THE PHYSICAL ENTROPY OF SINGLE CONSERVATION LAWS[*1)]

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Abstract

By means of the comparisons with the formulas in statistical mechanics and thermodynamics, in this paper it is demonstrated that for the single conservation law $\partial_t u + \partial_x f(u) = 0$, if the flux function $f(u)$ is convex (or concave), then, the physical entropy is $S = -f(u)$; Furthermore, if we assume this result can be generalized to any $f(u)$ with two order continuous derivative, from the thermodynamical principle that the local entropy production must be non-negative, one entropy inequality is derived, by which the O.A. Olejnik's famous E- condition can be explained successfully in physics.

Key words: Conservation laws, Entropy, Entropy production.

1. Introduction

As the simplest representation of general conservation laws, the single conservation laws with one space variable have been thoroughly discussed.In the cases that the flux function is convex or concave, P.D. Lax obtained a general expression of the solutions for Cauchy problems[2]; in order to guarantee the uniqueness of the solution, O.A. Olejnik presented her famous E-condition which can be applied to general conservation laws with one space variable[4]; The Lax's concepts of entropy functions and related inequality also can be used in this special case[3]. In fact, both for differential equation's theory and for numerical methods, the single conservation laws are the primitive discussed objects.

However, even for the single conservation laws, there are still something not thoroughly clear, the problems manifest especially when the entropy and entropy condition are concerned, which are related to the uniqueness of the generalized solution. According to the P.D. Lax's definition, there are a lot of entropy functions for a single conservation law, the entropy inequality must be satisfied for every convex entropy; however, at least for some equations, it is reasonable to expect that there exists a "physical entropy", which determines the uniqueness of the generalized solution. Thus a question has arisen: what is the physical entropy and what is the corresponding entropy condition. In addition, the Olejnik's E- condition has clear and definite geometrical meaning, and by use of the Lax's entropy inequalities with suitable entropy

functions, or by the Kružkov's theorem , the Olejnik's E-condition can be derived, but what is its physical significance, especially, how does it relate to the physical entropy.

In this paper we try to answer these questions. First, in the cases that the flux functions are convex (or concave), beginning from the Lax's general expressions of solutions for Cauchy problems, by comparisons with formulas in the thermodynamic and statistical mechanics, it is demonstrated that the negative flux function can be regarded as the physical entropy; Furthermore, it is assumed that the above conclusion still holds for the general single conservation laws, by means of the thermodynamic principle that the local entropy production must be non-negative, an entropy inequality different from the Lax's one is derived, from which the Olejnik's E- condition can be explained successfully in physics. Furthermore, it is demonstrated that in a sense a strong discontinuity of a single conservation law can be considered as a most simple mathematical model of the non-equilibrium phase transitions.

In [6], F. Rezakhanlou has studied the hydrodynamic behavior of certain stochastic particle systems, and proved that under Euler scaling, the microscopic particle density converges to a determinate limit that is characterized as the entropy solution of a nonlinear conservation law; Rezakhanlou's results are very interesting, and what used by him is the statistical mechanics method; However, in [6] the entropy condition is not derived from the micromechanism, it just be proved. As compared with [6], the method applied in the present paper can be considered as a thermodynamic one, it does not concern with the micromechanism, but its results reveal that the mathematical concept of entropy functions should have more direct physical origin.

In section 2 some preliminary knowledges about the single conservation laws, statistical mechanics and thermodynamics, which are necessary for the present paper, are briefly introduced. Section 3 contains our main results. Finally in section 4 there are some concise discussions.

2. Preliminary

The Cauchy problems for single conservation laws with one space variable can be expressed as follows[2,7]:

$$u_t + f(u)_x = 0, \quad -\infty < x < \infty, \, t > 0 \tag{2.1}$$

$$u(x,0) = \phi(x), \quad -\infty < x < \infty \tag{2.2}$$

where x and t are the independent variables, $u(x,t)$ is the unknown function, $f(u)$ is called flux. If for all smooth test functions $w(x,t)$ which vanish for $|x|+t$ large enough, the function $u(x,t)$ and $f(u)$ are integrable, and satisfy the following relation:

$$\int_0^\infty \int_{-\infty}^\infty [w_t u + w_x f] dx dt + \int_{-\infty}^\infty w(x,0)\phi(x) dx = 0 \tag{2.3}$$

then, function $u(x,t)$ is defined as a weak solution of (2.1) (2.2), as is well known for piecewise continuous solutions, (2.3) is equivalent to the Rankine-Hugoniot jump condition

$$s[u] - [f] = 0 \tag{2.4}$$

where s is the speed with which a discontinuity is propagating, and $[u]$ denotes the difference between the values of u on two sides of the discontinuity.

It is well known that the weak solutions of single conservation laws are not uniquely determined by their initial values. To pick up the generalized solution which is physically relevant and unique, O.A. Olejnik presented her famous E-condition[4]. We say a function $u(x,t)$ belongs to class K in above semi-plane $t \geq 0$, if $u(x,t)$ is continuously differential everywhere except only on finite number of smooth curves across which $u(x,t)$ has discontinuity. Olejnik has proved that if a weak solution of (2.1) (2.2) at the points of its discontinuity satisfies the following relations:

$$\frac{f(u_-) - f(w)}{u_- - w} \geq \frac{f(u_-) - f(u_+)}{u_- - u_+} \geq \frac{f(u_+) - f(w)}{u_+ - w} \quad \forall w \in I \tag{2.5}$$

$I = (\min(u_-, u_+), \max(u_-, u_+))$, then it is unique in class K, and can be defined as the generalized solution. Inequality (2.5) is the mathematical expression of the Olejnik's E- condition.

The concept of the entropy function and the related inequality presented by P.D. Lax are the another way to determine the unique generalized solution[3]. For a single conservation law according to P.D. Lax's definition, any convex function U of u is an entropy, let $U_u f_u = F_u$, $F(u)$ is called the corresponding entropy flux. Lax demands that for any convex entropy, in weak sense the generalized solution of (2.1) (2.2) should satisfy the following inequality, i.e.

$$\partial_t U(u) + \partial_x F(u) \leq 0 \tag{2.6}$$

for a piecewise smooth solution, on its discontinuity the inequality becomes

$$s(U(u_-) - U(u_+)) - (F(u_-) - F(u_+)) \leq 0 \tag{2.7}$$

where s is the propagation speed of the discontinuity.

Under the conditions that $f(u)$ is strictly convex and the initial function $\phi(x)$ is bounded measurable, it is proved in [2] that the generalized solution can be expressed as

$$u(x,t) = b\left(\frac{x - y_0(x,t)}{t}\right) \tag{2.8}$$

where $b(u)$ is the inverse of $a(u) = f_u(u)$, i.e., $a(b(u)) = u$ and $y_0 = y_0(x,t)$ is defined as following: $\nu(y_0; x, t) = \min_\xi, \nu(\xi; x, t), \nu(\xi; x, t) = \int_0^\xi \phi_0(\eta)\, d\eta + t\, g\left(\frac{x - \xi}{t}\right), \frac{d}{ds} g(s) = b(s)$, it can be proved that $(x - y_0)/t = a(\phi(y_0))$.

In our discussion, the following primitive knowledges of the thermodynamics and the statistical mechanics are needed.

For a thermodynamic system, a thermodynamic potential called Helmholtz free energy can be defined as

$$A = U - TS \tag{2.9}$$

where U is the inner energy, T is the absolute temperature, S is the entropy. If the volume V of the system and the temperature T are taken as the independent variables, then

$$dA = -P\, dV - S\, dT \tag{2.10}$$

where P denotes the pressure, thus,

$$P = -\Big(\frac{\partial A}{\partial V}\Big)_T \quad S = -\Big(\frac{\partial A}{\partial T}\Big)_V \tag{2.11}$$

and

$$\Big(\frac{\partial P}{\partial T}\Big)_V = \Big(\frac{\partial S}{\partial V}\Big)_T \tag{2.12}$$

in the thermodynamics, (2.12) is called one Maxwell relation [1].

It is demonstrated in the statistical mechanics that for a system containing N particles and having fixed temperature the free energy per particle is

$$A(V,T;N) = -\frac{1}{N} \log Z(V,T;N) \tag{2.13}$$

where $Z(V,T;N)$ is the partition function of the system and

$$Z(V,T;N) = \sum_{\{\mu_N\}} \exp(-\beta \mathcal{H}(V,T;\mu_N)) \tag{2.14}$$

in which $\beta = 1/kT$, k is the Boltzmann constant, $\mathcal{H}(V,T;\mu_N)$ is the Hamiltonia of the system consisting of N particles at the configuration μ_N. The meaning of quantity $\exp\{-\beta \mathcal{H}(V,T;\mu_N)\}$ is the relative probability with which the system is in configuration μ_N. For a real system, the thermodynamical limit should be considered, i.e. one should let $N \to \infty$.

The above contents belong to the equilibrium thermodynamics and the classical statistical mechanics. For a system which is not in equilibrium but satisfies the hypothesize of local equilibrium, the thermodynamics for irreversible process tells us that, the local entropy S_e should satisfy the following equation[5]:

$$\partial_t S_e = -\operatorname{div} j_s + \sigma \tag{2.15}$$

where j_s is the density of the entropy flow, so called entropy flow is the entropy change caused by the exchanges of the energies and materials between the system and the environment. σ is called the local entropy production, for a irreversible process, it must be $\sigma \geq 0$.

3. The entropy functions and the entropy inequalities of single conservation laws

In our discussion for the physical entropy of single conservation laws, the local equilibrium hypothesize is assumed, that means, although the whole system described by (2.1) (2.2) is not in equilibrium, the local subsystem in the neighborhood of every fixed point (x,t) can be considered to be in it, thus, the corresponding thermodynamical relations can be quoted, and the local thermodynamical quantities depending on (x,t) can be determined, the equation (2.1) (2.2) is considered as a constrained condition imposed on the local thermodynamical quantities. Of cause, the above hypothesize is made just for the smooth solution of (2.1) (2.2).

The independents x and t usually represent the coordinates of space and time, however, in order to apply the thermodynamical relations, they are endowed with the meaning of the volume and the temperature of a system, respectively. This point does

not contradict the local equilibrium hypothesize, the only possible doubt is that: the variable of the volume cannot become negative. But, in the following discussion, only a formal analogy is concerned, so there is no any obstacle.

First, assume in (2.1) $f_{uu}(u) \geq \alpha > 0$ and in (2.2) $\phi(x)$ is a bounded measurable function, under these conditions the results of [2] can be used. Enlightening by [2], we give

Definition. *Under the assumed conditions, the following quantity*

$$A(x,t) = - \lim_{N \to \infty} \frac{1}{N} \log \int_{-\infty}^{\infty} \exp\Big(- N\Big[\int_{0}^{\xi} \phi(\eta)\, d\eta + t\, g\Big(\frac{x-\xi}{t}\Big)\Big]\Big)\, d\xi \qquad (3.1)$$

is said to be the free energy of the system described by (2.1) (2.2) *in the state* (x,t), *the functions appearing in* (3.1) *are the same as in* (2.8).

It should be demonstrated that to call $A(x,t)$ free energy is reasonable, this can be done just by comparing (3.1) with (2.13) (2.14) and taking notice that $N \to \infty$ means the thermodynamical limit. From (3.1), by Laplace method and (2.8), we have

$$A(x,t) = - \min_{\xi} \Big\{ \int_{0}^{\xi} \phi(\eta)\, d\eta + tg\Big(\frac{x-\xi}{t}\Big)\Big\} = - \int_{0}^{y_0} \phi(\eta)\, d\eta + t\, g\Big(\frac{x-y_0}{t}\Big) \qquad (3.2)$$

When the variable x is regarded as the volume and t as the temperature, according to (2.11) and using those relations satisfied by y_0 in (2.8), by a direct computation we get

$$P = -\Big(\frac{\partial A}{\partial x}\Big)_t = u(x,t) \qquad (3.3)$$

$$S = -\Big(\frac{\partial A}{\partial t}\Big)_x = g(a(u)) - a(u)\, u \qquad (3.4)$$

because S is only the function of u, differentiating it one more time, we have

$$S_u = - f_u(u) \qquad (3.5)$$

The expressions (3.3) (3.5) demonstrate that from the point of view of the thermodynamics, the unknown function $u(x,t)$ can be regarded as the pressure, in the range of an arbitrary constant, $-f(u)$ is the entropy, and the equation (2.1) can be considered as the Maxwell relation expressed by (2.12).

In the following the function $u(x,t)$ will be released from the restriction of being convex (or concave), it is just assumed that $f_{uu}(u)$ is continuous, and the entropy condition for general single conservation laws with one space variable will be discussed. In this discussion, $-f(u)$ is still regarded as the physical entropy, the correctness of this point will be verified by the results derived from it.

In addition, only those solutions of (2.1) (2.2) are considered whose discontinuities occur in a finite range of $f(u)$; notice that for $f(u)$ plus an arbitrary constant, the solutions of (2.1) (2.2) are invariant, so it can be further assumed that at any discontinuity $f(u_+), f(u_-) > 0$.

Let us compute the entropy flux corresponding to the entropy $S = -f(u)$, it is easy to know

$$F_u = S_u f_u = -(f_u(u))^2 \qquad (3.6)$$

thus

$$F(u) = -\int_{u^*}^{u} f_\eta^2(\eta)d\eta + F(u^*) = -\int_{u^*}^{u}(ff_\eta)_\eta d\eta + \int_{u^*}^{u} ff_{\eta\eta}(\eta)d\eta + F(u^*)$$

$$= a(u)S(u) + \int_{u^*}^{u} f(\eta)df_\eta + \text{const.} \tag{3.7}$$

then,

$$\frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} = \frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(a(u)S(u)) + \Big(\int_{u^*}^{u} f(\eta)df_\eta\Big)_x = 0 \tag{3.8}$$

comparing (3.8) with (2.15), it is easy to know that if we consider (x, t) as the usual space and time variables, then, obviously $\frac{\partial}{\partial x}(a(u)f(u))$ represents the term of entropy flow; if we explain (x, t) as the volume and temperature, then, by thermodynamic relation $\Big(\frac{\partial S}{\partial P}\Big)_T = \Big(\frac{\partial V}{\partial T}\Big)_P$, this term corresponds to the entropy change because of the change of the system volume, it also does not concern with the entropy production; Thus, by the thermodynamical principle that the local entropy production must be nonnegative, in weak sense we have

$$\sigma = -\Big(\int_{u^*}^{u} f df_\eta\Big)_x \geq 0 \tag{3.9}$$

which is equivalent to in weak sense

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(a(u)S(u)) \geq 0 \tag{3.10}$$

or

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(a(u)f(u)) \leq 0 \tag{3.11}$$

Let (x, t) be a point on a curve Γ across which the generalized solution $u(x, t)$ of (2.1) (2.2) has a discontinuity, u_- and u_+ are the values of $u(x, t)$ at the two sides of Γ, Denote $\mathcal{D} = \Big\{u : u \in [\min(u_+, u_-), \max(u_+, u_-)] \text{ and } \frac{f(u) - f(u_-)}{u - u_-} = \frac{f(u_+) - f(u_-)}{u_+ - u_-}\Big\}$, we have the following proposition:

Proposition. *For the generalized solution of* (2.1) (2.2), *a discontinuity is permitted if and only if for any two states* $v, w \in \mathcal{D}$ *and* $\text{sgn}\,(v - w) = \text{sgn}\,(u_+ - u_-)$, *when regarding* v *as* u_+, w *as* u_-, *the inequality* (3.11) *in weak sense holds.*

Proof. It is only need to show that the above proposition is equivalent to the Olejnik' E- condition. From (3.11) , by the habitual practice and the Rankine- Hugoniot jump condition (2.4), we get

$$f(u_-)\Big(f_u(u_-) - \frac{f(u_-) - f(u_+)}{u_- - u_+}\Big) - f(u_+)\Big(f_u(u_+) - \frac{f(u_-) - f(u_+)}{u_- - u_+}\Big) \geq 0 \tag{3.12}$$

Previously, we have assumed $f(u_+), f(u_-) > 0$, so that if

$$f_u(u_-) \geq \frac{f(u_-) - f(u_+)}{u_- - u_+} \geq f_u(u_+) \tag{3.13}$$

then, (3.12) holds. It is easy to know if the Olejnik's E- condition (2.5) satisfies, (3.13) is correct, that is to say, under the E- condition the local entropy production across the discontinuity is nonnegative, the proposition holds;

Next, we discuss the opposite cases in which the Olejnik's E- condition does not hold. In order to avoid the overelaborate formal expression, without loss of generality, we consider the simple situation illustrated as in the figure 1 and assume $u_- > u_+$.

In this case there exist states $v, w \in \mathcal{D}$ and satisfy

$$\frac{f(u_+) - f(u_-)}{u_+ - u_-} = \frac{f(v) - f(w)}{v - w} \tag{3.14}$$

replacing u_- by w and u_+ by v in the left of (3.12), the resulting inequality is

$$f(w)\Big(f_u(w) - \frac{f(w) - f(v)}{w - v}\Big) - f(v)\Big(f_u(v) - \frac{f(w) - f(v)}{w - v}\Big) < 0 \tag{3.15}$$

which means that the entropy production for the state translation between v and w is negative, it contradicts (3.11), thus, the above proposition is proved.

From above discussion the physical meaning of the Olejnik's E- condition is clear, in the case shown as in fig.1, the states u_- and u_+ cannot be connected by a discontinuity, because if this connection were possible, it would be divided into three sections, i.e., the state successive translations between $(u_+, v), (v, w)$ and (w, u_-), but (3.15) has tolled us the translation between (v, w) through a discontinuity would bring out a negative entropy production, so, in physics, it cannot occur. Thus, the Olejnik's E- condition is non other than the mathematical expression of the thermodynamical principle that the local entropy production must be nonnegative.

The above argument strongly depends on the positiveness of $f(u_-)$ and $f(u_+)$, this point stems from the following physical and mathematical reasons: we think, only the conservation laws with convex flux functions describe the "real" physical processes and satisfy the "normal" physical laws, because only for a convex f, $S_{uu} = -f_{uu} < 0$, i.e. the entropy is a concave function of the pressure, which is the same as in the classical ideal gas model, for these conservation laws, the assumption $f(u) > 0$ is natural. For the general conservation laws, which will be considered as an mathematical generalizations of the real physical processes, if we want to explain them by the normal physical laws, of cause, we should let $f(u_-), f(u_+) > 0$.

Expression (3.12) can be derived by another way. We consider that on the interval $(\min(u_-, u_+), \max(u_-, u_+))$ the flux function $f(u)$ is altered by the chord connecting points $(u_-, f(u_-))$ and $(u_+, f(u_+))$, by use of the definition of Stieltjes integral, we have

$$\int_{x_-}^{x_+} \sigma dx = \int_{u_+}^{u_-} f df_\eta = f(u_-)\Big(f_u(u_-) - \frac{f(u_-) - f(u_+)}{u_- - u_+}\Big)$$
$$- f(u_+)\Big(f_u(u_+) - \frac{f(u_-) - f(u_+)}{u_- - u_+}\Big) \tag{3.16}$$

the right hand of (3.16) is just (3.12). This result can be understood as follows: at any strong discontinuity, the state transition from u_- to u_+ is carried out along the

chord connecting points $(u_-, f(u_-))$ and $(u_+, f(u_+))$; for any point in the chord the entropy production is zero, the non-negative entropy productions only happen at the two endpoints $(u_-, f(u_-))$ $(u_+, f(u_+))$. If we explain the variables x, t, and u as volume, temperature and pressure, respectively, then on the (x, u) plane, the chord connecting $(u_-, f(u_-))$and $(u_+, f(u_+))$ is a isotherm, which can be compared with the isotherm of gas-liquid transitions, just the pressure and volume exchange their positions; but the gas-liquid transitions belong to the equilibrium thermodynamics, a permitted discontinuity of single conservation laws describes irreversible process,its maintenance depends on the characteristics coming in on the two sides,thus, what happened in a strong discontinuity is not a ordinary phase transition, maybe, it could be considered as a most simple mathematical model of non-equilibrium transitions.

4. Discussion

Finally, we give a brief discussion: (1) From the above section, it seems that in general, regarding $-f(u)$ as the entropy of (2.1) (2.2) is reasonable; however, because $-f$ may not be convex, so it does not belong to the entropy in the Lax's sense. (2) Even f is concave, so $S = -f$ is a convex entropy, the entropy inequality (3.10) is still different from the (2.6) given by P.D. Lax. (3) The physical meaning of inequality (3.12) is obvious, it means for a permitted discontinuity, for the reference system moving with it, the negative entropy flowing into the discontinuity is greater than or equals to the negative entropy flowing out of it, which guarantees a positive entropy production.

Fig. 1

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