (\mathbf{A})_i = \mathbf{a}_i$, $\mathbf{K}\cdot\boldsymbol{\alpha} = (\boldsymbol{\alpha})_i = \alpha_i$ and $\mathbf{K}'\cdot\mathbf{A} = \mathbf{a}_i'$, $\mathbf{K}'\cdot\boldsymbol{\alpha} = \alpha_i'$ we get that $\mathbf{b} = \sum_{i=1}^n \lambda_i \mathbf{a}_i = \sum_{i=1}^n \lambda_i' \mathbf{a}_i'$. Thus $\lambda_i' = \mathbf{K}'^{*-1}\cdot\mathbf{K}^*\cdot\lambda_i$. Therefore, there is a $\boldsymbol{\lambda} \in \mathbb{U}$, independently of the coordinatization, with the components λ_i and λ_i' in the coordinatizations $\mathbf{K}$ and $\mathbf{K}'$. ■

The previously excluded degenerate case of $\mathbf{A} = \mathbf{0}$ deserves special attention. Now we require the validity of the aim inequality for all $\mathbf{p} \in \mathbb{V}^*$ without any constraint. The consequences can be formulated as previously and the proof is trivial.

THEOREM 5.5 (DEGENERATE LIU) *The following statements are equivalent for a $\mathbf{b} \in \mathbb{V}$ and a real number β:*

(i) $\mathbf{p}\cdot\mathbf{b} \ge \beta$ *for all* $\mathbf{p} \in \mathbb{V}^*$.

(ii) $\mathbf{b} = \mathbf{0}$ *and* $\beta \leq 0$.

REMARK 5.7 *The practical application rule is that if* $\mathbf{A} = \mathbf{0}$*, then the multiplier is zero.*

REMARK 5.8 *In continuum physics and thermodynamics the corresponding form of* (18) *and* (19) *are called* Liu equation(s) *and the* dissipation inequality*, respectively. We apply the same names for the degenerate case, too. There the Lagrange-Farkas multipliers are called simply Lagrange multipliers. Our nomenclature honors Farkas and emphasizes the difference between the two kinds of multipliers. It can be important also to make a clear distinction of a similar but different nomenclature and method in variational principle construction in continuum physics* [52].

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