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AN EXTENSION OF THE THEORY OF DIFFUSION AND HEAT CONDUCTION WITHIN LAGRANGE FORMALISM

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Abstract

Despite of the fact that a number of approaches exsists for the theory of diffusion and heat conduction within Lagrange formalisms, none of them solves the inverse problem without paying a high price. In this paper it is shown that a variational principle can easily be constructed for an extended theory based on a classical fluid model. This extended dynamics results in classical dynamics by the assumption of a local equilibrium. It is further shown that the resulting Lagrangians are generalizations of the Lagrangians proposed by Anthony for classical theories.

Keywords: Lagrangian formalism, complex matter field, thermion

1. Status Quo

The classical theory of diffusion is based on *Fick's law*. The evolution of the mass density ϱ of the diffusing substance is given by:

$$\partial_t \varrho - D\Delta\varrho = 0 \,. \tag{1}$$

$D > 0$ is the diffusion constant. It is well known that (1) is a non-selfadjoint equation, i.e. no Lagrangian of the form $l(\varrho, \partial_t\varrho, \nabla\varrho)$ can be constructed. However, there exist a lot of different approaches towards Variational Principles. I restrict myself to *Anthony's approach* [1].

By analogy to Schrödinger's matter field theory Anthony introduces a *complex matter field* ψ for the diffusing substance with the property

$$n = \frac{\varrho}{m} = |\psi|^2 = \psi^*\psi \,, \tag{2}$$

where n is the particle density and m the particle mass. To simplify the mathematical treatment, we switch over to real valued fields ϱ, ζ by the following substitution:

$$\psi = \sqrt{\frac{\varrho}{m}} \exp\left(i\frac{m}{k}\zeta\right) \,, \quad \psi^* = \sqrt{\frac{\varrho}{m}} \exp\left(-i\frac{m}{k}\zeta\right) \,. \tag{3}$$

Remark: I make use of a nomenclature different from Anthony's one. The quantity ζ appearing in *Eq.* (3) is connected with the quantities α, μ and ω appearing in ANTHONY's paper [1] by $\zeta = \mu\alpha/(m\omega)$. Since $m\zeta$ has the dimension of an action, I have to introduce the constant k with the same dimension in order to make the exponents in *Eq.* (3) dimensionless.

Anthony proposes a Lagrangian (see *Eq.* (19) in his paper) for a multicomponent system containing also thermal degrees of freedom and chemical reactions. For an isothermic one-component system we set $T = T_0$, $\varphi = \varphi_0$ and $R = 0$. The Lagrangian then takes the form:

$$l(\varrho, \nabla\varrho, \partial_t\zeta, \nabla\zeta) = -\varrho\partial_t\zeta + D\nabla\varrho \cdot \nabla\zeta \,. \tag{4}$$

It also can be written in terms of the complex matter field ψ after reversing substitution (3):

$$l = -\frac{k}{2i}\left[\psi^*\partial_t\psi - \psi\partial_t\psi^*\right] + D\frac{k}{2i\psi^*\psi}\left[(\psi^*\nabla\psi)^2 - (\psi\nabla\psi^*)^2\right] \,. \tag{5}$$

The arbitrary constant k having the same dimension ('action') as Planck's constant makes the Lagrangian energy-valued. Apart from this its value has no effect on the dynamics defined by (5)!

The variational procedure with respect to ζ, ϱ applied to the Lagrangian (4) results in the Euler–Lagrange equations

$$\partial_t\varrho - D\Delta\varrho = 0 \,, \tag{6}$$

$$\partial_t\zeta + D\Delta\zeta = 0 \,. \tag{7}$$

On the one hand, Fick's law of Diffusion is reproduced, but on the other hand, the field ζ appears as a second quantity, the interpretation of which is difficult. Looking at *Eq.* (7), a physical meaning of ζ becomes doubtful, because this equation is a time-reversed diffusion law! So some questions arise:

- What is the meaning of the second field ζ which by means of (3) is connected with the phase of the matter field ψ?
- Is it possible to modify the Lagrangian (4) in such a way as to make the equation for ζ acceptable?
- Is there any experimental evidence for the existence of a second field quantity ζ?

Anthony himself supposes that the phase function is a measure for the deviation of the process from local thermodynamical equilibrium. I try to answer the questions by extending the Lagrangian (4).

2. A Macroscopic Model for Diffusion

To get an idea how to extend classical diffusion theory we need a suitable model. In my opinion, a good approach is given by using an analogy to a compressible, barotropic[1] fluid motion through a rigid, porous body. The dynamics of this kind of system, illustrated in *Fig. 1* is well known from classical hydrodynamics. It is ruled by the mass balance equation and Euler's equation with an exterior frictional force proportional to the velocity:

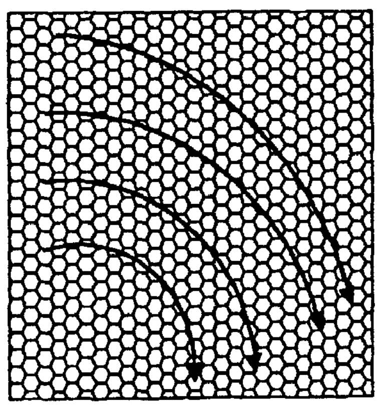

Fig. 1. Fluid motion with exterior friction

$$\partial_t \varrho + \nabla \cdot (\varrho \vec{v}) = 0 \, , \tag{8}$$

$$\varrho \partial_t \vec{v} - \varrho \vec{v} \times (\nabla \times \vec{v}) + \varrho \nabla \left[\frac{1}{2} \vec{v}^2 + P(\varrho) \right] = -\eta \varrho \vec{v} \, . \tag{9}$$

η is the friction constant and $P(\varrho)$ the pressure function given by:

$$P(\varrho) := \int_{\varrho_0}^{\varrho} \frac{p'(\tilde{\varrho})}{\tilde{\varrho}} d\tilde{\varrho} \, . \tag{10}$$

$p(\varrho)$ is the hydroelastic pressure and ϱ_0 a reference density. In the special *irrotational case*, $\nabla \times \vec{v} = 0$, the velocity can be expressed by a potential

$$\vec{v} = \nabla \Phi \, , \tag{11}$$

[1] 'barotropic': the hydroelastic pressure depends on the mass density only.

so that Euler's equation (9) can be integrated to the *modified Bernoulli's equation* (13). Together with the mass balance equation the complete dynamics of the irrotational case is given by the two equations

$$\partial_t \varrho + \nabla \cdot (\varrho \vec{v}) = 0 \,, \tag{12}$$

$$\partial_t \Phi + \eta \Phi + \frac{1}{2}(\nabla \Phi)^2 + P(\varrho) = 0 \,. \tag{13}$$

WAGNER [4] has shown that a flow with exterior friction can be derived from a *variational principle.* For irrotational motion he proposes the Lagrangian:

$$l(\varrho, \Phi, \partial_t \Phi, \nabla \Phi, t) = -e^{\eta t} \varrho \left[\partial_t \Phi + \eta \Phi + \frac{1}{2}(\nabla \Phi)^2 \right] - e^{\eta t} \int\limits_{\varrho_0}^{\varrho} P(\tilde{\varrho}) d\tilde{\varrho} \,. \tag{14}$$

This Lagrangian is time-dependent, because there is dissipation of energy and an exchange of momentum between the fluid and the rigid body. Variation with respect to Φ, ϱ reproduces conservation of mass (12) and the modified Bernoulli's equation (13).

I shall prove now that our fluid model leads to a suitable extension of Fick's law of Diffusion. In the special case of a *throttled motion*[2] the two terms $\partial_t \Phi$ and $\vec{v}^2$, which describe inertia effects, can be neglected in *Eq.* (13) so that we obtain the following simplified Bernoulli's equation:

$$\eta \Phi + P(\varrho) = 0 \,. \tag{15}$$

Eq. (15) can be interpreted as a *local equilibrium* of acting forces: the sum of the driving pressure-induced force and the frictional force vanishes. With regard to (15) the velocity potential Φ can completely be expressed by the mass density, i.e. the state of the throttled system is determined by the mass density, only. Using (15, 10) *Eq.* (12) then takes the form:

$$\begin{aligned} 0 &= \partial_t \varrho + \nabla \cdot [\varrho \nabla \Phi] \\ &= \partial_t \varrho + \nabla \cdot \left[\varrho \nabla \left(-\frac{P(\varrho)}{\eta} \right) \right] \\ &= \partial_t \varrho - \nabla \cdot \left[\frac{p'(\varrho)}{\eta} \nabla \varrho \right] \,. \end{aligned} \tag{16}$$

In the special linear case

$$p = p_0 + K(\varrho - \varrho_0) \tag{17}$$

[2] i.e. a flow with sufficiently small acceleration $\{\partial_t + \vec{v} \cdot \nabla\} \vec{v} = \nabla \left[\partial_t \Phi + \frac{1}{2}(\nabla \Phi)^2 \right]$

with the *compression modulus* K the quantity

$$D := \frac{p'(\varrho)}{\eta} = \frac{K}{\eta} \tag{18}$$

is constant, and so *Eq.* (16) turns out to be Fick's law of diffusion (1). The conclusion can be drawn that a **flow suffering exterior friction results in diffusion, if inertia effects are neglected!**

Taking now into account inertia I define the function

$$\bar{\zeta} := e^{\eta t}\left[\Phi + \frac{P(\varrho)}{\eta}\right] \tag{19}$$

as a measure for the *deviation of the process from local equilibrium.* Obviously I take 'local equilibrium' as a synonym for the throttled motion, which is characterized by (15) and for which $\bar{\zeta}$ vanishes. Substituting the velocity potential Φ by $\bar{\zeta}$ by means of (14) I get the Lagrangian (14) in the form

$$l = l_0(\varrho, \partial_t\bar{\zeta}, \nabla\varrho, \nabla\bar{\zeta}) + l_I(\varrho, \nabla\varrho, \nabla\bar{\zeta}, t) + \partial_t G(\varrho, t)$$

with

$$\begin{aligned} l_0(\varrho, \partial_t\bar{\zeta}, \nabla\varrho, \nabla\bar{\zeta}) &:= -\varrho\partial_t\bar{\zeta} + D\nabla\varrho\cdot\nabla\bar{\zeta}\,, \\ l_I(\varrho, \nabla\varrho, \nabla\bar{\zeta}, t) &:= -\frac{1}{2}\varrho\left[e^{-\eta t}(\nabla\bar{\zeta})^2 + e^{\eta t}\left(\frac{D}{\varrho}\nabla\varrho\right)^2\right]\,, \\ G(\varrho, t) &:= \frac{e^{\eta t}}{\eta}p(\varrho)\,, \end{aligned} \tag{20}$$

which divides into three parts. The first part l_0 is identical with Anthony's Lagrangian (4) if the deviation from equilibrium is identified $\bar{\zeta}$ with the quantity ζ of ch. 2 defined by (3):

$$\zeta \equiv \bar{\zeta}\,. \tag{21}$$

The second part l_I is associated with inertia effects and with external friction. Its explicit time-dependence gets clear, if one keeps in mind that the fluid is but a partial, open system which interacts with the rigid body. The third part is a total time derivative and has no effect on the Euler–Lagrange equations.

So the following conclusions can be drawn:

- Anthony's Lagrangian (4) can be extended to another Lagrangian (20) which takes inertia effects into account.

- The function ζ can be physically associated with the *deviation from local equilibrium* (15). The whole system is described by both fields, ϱ and ζ, and, thus, finally by the matter field ψ (see *Eq.* 3).
- The Euler–Lagrange equations due to (20) are equivalent to the mass balance (12) and to the modified Bernoulli's equation (13) by substitution (19). So, the equation for $\tilde{\zeta}$ can physically be accepted!

Reversing substitution (3) and taking account of (21) the Lagrangian (20) of the fluid with exterior friction can be put into the form:

$$l = -\frac{k}{2i}\left[\psi^*\partial_t\psi - \psi\partial_t\psi^*\right] + D\frac{k}{2i\psi^*\psi}\left[(\psi^*\nabla\psi)^2 - (\psi\nabla\psi^*)^2\right] - e^{-\eta t}\frac{k^2}{2m}\nabla\psi^*\cdot\nabla\psi + \left(\frac{k^2}{4m}e^{-\eta t} - mDe^{\eta t}\right)\frac{[\nabla(\psi^*\psi)]^2}{2\psi^*\psi} \tag{22}$$

depending on the matter field ψ. The term $\partial_t G$ has been cancelled.

3. Extended Fourier's Law of Heat Conduction

Let c be the specific heat and λ the coefficient of heat conductivity. Because of the fact, that Fick's law of diffusion and Fourier's law of heat conduction

$$c\partial_t T - \lambda\Delta T = 0 \tag{23}$$

are of the same type, the question arises if the extended model of diffusion presented in ch. 3 can be transferred to the case of heat conduction.

For this purpose the description of thermal processes is based on a *particle model.* Starting from a Lagrangian of heat conduction and using a complex *field of thermal excitation* as the fundamental variable Azirhi [5] has already established a model for heat conduction within the framework of quantum field theory. He associates thermal excitation with an ensemble of quasi-particles which he calls **thermions**.

In contrast to Azirhi's quantum field theoretical approach I make use of the classical fluid model in ch. 3: Heat is interpreted as a classical gas of thermions diffusing through a material body. Let m^* be the effective mass of a thermion, $\hbar\omega_0$ its energy, $u = cT$ the density of internal energy and n the particle density of thermions. Then, the following identifications lead from the quantum theoretical concept to the classical model of heat:

$$n\hbar\omega_0 = u = cT\ , \tag{24}$$

$$nm^* = \varrho\ . \tag{25}$$

So the mass density ϱ of thermions is connected with the temperature by

$$\varrho = \frac{m^*}{\hbar\omega_0} cT \, . \tag{26}$$

Together with another substitution

$$\frac{m^*}{\hbar}\bar{\zeta} = \varphi + \omega_0 t \, , \tag{27}$$

which connects the deviation from local equilibrium $\bar{\zeta}$ with the phase function φ of the thermal excitation field, and with the definition $\lambda := cD$ the Lagrangian (20) reads after neglecting the term $\partial_t G$:

$$l = l_0(T, \partial_t\varphi, \nabla T, \nabla\varphi) + l_{Tr}(T, \nabla T, \nabla\varphi, t)$$

with

$$l_0 := -cT - \frac{c}{\omega_0} T\partial_t\varphi + \frac{\lambda}{\omega_0}\nabla T \cdot \nabla\varphi \, , \tag{28}$$

$$l_I := -\frac{cT}{\hbar\omega_0}\left[\frac{\hbar^2}{2m^*}e^{-\eta t}(\nabla\varphi)^2 + \frac{m^*\lambda^2}{2c^2}e^{\eta t}\left(\frac{\nabla T}{T}\right)^2\right] .$$

The first part l_0 is identical to the Lagrangian for Fourier's law proposed by ANTHONY [2]. In analogy with the case of diffusion the second part takes effects of *thermal inertia* into account. Its explicit time-dependence is due to the open system of thermions.

The Euler–Lagrange equations read:

$$c\partial_t T - \lambda\Delta T + \frac{c\hbar}{m^*\omega_0}e^{-\eta t}\nabla \cdot (T\nabla\varphi) = 0 \, , \tag{29}$$

$$\partial\varphi + \frac{\lambda}{c}\Delta\varphi + \frac{\hbar}{2m^*}e^{-\eta t}(\nabla\varphi)^2 + \omega_0 - \frac{2m^*\lambda^2}{\hbar c^2}e^{\eta t}\frac{\Delta\sqrt{T}}{\sqrt{T}} = 0 \, . \tag{30}$$

The explicit time-dependence of these equations can be eliminated completely by substituting

$$\varphi = e^{\eta t}\varphi - \omega_0 t \tag{31}$$

and multiplying *Eq.* (30) with $e^{-\eta t}$:

$$c\partial_t T - \lambda\Delta T = -\frac{c\hbar}{m^*\omega_0}\nabla \cdot (T\nabla\varphi) \, , \tag{32}$$

$$\partial_t\phi + \eta\phi + \frac{\lambda}{c}\Delta\phi + \frac{\hbar}{2m^*}(\nabla\phi)^2 = \frac{2m^*\lambda^2}{\hbar c^2}\frac{\Delta\sqrt{T}}{\sqrt{T}} \, . \tag{33}$$

As in the case of extended diffusion ϕ has the meaning of a deviation from local equilibrium (apart from the factor $m^*/\hbar$). If $\nabla\phi$ is assumed to be sufficiently small, (32) results in Fourier's law, as it should be! Outside local equilibrium the second equation (33) describes the relaxation of the system to local equilibrium. Obviously the production rate on the left hand side of (33) shows that the system is thrown out of local equilibrium by strong spatial fluctuations of the temperature!

ANTHONY and KNOPPE [3] have also constructed an extended theory for heat conduction, but they make use of a different ansatz.

4. Consequences

The question arises, if there are any observable effects for experimental investigations. The fluid model of extended heat conduction differs in two significant points from classical Fourier's theory:

Finite signal speed: *Fig. 2* shows the evolution of a temperature profile given by a Heaviside function at the time $t = t_0$. Some time later the profile has changed by heat conduction. Fourier's law gives rise to a temperature change in any point x. This can also be interpreted as a kind of 'thermal signal' which propagates from the singular point of discontinuity to infinity in an arbitrary short time. This phenomenon is called the *paradoxon of infinite signal speed.*

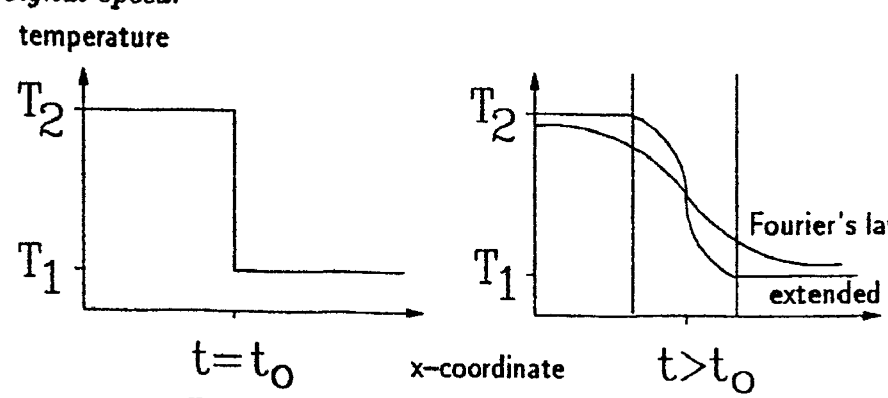

Fig. 2. Paradoxon of infinite signal speed

Contrary to this the extended theory predicts a temperature change only inside a limited region. The extension of this region is approximately given by the product of the passed time and the speed of sound of the thermion gas. Within the proposed model the finite signal speed is a result of the analogy with classical hydrodynamics: After linearization of *Eqs.* (32, 33) and after some manipulations of both equations and finally taking account of derivatives up to the 2nd it can be shown that near local equilibrium the evolution of the temperature is ruled by *Cattaneo's equation*

$$\frac{\lambda}{K}\partial_t^2 T + c\partial_t T - \lambda\Delta T = 0 \,. \tag{34}$$

The solutions of this well-known type of equation (telegraph equation) are *damped waves* of a signal speed limited by

$$v_{th} = \sqrt{K} \,. \tag{35}$$

For further details see forthcoming paper!

Speculations on momentum exchange: In contrast with Fourier's theory, which considers a heat flux without any associated mechanical forces, the extended theory predicts an exchange of momentum between the thermion gas and the rigid body, so that any heat flux causes force acting on the body. Starting again from the theory of classical gases the density of this force is determined by the frictional term in Euler's equation (9)

$$\vec{f} = \eta\varrho\vec{v} = \eta\varrho\nabla\Phi \,. \tag{36}$$

Near local equilibrium the velocity potential Φ can be approximated by (15). So, the friction force density is simply given by

$$\vec{f} = -\eta\varrho\nabla\left(\frac{P(\varrho)}{\eta}\right) = -p'(\varrho)\nabla\varrho \,. \tag{37}$$

Restricting ourselves again to the linear case $p'(\varrho) = K$ and substituting the mass density of the thermion gas by the temperature by means of (26), we result in

$$\vec{f} = -\frac{m^* K c}{\hbar\omega_0}\nabla T \,. \tag{38}$$

Let V be the spatial region filled by the body. Then the total force on the body reads

$$\vec{F} = -\frac{m^* K c}{\hbar\omega_0}\int\limits_V \nabla T dV = -\frac{m^* K c}{\hbar\omega_0}\int\limits_{\partial V} T \cdot d\vec{S} \,. \tag{39}$$

∂V is the surface of the body. To estimate this force let us assume that the thermion energy is connected with the thermion mass by the relativistic relation

$$\hbar\omega_0 = m^* v_c^2 \,, \tag{40}$$

where v_c is the speed of light. The compression modulus K of the thermion gas is associated with the speed v_{th} of waves in the thermion gas being an analogue of a hydroelastic fluid:

$$K = v_{th}^2 \, . \tag{41}$$

Keeping in mind the microscopic picture, which associates thermal excitations with phonons, we estimate v_{th} by the *sound velocity*. Thus, we finally result in

$$\vec{F} = -c\left(\frac{v_{th}}{v_c}\right)^2 \int\limits_{\partial V} T \cdot d\vec{S} \, . \tag{42}$$

To exemplify *Eq.* (42) let us look at a cylindrical body between two heat baths (*Fig. 3*). In the stationary state the temperature varies only along the cylindric axis. Then the amount of the reaction force is given by:

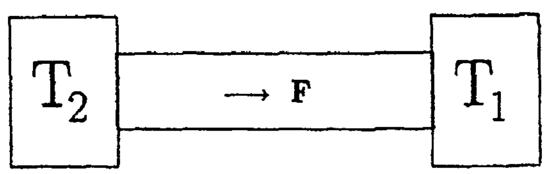

Fig. 3. Reaction force of a heat flux

$$F = \frac{m^* K c}{\hbar\omega_0} A|T_2 - T_1| = c\left(\frac{v_{th}}{v_c}\right)^2 A|T_2 - T_1| \, . \tag{43}$$

A is the area of the cross-section. Because of the square of the velocity quotient v_{th}/v_c this force is expected to be very small!

5. Perspectives

One critical point of the theory presented in this paper is the explicit time-dependence of the Lagrangians. This is due to the fact that the Lagrangian (14) explicitly involves only degrees of freedom of the fluid whereas the degrees of freedom of the material background are disregarded. This motivates us to go a step further towards an extended Lagrangian containing some supplementary fields in order to take the body's dynamics into account. The dynamical equations for these fields are expected to describe elastic, plastic or fluid motion of the material background. Such a Lagrangian would be time-independent and adequate for diffusion and heat conduction in deformable bodies.

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