WEAKLY NONLOCAL CONTINUUM PHYSICS - THE GINZBURG-LANDAU EQUATION

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

1. Introduction

Ginzburg-Landau equation and its variants appear in different fields of physics and are applied to several phenomena. 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. [1])

- The static, equilibrium part of the equation 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 nonrelativistic space-time, the Ginzburg-Landau equation should be compatible with the general balance and constitutive structure of continuum physics. Recently there has been several efforts to give a uniform reasoning of the equation on pure thermodynamic ground and to generalize the method of the derivation [2, 3, 4, 5]. The treatment of Ginzburg-Landau equation is a kind of test of weakly nonlocal (gradient) thermodynamic theories.

In some previous works the possible role of internal, dynamic variables in weakly nonlocal extensions of the constitutive state space was investigated both with the heuristic method of classical irreversible thermodynamics and with the more exact Liu procedure [4, 5]. It was found that with the help of special dynamic variables (current multipliers) appearing in a generalized entropy current one can find an equation that is similar to the Ginzburg-Landau equation, but is not the same. The equation was called thermodynamic Ginzburg-Landau equation. The static part of the Ginzburg-Landau equation gives nonhomogeneous solutions in case of uniform boundary conditions, therefore it is a pattern forming equation. On the other hand, thermodynamic Ginzburg-Landau is not a pattern forming equation, its corresponding solutions are homogeneous. This is an important difference and corresponds well to the fact that with internal variables one introduces a local theory, all the functions in the basic state space are local. Therefore any nonlocalities formulated by an internal variable theory are relocalized in this sense. Pattern forming theories, like those based on the Ginzburg-Landau equation, cannot be relocalized.

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In this paper it is shown, that there is a non-equilibrium thermodynamic approach also for pattern forming equations, however, it is not relocatable, independent of any kind of internal variables. A pure thermodynamic derivation can unify the mentioned two parts of the derivation, there is no need to postulate any kind of variational principle. The Euler-Lagrange form of the static part of the equation turns out to be a consequence of the Second Law.

In the paper the key ingredients of the methodology and the mathematical background to exploit the Second Law inequality is shortly summarized in weakly non-local continuum theories (gradient theories, theories with coarse grained thermodynamic potentials, phase-field models, etc...). After the introduction, an overview of the methods to exploit the Second Law inequality is given. We call the attention to the essential differences between the local and weakly nonlocal theories and a constructive way to arrive solvable Liu equations is given. The most important difference is that the weakly nonlocal extension of the constitutive state space, implies that some space derivatives of the constraints (evolution equations) are to be considered as constraints, too. A simple example show the application of Liu procedure. In the following section Liu procedure is applied to derive the Ginzburg-Landau equation. Different kind of generalizations are treated, the difference between the relocalized and pattern forming (non relocalizable) theories is formulated. A new, generalized formulation of Liu’s theorem and its direct proof from Farkas’ lemma is given in an Appendix.

2. Methods to exploit the Second Law inequality - procedures of CIT, Coleman-Noll and Liu

In every non-equilibrium thermodynamic theories 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 far from being trivial and originated from Coleman and Mizel. They essentially reverse the way of thinking: one should look for the solution of the entropy inequality taking into account the evolution equations as constraints [6, 7]. In continuum physics the dynamic equations are given in a determined form (e.g. as balances of extensives), except some constitutive, material functions. The task is to ensure the nonnegativity of the entropy production with appropriate constitutive assumptions. Therefore one should specify the undetermined material functions such, that in case of all possible solutions of the dynamic equations the form of the constitutive functions, the material properties, ensure the nonnegativity of the entropy production. In case of weakly nonlocal theories the entropy current plays a distinguished role. The entropy and the entropy current are both constitutive and are to be determined according to the above requirement (as it was suggested in extended rational thermodynamics [8]). The entropy possibly should preserve its potential character in a general sense, therefore solving the above problem (e.g. Liu equations) the practical aim is a simplification in such a way that every constitutive quantity including the entropy current 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 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 the Liu procedure in case of the traditional, simplest state spaces [9], and the method can be generalized to include non-classical entropy currents [9, 10].
– 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 (T5.5) 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 (j_s = j_q/T), or a generalized one. In weakly nonlocal considerations both classical (see e.g. [2, 11]) and generalized forms are applied. 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 [12, 3].

– Liu procedure. With Liu procedure one applies Liu’s theorem with Lagrange-Farkas multipliers (T5.3 in the Appendix). At the 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 extremum problems, with Lagrange-Farkas multipliers one can preserve and exploit the structure of the constraint 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 possible to solve completely the physical problem.

The train of thought is the following. The entropy current is considered as an independent constitutive quantity. With a proper choice of the constitutive space we can solve the Liu equations and determine the entropy current. Hence the entropy inequality simplifies considerably. The point of view of Onsagerian CIT is important here: with a proper identification of thermodynamic currents and forces the resulted entropy inequality can be solved, determining all constitutive quantities. This ensures, that our theory is independent of further artificial constraints, the entropy inequality becomes a consequence of material properties.

In weakly nonlocal continuum physical calculations with Liu procedure one should consider some additional practical rules. There the constraints are (partial) differential equations. The functions in the differential equations form the basic state space. The constitutive quantities depend on these functions, on the basic state and on some of its derivatives. These derivatives are locally independent therefore the problem is algebraically manageable. The basic state variables and some of its derivatives can be included into the constitutive state space (or simply state space [13]), into 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, the so called process directions. The choice of the constitutive state space is crucial and determines the restricted constitutive functions, after applying Liu procedure, the peculiarity of weakly nonlocal theories is that 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. In the following we will show some examples to clarify the most important practical rules in the application of the formalism. One can find other examples on the application of derivative constraints in [14, 15].

Remark 2.1. The mentioned exploitation methods of the Second Law, being algebraic, are essentially independent of the solvability of the dynamic equations, whether the associated problems are 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.

Example 1. In this example the basic state space is formed by two times differentiable real functions \( x : \mathbb{R} \rightarrow \mathbb{R} \). 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

\[
F(x, x') = 0.
\]  

Evidently \( S'(x, x') = \partial_1 S x' + \partial_2 S x'' \), where \( \partial_n \) 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 \( F \) 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 \((T5.5)\) gives some conditions. The single Liu equation is

\[
\partial_2 S = 0.
\]

Therefore \( S \) is independent on \( x' \). The dissipation inequality can be written in the following simple form

\[
\partial_1 S x' = \frac{dS}{dx}(x) x' \geq 0
\]

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 on the state space, the derivative of \((1)\) gives a further restriction

\[
\partial_1 F x' + \partial_2 F x'' = 0.
\]

Considering this condition we apply Liu’s theorem \((T5.3)\) with the multiplier method, introducing the multipliers \( \lambda_1 \) and \( \lambda_2 \) for the constraints \((1)\) and \((3)\) respectively

\[
\partial_1 S x' + \partial_2 S x'' - \lambda_2 (\partial_1 F x' + \partial_2 F x'') - \lambda_1 F = (\partial_1 S - \lambda_2 \partial_1 F) x' + (\partial_2 S - \lambda_2 \partial_2 F) x'' - \lambda_1 F \geq 0
\]

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 to 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 nonnegative. Given a function \( S \) we can calculate \( F \), with appropriate conditions on \( L \). For example if \( S(x, x') = x \cdot x' \) and \( L = \text{constant} \), then \( F(x, x') = f(x^{L-1} x') \) is a solution of the above equation for any \( f : \mathbb{R} \rightarrow \mathbb{R} \).
Let us denote an internal variable (e.g., an order parameter of a second order phase transition) characterizing the microstructure of the material by $\xi$. In this case the Ginzburg-Landau equation can be written as

$$\partial_t \xi = -\gamma_1 \Gamma_\xi + \gamma_2 \Delta \xi,$$

where $\Gamma_\xi$ is the partial derivative of the appropriate thermodynamic potential (e.g. $\Gamma_\xi = \partial_\xi f$, where $f$ is the free energy), and $\partial_t$ denotes the partial time derivative. Here we assumed that the internal variable $\xi$ is not related to the mechanical motion, therefore the choice of the frame (partial or substantial time derivatives) is irrelevant. $\gamma_1$ and $\gamma_2$ are material coefficients. The usual form of the Ginzburg-Landau free energy density is

$$f(\xi, \nabla \xi) = f_0(\xi) - \gamma (\nabla \xi)^2 / 2,$$

where $\gamma$ is a material coefficient, $f_0$ is the static (equilibrium) free energy and so $\Gamma_\xi = f'(\xi)$. Gurtin gave a method to deduce equation (4) from pure thermodynamic considerations, with the concept of microforce balance and showed that some additional terms should appear with a characteristic structure [2, 16]. The generalized form of the equation together with the characteristic term is the following

$$\partial_t \xi = -\gamma_1 \Gamma_\xi + \gamma_2 \Delta \xi + \gamma_3 \Delta \partial_t \xi,$$

Such kind of terms appear in connection of several different phenomena and not only in case of the Ginzburg-Landau equation [17, 18]. E.g. the Guyer-Krumhansl equation of heat conduction can be considered as a Cattaneo-Vernotte type wave heat conduction equation supplemented by a Gurtin term.

It was argued that the Ginzburg-Landau equation is the first nonlocal extension of any kind of equation for an internal variable [4, 5] and its characteristic functional form can be derived from the requirement of compatibility with the Second Law, without referring to variational principles. Hence, the reason of its wide-range applicability is well founded, because any internal variable that can characterize a material structure and is independent of other requirements should fulfill a Ginzburg-Landau equation in the first nonlocal approximation. The arguments were supported by calculations based on Liu’s theorem. However, in an internal variable, completely relocalized theory one cannot derive directly (4), but only a very similar equation, that was called thermodynamic Ginzburg-Landau equation

$$\partial_t \xi = -\gamma_T1 \Gamma_\xi + \gamma_T2 \Delta \Gamma_\xi,$$

where $\gamma_T1$ and $\gamma_T2$ are material coefficients. Moreover, the entropy (free energy) was proved to be gradient independent. One can see, that the equations (4) and (7) are similar but not the same at all. The essential qualitative difference is that static (equilibrium) solutions of the thermodynamic Ginzburg-Landau equation with homogeneous boundary conditions are homogeneous but static solutions of the original Ginzburg-Landau equation with the same boundary conditions are not, they can form structures. The situation is well known and understood in superconductors. The London equation (corresponding to the thermodynamic Ginzburg-Landau) does not determine the penetration length of the magnetic field, however, the Ginzburg-Landau equation gives that [19].

In the following, applying Liu’s procedure with the methodology described in the previous section, we will derive the Ginzburg-Landau equations from very general
assumptions and show that the Gurtin terms are consequences of pure thermodynamic considerations, without referring new concepts, like the configurational force balance or virtual power, etc..

We are looking for a dynamic equation of $\xi$ in the following general form

$$\frac{\partial}{\partial t} \xi - F = 0,$$

where $F$ is a constitutive function, which form is to be restricted by the Second Law. The basic state space is spanned by $\xi$. Let us assume that the constitutive space is spanned by $\xi$, $\nabla \xi$, and $\nabla^2 \xi$. In this case the entropy inequality will be

$$\partial_t s + \nabla \cdot j_s = \partial_1 s \partial_t \xi + \partial_2 s \cdot \nabla \partial_t \xi + \partial_3 s : \nabla^2 \partial_t \xi + \partial_4 j_s \cdot \nabla \partial_t \xi + \partial_5 j_s : \nabla^3 \xi \geq 0.$$

One can see, that the space of the process directions (independent variables) is spanned by $\partial_t \xi$, $\nabla \partial_t \xi$, $\nabla^2 \partial_t \xi$ and $\nabla^3 \xi$. Moreover, let us observe that these variables are not really independent, the gradient of (8) connect them. Therefore, in addition to (8) one should consider the following constraint

$$\nabla \partial_t \xi + \nabla F = \nabla \partial_1 \xi + \partial_1 F \nabla \xi + \partial_2 F \cdot \nabla^2 \xi + \partial_3 F : \nabla^3 \xi = 0.$$

Introducing $\Gamma_1$ and $\Gamma_2$ Lagrange-Farkas multipliers for the constraints (8) and (9) respectively, one can get the following Liu equations

$$\begin{align*}
\partial_1 s &= \Gamma_1, \\
\partial_2 s &= \Gamma_2, \\
\partial_3 s &= 0, \\
(\partial_4 j_s - \Gamma_2 \partial_3 F)^s &= 0.
\end{align*}$$

Here the superscript $^s$ denotes the symmetric part of the corresponding tensor. The first two equations determine the multipliers. From the third equation follows, that the entropy does not depend on the second derivative of $\xi$. Taking into account these requirements one can give a solution of the fourth equation and determine the entropy current as

$$j_s(\xi, \nabla \xi, \nabla^2 \xi) = \partial_2 s(\xi, \nabla \xi) F(\xi, \nabla \xi, \nabla^2 \xi) + j_0(\xi, \nabla \xi).$$

For the sake of clarity we explicitly denoted the variables of the corresponding functions. With the above solution of the Liu equations the dissipation inequality can be simplified considerably

$$\nabla \cdot j_0 + (\nabla \cdot \partial_2 s - \partial_1 s) \cdot F \geq 0.$$

Assuming, that $j_0 \equiv 0$ 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. Therefore, $F$ is the constitutive quantity to be determined (thermodynamic current) and it should be proportional to the given one (force)

$$\partial_t \xi = F = L(\nabla \cdot \partial_2 s - \partial_1 s)$$

with a nonnegative state dependent constitutive function $L$. $s(\xi, \nabla \xi)$ is a given entropy function (determined from static measurements). (12) is the Ginzburg-Landau equation, and one can get back the very traditional form using the specific entropy functional with a form like (5) and dealing with a strictly linear theory in a thermodynamic sense, where $L$ is a constant function. The choice of the right thermodynamic potential (e.g. entropy or free energy) depends on the boundary conditions (11).
If we do not restrict the space of the independent variables by (9), by the derivative of the original constraint, then after an easy calculation one can get the following form of the dissipation inequality

\[ \nabla \cdot j_0(\xi, \nabla \xi) - \partial_t s(\xi) F(\xi, \nabla \xi, \nabla^2 \xi) \geq 0. \]  

The Liu equations require, that the entropy must not depend on the gradients of the basic state. However, the dissipation inequality still can be solved, if one considers two additional physical requirements, prerequisites of relocalizability [5].

1. \( \xi \) is a dynamic variable in a thermodynamic sense therefore \( \xi \) is zero in equilibrium,
2. there is no entropy flow connected to the dynamic variable if its value is zero.

It was argued that these requirements are weak from a physical point of view. With these assumptions one can specify \( j_0 \) in the entropy current with the Nyíri-form as \( j_0(\xi, \nabla \xi) = A(\xi, \nabla \xi) \xi \), or equivalently \( j_0(\xi, \nabla \xi) = \hat{A}(\xi, \nabla \xi) \partial_\xi s \) [10], according to the mean value theorem. Here the current multipliers \( A \) or \( \hat{A} \) are constitutive functions to be determined. With the second form of \( j_0 \) the dissipation inequality (13) can be solved and gives the thermodynamic Ginzburg-Landau equation (7).

Introducing an additional, new dynamic variable one can recover the additional Gurtin-term in the thermodynamic Ginzburg-Landau equation [4]. Let us observe, that the key assumption determining the form of the additional entropy current was that the entropy current should not affect the equilibrium solutions. Because the entropy is a local function in this case, the special internal variables, the current multipliers in a sense relocalize the nonlocalities.

We can apply similar reasoning in the previous non relocalizable case, too. However, first we should extend the previous constitutive state space considering a derivative one order higher then before. Therefore, let be our constitutive space spanned by \( (\xi, \nabla \xi, \nabla^2 \xi, \nabla^3 \xi) \). After a short calculation we can recover the validity of (11) in these new variables. The only difference is that the final constitutive quantities e.g. \( j_0 \) and \( L \) will depend on the larger constitutive state. Now we assume that \( j_0 \) has the following form

\[ j_0(\xi, \nabla \xi, \nabla^2 \xi) = \hat{B}(\xi, \nabla \xi, \nabla^2 \xi) F(\xi, \nabla \xi, \nabla^2 \xi), \]

were \( \hat{B} \) is a current multiplier. The above form is a direct application of the requirement that the entropy current should not change the equilibrium solutions (with some minor additional restrictions on the possible constitutive dependencies). In this case the entropy production (11) is

\[ \hat{B} \cdot \nabla F + (\nabla \cdot \hat{B} + \nabla \cdot \partial_2 s - \partial_1 s) \cdot F \geq 0. \]

With two undetermined constitutive functions \( (\hat{B}, F) \) the inequality has a general solution, the currents and forces are determined by the constitutive dependencies. In case of isotropic materials

\[ \hat{B} = L_1 \nabla F \]
\[ F = L_2 (\nabla \cdot \hat{B} + \nabla \cdot \partial_2 s - \partial_1 s). \]

Here \( L_1 \) and \( L_2 \) are nonnegative scalar constitutive functions. \( \hat{B} \) can be eliminated from the above equations and finally we get

\[ \partial_t \xi = F = L_2 (\nabla \cdot \partial_2 s - \partial_1 s) + L_2 \nabla \cdot (L_1 \nabla \partial_1 \xi). \]

This is the Ginzburg-Landau equation with a characteristic additional Gurtin-term.
4. Conclusions and discussion

The requirement of a nonnegative entropy production is a relatively strong and not a complete form of the Second Law. Strong form because it is a local requirement and other weaker formulations require only the validity of integral inequalities. Not a complete one because an increasing entropy is only a part of the physical content of the Second Law. The stability of materials in isolated systems incorporates some other conditions (e.g., concave entropy function), too [20]. 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) ensuring 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 Nonequilibrium Reversible-Irreversible Coupling (GENERIC) [21, 22, 23], 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 Hamiltonian type [24]. 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.

Weakly nonlocal, pattern forming equations emerge in different fields of physics independently of thermodynamic argumentation. Understanding their compatibility with the Second Law can be considered as one of the most important 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, is a straightforward consequence of the entropy inequality alone in a nonlocally extended constitutive space. On the other hand the outline of the mathematical background and all the key ingredients of an efficient formalism to exploit the Second Law inequality in weakly nonlocal continuum theories (gradient theories, theories with coarse grained thermodynamic potentials, phase-field models, etc.) is given.

5. Appendix: Liu 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 [25]. 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 [8, 13] 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 so called Farkas’ lemma [26]. That theorem was proved first by Farkas in 1894 [27] and independently by Minkowski in 1896 [28]. In this appendix we formulate and generalize Liu’s theorem in a way that is best adapted for 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 \[29, 30\]. Here we start from a simple variant.

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

(i) \( \mathbf{p} \cdot \mathbf{b} \geq 0 \), for all \( \mathbf{p} \in S \).

(ii) There are nonnegative real numbers \( \lambda_1, ..., \lambda_n \) such that \( \mathbf{b} = \sum_{i=1}^{n} \lambda_i \mathbf{a}_i \).

Proof: \( S \) is not empty. In fact, for all \( k, i \in \{1, ..., n\} \) there is a \( \mathbf{p}_k \in V^* \) 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 \( S_0 = \{ \mathbf{y} \in V^* | \mathbf{y} \cdot \mathbf{a}_i = 0, i = 1...n \} \). 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 nonnegative, because with the previously defined \( \mathbf{p}_k \in S \), \( 0 \leq \mathbf{p}_k \cdot \mathbf{b} = \mathbf{p}_k \cdot \sum_{i=1}^{n} \lambda_i \mathbf{a}_i = \lambda_1 \mathbf{p}_k \cdot \mathbf{a}_1 = \lambda_k \) is valid for all \( k \).

**Remark 5.1.** In the following the elements of \( V^* \) are called independent variables and \( V^* \) itself is called the space of independent variables. The inequality in the first statement of the lemma is called aim inequality and the nonnegative 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 case of conditional extremum problems:

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

From this form we can read out 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 the vector \( \mathbf{b} \) belongs to the cone generated finitely by the vectors \( \mathbf{a}_i \) \((\text{Cone}(\mathbf{a}_1, ..., \mathbf{a}_n) = \{ \lambda_1 \mathbf{a}_1 + ... + \lambda_n \mathbf{a}_n | (\lambda_1, ..., \lambda_n) \in \mathbb{R}^{+n} \})\), 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 \[31, 32\]. Later it was reproved independently by others several times (e.g. \[33, 30\]). Here we give a simple version again.

**Theorem 5.2. (Affine Farkas)** Let \( \mathbf{a}_i \neq 0 \) be independent vectors in a finite dimensional vector space \( V \) and \( \alpha_i \) real numbers, \( i = 1...n \) and \( S_A = \{ \mathbf{p} \in V^* | \mathbf{p} \cdot \mathbf{a}_i \geq \alpha_i, i = 1...n \} \). The following statements are equivalent for a \( \mathbf{b} \in V \) and a real number \( \beta \):

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

(ii) There are nonnegative 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).
Remark 5.3. The geometric interpretation is similar to the previous one, but

Remark 5.4. \[ \lambda \] multipliers everything is affine.

Theorem 5.3. \[ \lambda \in V \] \[ p \in S \] and \[ (ii) \] There are real numbers \[ \lambda = (\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^n \] such that \[ b = \sum_{i=1}^{n} \lambda_i a_i \]. Hence \[ \beta \leq \inf_{p \in \mathcal{L}} \{ p \cdot b \mid \sum_{i=1}^{n} \lambda_i a_i \} = \sum_{i=1}^{n} \lambda_i a_i \].

Remark 5.3. The multiplier form is a good reminder again

\[ (p \cdot b - \beta) - \sum_{i=1}^{n} \lambda_i (p \cdot a_i - \alpha_i) = p \cdot (b - \sum_{i=1}^{n} \lambda_i \cdot a_i) - \beta + \sum_{i=1}^{n} \lambda_i \alpha_i \geq 0, \ \forall p \in V^* \].

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 \( a_i \neq 0 \) be independent vectors in a finite dimensional vector space \( V \) and \( \alpha_i \) real numbers, \( i = 1 \ldots n \) and \( S_L = \{ p \in V^* \mid p \cdot a_i \geq \alpha_i, i = 1 \ldots n \} \). The following statements are equivalent for a \( b \in V \) and a real number \( \beta \):

(i) \( p \cdot b \geq \beta \), for all \( p \in S_L \),

(ii) There are real numbers \( \lambda_1, \ldots, \lambda_n \) such that

\[ b = \sum_{i=1}^{n} \lambda_i a_i, \]

and

\[ \beta \leq \sum_{i=1}^{n} \lambda_i \alpha_i. \]

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 \( a_i \) and \( -a_i, i = 1, \ldots, n; \) \( S_A = \{ p \in V^* \mid p \cdot a_i \geq \alpha_i, \ \text{and} \ \ p \cdot (-a_i) \geq -\alpha_i, i = 1 \ldots n \} \).

Therefore there are nonnegative real numbers \( \lambda_1^+, \ldots, \lambda_n^+ \) and \( \lambda_1^-, \ldots, \lambda_n^- \) such that \[ b = \sum_{i=1}^{n} (\lambda_i^+ a_i - \lambda_i^- a_i) = \sum_{i=1}^{n} (\lambda_i^+ - \lambda_i^-) a_i = \sum_{i=1}^{n} \lambda_i a_i \] and \[ \beta \leq \sum_{i=1}^{n} (\lambda_i^+ \alpha_i - \lambda_i^- \alpha_i). \]

Remark 5.5. The multiplier form is a help in the applications again

\[ 0 \leq (p \cdot b - \beta) - \sum_{i=1}^{n} \lambda_i (p \cdot a_i - \alpha_i) = p \cdot (b - \sum_{i=1}^{n} \lambda_i \cdot a_i) - \beta + \sum_{i=1}^{n} \lambda_i \alpha_i, \ \forall p \in V^*. \]

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 account vectorial constraints. First of all let us remember some well known identifications of linear algebra: \( \text{Lin}(U^*, V) \equiv \text{Bilin}(U^* \times V^*, \mathbb{R}) \equiv V \otimes U \), where \( \text{Bilin} \) denotes the bilinear mappings of the corresponding spaces (see e.g. [34]).
Theorem 5.4. (vector Liu) Let $A \neq 0$ in a tensor product $V \otimes U$ of finite dimensional vector spaces $V$ and $U$. Let $\alpha \in U$ and $S_{VL} = \{ p \in V^* | p \cdot A = \alpha \}$. The following statements are equivalent for a $b \in V$ and a real number $\beta$:

(i) $p \cdot b \geq \beta$, for all $p \in S_{VL}$.

(ii) There is a $\lambda \in U^*$ such that

\begin{align}
    b &= A \cdot \lambda, \\
    \beta &\leq \lambda \cdot \alpha.
\end{align}

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

The previously excluded degenerate case of $A = 0$ deserves a special attention. Now we require the validity of the aim inequality for all $p \in V^*$ 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 $b \in V$ and a real number $\beta$:

(i) $p \cdot b \geq \beta$ for all $p \in V^*$.

(ii) $b = 0$ and $\beta \leq 0$.

Remark 5.7. The practical application rule is that if $A = 0$ 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 kind 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 [35].

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References

[1] O. Penrose and P. C. Fife. Thermodynamically consistent models of phase-field type for the kinetics of phase transitions. Physica D, 43:44–62, 1990.
[2] M. G. Gurtin. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance. Physica D, 92:178–192, 1996.
[3] P. M. Mariano. Multifield theories in mechanics of solids. Advances in Applied Mechanics, 38:1–94, 2002.
[4] P. Ván. Weakly nonlocal irreversible thermodynamics - the Ginzburg-Landau equation. Technische Mechanik, 22(2):104–110, 2002. [cond-mat/0111307].
[5] P. Ván. Weakly nonlocal irreversible thermodynamics. Annalen der Physik (Leipzig), 12(3):142–169, 2003. [cond-mat/0112214].
[6] B. D. Coleman and V. J. Mizel. Existence of caloric equation of state in thermodynamics. Journal of Chemical Physics, 40:1116–1125, 1964.
