

## On the Lagrange functional for dissipative processes(\*)

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THE CONDITIONS are given for the nonlinear potential in Schrödinger-like equations, describing the diffusion of point defects in crystals, to be self-adjoint. The conservation laws following from the constructed Lagrange functional and Noether theorem are discussed. The second variation is investigated, too.

Podano warunki jakie musi spełniać nieliniowy potencjał w równaniach typu Schrödingera (opisujące dyfuzję defektów punktowych w kryształach), aby te równania były samosprężone. Przedyskutowano prawa zachowania wynikające ze skonstruowanego funkcjonału Lagrange'a oraz z twierdzenia Noether. Zbadano również zachowanie się drugiej wariacji.

Приведены условия каким должен удовлетворять нелинейный потенциал в уравнениях типа Шредингера (описывающие диффузию точечных дефектов), чтобы эти уравнения были самосогласованными. Рассматривались законы поведения, вытекающие из построенного функционала Лагранжа, а также из теоремы Нетер. Исследовалось также поведение второй вариации.

### 1. Introduction

THE FACT that it is impossible to describe the irreversible processes with the help of Lagrange formalism is almost commonly accepted. Nevertheless, it is a fascinating idea to incorporate this class of processes into the general scheme of the Hamilton variational principle. The first attempt to construct a variational principle for the thermodynamics of irreversible processes was made by the Polish physicist W. NATANSON in 1986. His approach is very general and includes the variational principles constructed by I. GYARMATI (1969) and C. VOJTA (1967) for the linear Onsager thermodynamics of irreversible processes as special cases [1]. Recently, a new and very promising variational theory of dissipative processes has been proposed by K. -H. ANTHONY [2-5].

In order to be able to construct the proper Hamilton principle for the thermal conductivity process, ANTHONY [2] introduced a scalar field of thermal excitations

$$(1.1) \quad \psi(\mathbf{x}, t) = \sqrt{T(\mathbf{x}, t)} e^{i\varphi(\mathbf{x}, t)},$$

where  $T = T(\mathbf{x}, t)$  is the absolute temperature. The new variable, the phase  $\varphi(\mathbf{x}, t)$  of the complex field  $\psi(\mathbf{x}, t)$ , has not found satisfactory interpretation till now. In this paper we deal with diffusion of crystal lattice defects. Anthony has described diffusion with chemical reactions in [5] and he has introduced there the proper  $\varphi$  functions, too. The

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approach to diffusion in this paper is based on the nonlinear Schrödinger-like equation [7–9]. It occurs that the formal resemblance to the true Schrödinger equation, for which the Lagrange density function (Lagrangian) is well known, is not sufficient to build the Lagrangian for the Schrödinger-like equation. We discuss these two theories in certain aspects, and propose to interpret the phase  $\varphi(\mathbf{x}, t)$  as a parameter describing the interaction of the system with the hidden degrees of freedom (the variables not explicitly taken into the description of the system). It allows to consider within the framework of Lagrange formalism the deviation of the system from equilibrium state.

Let us very shortly recall the basic points of Lagrange formalism (for more details see the papers of ANTHONY [2]–[6] or elsewhere).

The Hamilton principle says that complete information about the physical system is contained in the Lagrange density function

$$(1.2) \quad l(\psi_i(\mathbf{x}, t), \partial_t \psi_i(\mathbf{x}, t), \partial_\alpha \psi_i(\mathbf{x}, t)),$$

where  $\psi_i(\mathbf{x}, t)$  are (in general) complex field process variables,  $i = 1, \dots, N$  and  $\partial_t = \frac{\partial}{\partial t}$ ,

$\partial_\alpha = \frac{\partial}{\partial x^\alpha}$ ,  $\alpha = 1, 2, 3$ , and also that the true process causes the Lagrange functional (called also an action integral) to have an extremum. This fact is mathematically expressed as vanishing of the first variation of the integral

$$(1.3) \quad \delta^1 J = \delta^1 \int_{t_1}^{t_2} dt \int_{\mathcal{P}} dV(\mathbf{x}) l(\psi_i(\mathbf{x}, t), \partial_t \psi_i(\mathbf{x}, t), \partial_\alpha \psi_i(\mathbf{x}, t)) = 0,$$

for arbitrary, free variations of the field variables  $\psi_i(\mathbf{x}, t)$  at the time interval  $[t_1, t_2]$ , keeping fixed the field variables at the end points of the time interval, i.e.  $\delta\psi_i(\mathbf{x}, t_1) = \delta\psi_i(\mathbf{x}, t_2) = 0$ . Here  $\mathcal{P}$  is the space volume of integration.

As a result of applying the Hamilton principle to  $J$ , one obtains the set of  $N$  Euler–Lagrange equations<sup>(1)</sup>

$$(1.4) \quad l_i = d_t \frac{\partial l}{\partial(\partial_t \psi_i)} + \sum_{\alpha=1}^3 d_\alpha \frac{\partial l}{\partial(\partial_\alpha \psi_i)} - \frac{\partial l}{\partial \psi_i} = 0, \quad i = 1, \dots, N.$$

These are the equations of evolution (of motion) of the physical system.

A very important feature of the Lagrangian is its invariance with respect to various continuous groups of transformations. The most important role is played by the space-time coordinate transformations (e.g., the Galilean or Lorentz transformations), which assume the homogeneity and isotropy of the Universe — the physical laws do not depend on the translations and rotations of the physical system in the space-time. The prominent Noether theorem assures that a conservation law corresponds to each invariance group parameter  $\varepsilon$ , namely

$$(1.5) \quad \partial_t \rho_{(\varepsilon)} + \sum_{\alpha=1}^3 \partial_\alpha J_{\alpha(\varepsilon)} = 0,$$

<sup>(1)</sup> We use here the symbols of the total derivative  $d_t$  (with  $\mathbf{x} = \text{const}$ ) and  $d_\alpha$  (with  $t = \text{const}$ ) rather than the partial derivatives  $\partial_t$  and  $\partial_\alpha$ , because the latter can cause misunderstandings, see e.g. [12].

where  $\underset{(\epsilon)}{\rho}$  and  $\underset{(\epsilon)}{J_\alpha}$  are, respectively, the density and flux of the conserved quantity. We give here some examples of the conservation laws.

### 1.1. Conservation of energy

One obtains the law of conservation of energy (the first law of thermodynamics) by studying the invariance of the Lagrangian with respect to the time translations — the result of any experiment does not depend on the choice of the instant of time. In this case one has

the energy density

$$(1.6) \quad \epsilon = \sum_{i=1}^N \frac{\partial l}{\partial(\partial_t \psi_i)} \partial_t \psi_i - l,$$

the energy flux density

$$(1.7) \quad J_\alpha = \sum_{i=1}^N \frac{\partial l}{\partial(\partial_\alpha \psi_i)} \partial_t \psi_i.$$

### 1.2. Conservation of linear momentum

The law of conservation of the linear momentum (the second Newton law) follows from the invariance of the Lagrangian on the space translations — the result of any experiment does not depend on the point of the Universe. In this case one has

density vector of linear momentum

$$(1.8) \quad p_\alpha = - \sum_{i=1}^N \frac{\partial l}{\partial(\partial_t \psi_i)} \partial_\alpha \psi_i,$$

density tensor of flux of linear momentum (stress)

$$(1.9) \quad \sigma_{\alpha\beta} = - \sum_{i=1}^N \frac{\partial l}{\partial(\partial_\alpha \psi_i)} \partial_\beta \psi_i + \delta_{\alpha\beta} l.$$

### 1.3. Conservation of mass-like observables

This type of conservation laws follows from the invariance of the Lagrangian with respect to the change of the variables. For the complex field variables one introduces the so-called gauge transformations

$$(1.10) \quad \bar{\psi}(\mathbf{x}, t) = \psi(\mathbf{x}, t) e^{i\Lambda t},$$

$$(1.11) \quad \bar{\psi}^*(\mathbf{x}, t) = \psi^*(\mathbf{x}, t) e^{-i\Lambda t},$$

and, as a result, one obtains the following expressions for the mass-like density:

$$(1.12) \quad \varrho = i\Lambda \left[ \frac{\partial l}{\partial(\partial_t \psi)} \psi - \frac{\partial l}{\partial(\partial_t \psi^*)} \psi^* \right],$$

mass-like flux density function

$$(1.13) \quad J_\alpha = i\Lambda \left[ \frac{\partial l}{\partial(\partial_\alpha \psi)} \psi - \frac{\partial l}{\partial(\partial_\alpha \psi^*)} \psi^* \right].$$

In the case of the Schrödinger wave function  $\psi(\mathbf{x}, t)$ , one obtains the conservation of mass or conservation of the electric charge laws in dependence on the choice of the gauge factor  $\Lambda$ .

## 2. Diffusion and Nelson–Brown process

Diffusion is one of the most interesting processes which proceeds on the microlevel and gives very important macroeffects. Modern electronics and nuclear energetics are the most spectacular examples where the diffusion plays the pivotal part.

In the papers [7]–[9] a new approach is proposed to describe the diffusion of point defects in a crystal lattice. Here we give the outline of the main results only.

The process of diffusion is described by the so-called Nelson relation

$$(2.1) \quad m(\partial_t \mathbf{v} + (\mathbf{v}\nabla)\mathbf{v} - (\mathbf{u}\nabla)\mathbf{u} + D\Delta\mathbf{u}) = -\zeta\mathbf{b} + \mathbf{F},$$

where  $m$  is the mass of the diffusing defect,

$$(2.2) \quad \mathbf{u}(\mathbf{x}, t) = -D \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)},$$

is the osmotic velocity,  $D$  is the diffusion coefficient and  $p(\mathbf{x}, t)$  is the probability density of observing at the instant of time  $t > 0$  a diffusing defect in the neighborhood of a point  $\mathbf{x}$  within a volume  $dV(\mathbf{x})$ . The probability density  $p(\mathbf{x}, t)$  satisfies Eq. (2.1) and the Fokker–Planck equation

$$(2.3) \quad \partial_t p = D\Delta p - \text{div}(p\mathbf{b}).$$

The quantity  $\mathbf{b}(\mathbf{x}, t)$  is the so-called forward velocity with which the particle starts from the point  $\mathbf{x}$ . The peculiar velocity  $\mathbf{v}$  is connected with  $\mathbf{b}$  and  $\mathbf{u}$  by the formula

$$(2.4) \quad \mathbf{u} = \mathbf{v} - \mathbf{b}.$$

The number  $n(\mathbf{x}, t)$  of diffusing crystal defects on the unit of volume is connected with the probability density  $p(\mathbf{x}, t)$  in the following way:

$$(2.5) \quad p(\mathbf{x}, t) = \frac{n(\mathbf{x}, t)}{N},$$

where  $N$  is the number of all diffusing particles. On the other hand, the mass density of defects is given by the formula

$$(2.6) \quad \varrho(\mathbf{x}, t) = mn(\mathbf{x}, t),$$

and it follows that

$$(2.7) \quad p(\mathbf{x}, t) = \frac{\varrho(\mathbf{x}, t)}{mN} = \frac{\varrho(\mathbf{x}, t)}{M},$$

where  $M$  is the total mass of diffusing matter.

It follows from Eq. (2.1) that in the asymptotic case for the kinetic relaxation time

$$(2.8) \quad \tau = \frac{m}{\zeta} \rightarrow 0,$$

with  $\zeta = \text{const}$ , the total force acting on the diffusing particle is given by the Stokes relation

$$(2.9) \quad \mathbf{F} = \zeta \mathbf{b},$$

where  $1/\zeta$  is called the mobility of the defect, and the diffusion process can be considered as a throttled process.

In the general case, the Stokes relation is not valid, the total force is given by the formula

$$(2.10) \quad \mathbf{K}(\mathbf{x}, t) = -\zeta \mathbf{b}(\mathbf{x}, t) + \mathbf{F}(\mathbf{x}, t) \neq \mathbf{0},$$

and then the diffusion should be described by the Nelson relation (2.1). Following the lines of the stochastic quantization method of NELSON [10], it is assumed that the peculiar velocity  $\mathbf{v}(\mathbf{x}, t)$  and the external force  $\mathbf{F}(\mathbf{x}, t)$  are the potential fields

$$(2.11) \quad \begin{aligned} \mathbf{v}(\mathbf{x}, t) &= 2D\nabla S(\mathbf{x}, t), \\ \mathbf{F}(\mathbf{x}, t) &= -\nabla U(\mathbf{x}, t), \end{aligned}$$

The osmotic velocity  $\mathbf{u}(\mathbf{x}, t)$  is potential from the very beginning;

$$(2.12) \quad \mathbf{u}(\mathbf{x}, t) = -2D\nabla R(\mathbf{x}, t),$$

where

$$(2.13) \quad R(\mathbf{x}, t) = \frac{1}{2} \ln \frac{p(\mathbf{x}, t)}{p_0}.$$

In these variables the Nelson relation (2.1) takes the form

$$(2.14) \quad \partial_t S = D\Delta R - D[(\nabla S)^2 - (\nabla R)^2] - \frac{V}{2Dm},$$

where

$$(2.15) \quad V = U + \frac{2Dm}{\tau} (R + S + C(t)).$$

Here  $C(t)$  is a certain integration constant.

If one introduces the new variable

$$(2.16) \quad \psi(\mathbf{x}, t) = e^{R+iS},$$

then Eq. (2.1) together with the continuity equation

$$(2.17) \quad \partial_t p + \text{div}(p\mathbf{v}) = 0,$$

(for more details, see [7]) give

$$(2.18) \quad i\tilde{h}\partial_t\psi = -\frac{\tilde{h}^2}{2m}\Delta\psi + V\psi,$$

where

$$(2.19) \quad V = U + \frac{\tilde{h}}{2\tau} \left[ \ln|\psi|^2 + i\ln\left(\frac{\psi^*}{\psi}\right) + C(t) \right],$$

and

$$(2.20) \quad \tilde{h} = 2Dm.$$

Equation (2.18) is a Schrödinger-like equation only. It is not a true Schrödinger equation because the potential  $V$  is a nonlinear one and the constant  $\tilde{h}$  cannot reach the value of the reduced Planck constant  $h/2\pi$ . This is easy to see because the temperatures calculated from Eq. (2.20) and the Arrhenius formula

$$(2.21) \quad D = D(T) = D_0 \exp\left[-\frac{E_a}{kT}\right],$$

with the assumption  $2\pi\tilde{h} = h$ , the experimental data of  $D_0$

$$(2.22) \quad D_0 = (10^{-2} \div 10^0) \frac{\text{cm}^2}{\text{s}},$$

and the activation energy  $E_a$  for various metals, are much greater than the corresponding melting temperatures.

### 3. Lagrange function for the nonlinear Schrödinger-like equation

Not every  $N$  equations for  $N$  field process variables make it possible to build up the Lagrange function. It is known from the theory of the so-called inverse Lagrange problem (see, e.g., [12]) that this set of equations should possess the property of being self-adjoint. The conditions to be satisfied so that the set of equations

$$(3.1) \quad l_k \equiv \sum_{i=1}^N \sum_{\alpha, \beta=0}^3 (A_{ki}^{\alpha\beta}(\mathbf{x}, \psi, \partial\psi) \partial_\alpha \partial_\beta \psi^i + B_k(\mathbf{x}, \psi, \partial\psi)) = 0$$

is self-adjoint are given by K. -H. ANTHONY [11], and this theorem (without proof) is quoted in Appendix<sup>(2)</sup>.

Let us try to find the Lagrange function for our nonlinear Schrödinger-like equation (2.18) (we put for the time being  $C(t) = 0$  as not essential to our prospective considerations). We see that in Eq. (2.18) there are two field variables  $\psi_1 = \psi(\mathbf{x}, t)$  and  $\psi_2 = \psi^*(\mathbf{x}, t)$  ( $\psi^*(\mathbf{x}, t)$  is complex conjugated to  $\psi(\mathbf{x}, t)$ ). Therefore additionally to Eq.

<sup>(2)</sup> For the other formulations of this theorem compare, e.g., the book of SANTILLI [12] or the paper [13].

(2.18) we need one more equation as to get a self-adjoint set of field equation. Using the statements of the Appendix we find that

$$(3.2)_1 \quad l_1 = i\tilde{\hbar}\partial_t\psi^* - \frac{\tilde{\hbar}^2}{2m}\partial_\alpha\partial_\alpha\psi^* + U(\mathbf{x})\psi^* + \frac{\tilde{\hbar}}{2\tau}\left[\ln(\psi\psi^*) + i\left(\ln\left(\frac{\psi^*}{\psi}\right) - 2\right)\right]\psi^*,$$

and

$$(3.2)_2 \quad l_2 = -i\tilde{\hbar}\partial_t\psi - \frac{\tilde{\hbar}^2}{2m}\partial_\alpha\partial_\alpha\psi + U(\mathbf{x})\psi + \frac{\tilde{\hbar}}{2\tau}\left[\ln(\psi\psi^*) + i\ln\left(\frac{\psi^*}{\psi}\right)\right]\psi.$$

These two equations are self-adjoint and using Eq. (1.4) they can be formally obtained as the Euler–Lagrange equations of the Lagrange functional with the Lagrange density

$$(3.3) \quad l = \frac{i\tilde{\hbar}}{2}(\psi^*\partial_t\psi - \psi\partial_t\psi^*) - \frac{\tilde{\hbar}^2}{2m}\partial_\alpha\psi\partial_\alpha\psi^* - U(\mathbf{x})\psi\psi^* - M(\psi, \psi^*)\psi\psi^*,$$

where

$$(3.4) \quad M(\psi, \psi^*) = \frac{\tilde{\hbar}}{2\tau}\left[(\ln(\psi\psi^*) - 1) + i\left(\ln\left(\frac{\psi^*}{\psi}\right) - 1\right)\right].$$

The last term of the function  $M(\psi, \psi^*)$  is purely imaginary and that is not admissible from our point of view. A Lagrangian of the form like Eqs. (3.3) and (3.4) can be found in the literature [15], however its imaginarity is not commented upon<sup>(3)</sup>.

The obtained result forces to look for the most general form of the potential depending on  $\psi$  and  $\psi^*$  and admissible by Lagrange formalism. The possibility of applying the other form of the nonlinear potential to describe the process of diffusion, as considered in this paper, is discussed in [9].

The requirement of reality of the Lagrange density

$$(3.5) \quad l(\psi, \psi^*, \partial\psi, \partial\psi^*) = l^*(\psi, \psi^*, \partial\psi, \partial\psi^*),$$

gives additional constraints on the Euler–Lagrange equations

$$(3.6) \quad \begin{aligned} l_1 &= d_t \frac{\partial l}{\partial(\partial_t\psi)} + d_\alpha \frac{\partial l}{\partial(\partial_\alpha\psi)} - \frac{\partial l}{\partial\psi}, \\ l_2 &= d_t \frac{\partial l}{\partial(\partial_t\psi^*)} + d_\alpha \frac{\partial l}{\partial(\partial_\alpha\psi^*)} - \frac{\partial l}{\partial\psi^*}, \end{aligned}$$

and it follows that

$$(3.7) \quad l_1 = l_2^*$$

because of Eq. (3.5)

$$(3.8) \quad \frac{\partial l(\psi, \psi^*, \partial\psi, \partial\psi^*)}{\partial\psi^*} = \frac{\partial l^*(\psi, \psi^*, \partial\psi, \partial\psi^*)}{\partial\psi^*} = \left[ \frac{\partial l(\psi, \psi^*, \partial\psi, \partial\psi^*)}{\partial\psi} \right]^*.$$

<sup>(3)</sup> Complex potentials are considered in quantum mechanics [14] to describe, e.g., the inelastic scattering of neutrons. We make use of the theorems of the theory of the calculus of variations valid for the real functionals.

A similar argument holds also for the terms  $\partial l/\partial(\partial_t \psi^*)$  and  $\partial l/\partial(\partial_\alpha \psi^*)$ .

The conditions (3.5) and (3.7) are not fulfilled for Eqs. (3.3) and (3.2).

We rewrite now Eqs. (3.2) in a more general form

$$(3.9) \quad \begin{aligned} l_1 &= i\tilde{h}\partial_t \psi^* + \hat{H}\psi^* + G_1(\psi, \psi^*)\psi^* = 0, \\ l_2 &= -i\tilde{h}\partial_t \psi + \hat{H}\psi + G_2(\psi, \psi^*)\psi = 0, \end{aligned}$$

where

$$(3.10) \quad \hat{H} = -\frac{\tilde{h}^2}{2m} \partial_\alpha \partial_\alpha + U(\mathbf{x}).$$

The condition (3.7) holds if

$$(3.11) \quad G_1(\psi, \psi^*) = G_2^*(\psi, \psi^*).$$

From now on we omit the indices of the function  $G_i(\psi, \psi^*)$  and put

$$(3.12) \quad \begin{aligned} G_1(\psi, \psi^*) &= G^*(\psi, \psi^*), \\ G_2(\psi, \psi^*) &= G(\psi, \psi^*). \end{aligned}$$

In our case, the only non-trivial identity (A.5) from the theorem results in the following condition for  $G$

$$(3.13) \quad \frac{\partial(\psi^* G^*(\psi, \psi^*))}{\partial \psi^*} = \frac{\partial(\psi G(\psi, \psi^*))}{\partial \psi},$$

which has to be fulfilled in order to get self-adjoint set of Eqs. (3.9).

We see that the Lagrange density function for the system of equations (3.9) has the form

$$(3.14) \quad l = \frac{i\tilde{h}}{2} (\psi^* \partial_t \psi - \psi \partial_t \psi^*) - \frac{\tilde{h}^2}{2m} \partial_\alpha \psi \partial_\alpha \psi^* - U(\mathbf{x}) \psi \psi^* - L(\psi, \psi^*) \psi \psi^*.$$

It follows from Eq. (3.5) that  $L(\psi, \psi^*)$  is real. The Euler-Lagrange equations for this Lagrangian read

$$(3.15) \quad \begin{aligned} l_1 &= i\tilde{h}\partial_t \psi^* - \frac{\tilde{h}^2}{2m} \partial_\alpha \partial_\alpha \psi^* + U(\mathbf{x}) \psi^* + L(\psi, \psi^*) \psi^* + \frac{\partial L(\psi, \psi^*)}{\partial \psi} \psi \psi^* = 0, \\ l_2 &= -i\tilde{h}\partial_t \psi - \frac{\tilde{h}^2}{2m} \partial_\alpha \partial_\alpha \psi + U(\mathbf{x}) \psi + L(\psi, \psi^*) \psi + \frac{\partial L(\psi, \psi^*)}{\partial \psi^*} \psi \psi^* = 0. \end{aligned}$$

Comparison of Eqs. (3.15) and (3.9), with taking into account Eq. (3.12) gives

$$(3.16) \quad G^*(\psi, \psi^*) = \frac{\partial}{\partial \psi} (\psi L(\psi, \psi^*)) = \frac{\partial}{\partial \psi^*} (\psi^* L(\psi, \psi^*)) = G(\psi, \psi^*).$$

what implies that  $G(\psi, \psi^*)$  is real, too. When we put, for example,

$$(3.17) \quad L(\psi, \psi^*) = A(\ln(\psi \psi^*) - 1),$$

then

$$(3.18) \quad G(\psi, \psi^*) = A \ln(\psi \psi^*).$$



The application of the Noether theorem to the Lagrangian (3.14) gives us the following results:

1. *Conservation of energy*

the energy density

$$(3.19) \quad \epsilon = \frac{\tilde{\hbar}^2}{2m} \partial_\alpha \psi \partial_\alpha \psi^* + U(\mathbf{x}) \psi \psi^* + L(\psi, \psi^*) \psi \psi^*,$$

the energy flux density

$$(3.20) \quad J_\alpha = -\frac{\tilde{\hbar}^2}{2m} (\partial_\alpha \psi \partial_t \psi^* + \partial_\alpha \psi^* \partial_t \psi),$$

and the conservation law gives us the known Euler-Lagrange equations (3.15) again.

2. *Conservation of linear momentum*

density vector of the linear momentum

$$(3.21) \quad p_\alpha = -\frac{i\tilde{\hbar}}{2} (\psi^* \partial_\alpha \psi - \psi \partial_\alpha \psi^*),$$

density tensor of the flux of the linear momentum (stress)

$$(3.22) \quad \sigma_{\alpha\beta} = \frac{\tilde{\hbar}^2}{2m} (\partial_\alpha \psi^* \partial_\beta \psi + \partial_\alpha \psi \partial_\beta \psi^*) + l \delta_{\alpha\beta}.$$

Momentum balance is due, of course, to a vanishing external force

$$(3.23) \quad \mathbf{F}(\mathbf{x}, t) = -\nabla U(\mathbf{x}, t) = \mathbf{0}.$$

3. *Conservation of mass*

mass-like density

$$(3.24) \quad \rho = -\tilde{\hbar} \Lambda \psi \psi^*,$$

mass-like flux density

$$(3.25) \quad j_\alpha = -i\Lambda \frac{\tilde{\hbar}^2}{2m} (\psi \partial_\alpha \psi^* - \psi^* \partial_\alpha \psi).$$

When we put

$$(3.26) \quad \Lambda = -\frac{\rho_0}{\tilde{\hbar}},$$

then

$$(3.27) \quad \begin{aligned} \rho &= \rho_0 \psi \psi^*, \\ j_\alpha &= -\frac{i\tilde{\hbar}}{2m} \rho_0 (\psi \partial_\alpha \psi^* - \psi^* \partial_\alpha \psi). \end{aligned}$$

The conservation law gives the law of the mass conservation (the continuity equation)

$$(3.28) \quad \partial_t \rho + \operatorname{div}(\rho \mathbf{v}) = 0,$$

where

$$(3.29) \quad v_\alpha = \frac{i\hbar}{2m} \left( \frac{1}{\psi^*} \partial_\alpha \psi^* - \frac{1}{\psi} \partial_\alpha \psi \right) = \frac{i\hbar}{2m} \partial_\alpha \ln \left( \frac{\psi^*}{\psi} \right) = 2D \partial_\alpha S(\mathbf{x}, t).$$

To complete our analysis we rewrite the rest of densities and fluxes as expressed in the old system of variables:

energy

$$(3.30) \quad \begin{aligned} \varrho_0 \epsilon &= \varrho \left( \frac{1}{2} m(u^2 + v^2) + U(\mathbf{x}) + L(\psi, \psi^*) \right), \\ \varrho_0 J_\alpha &= -\varrho 2mD^2 (v_\alpha \partial_t S(\mathbf{x}, t) - u_\alpha \partial_t R(\mathbf{x}, t)), \end{aligned}$$

momentum

$$(3.31) \quad \begin{aligned} \varrho_0 p_\alpha &= \varrho m v_\alpha, \\ \varrho_0 \sigma_{\alpha\beta} &= -\varrho \delta_{\alpha\beta} \left( 2mD \partial_t S + \frac{1}{2} m(u^2 + v^2) + U + L \right) + m\varrho (u_\alpha u_\beta + v_\alpha v_\beta). \end{aligned}$$

#### 4. The second variation

We use in our analysis the tools applicable in the calculus of variations. It is known from the ordinary theory of maxima and minima that the necessary condition for the functional to have an extremum is the vanishing of its first variation (what is ensured by the Euler–Lagrange equations) and that its second variation for the solutions of the Euler–Lagrange equations should be [16]

$$(4.1) \quad \delta^2 J = \begin{cases} \geq 0 & \text{for the minimum,} \\ \leq 0 & \text{for the maximum.} \end{cases}$$

Let us assume the following form of the variation of the process [12]

$$(4.2) \quad \delta\psi_i(\mathbf{x}, t) = \varepsilon \eta_i(\mathbf{x}, t), \quad i = 1, \dots, N,$$

where

$$(4.3) \quad \eta_i(\mathbf{x}, t) = \left. \frac{\partial \psi_i(\mathbf{x}, t, \varepsilon)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad i = 1, \dots, N,$$

and  $\psi_i(\mathbf{x}, t, \varepsilon)$  is the one-parameter family of real processes, such that

$$(4.4) \quad \psi_i(\mathbf{x}, t, 0) = \psi_i(\mathbf{x}, t).$$

It follows that

$$(4.5) \quad \delta(\partial_\alpha \psi_i(\mathbf{x}, t)) = \varepsilon \partial_\alpha \eta_i(\mathbf{x}, t) = \partial_\alpha (\delta\psi_i(\mathbf{x}, t)).$$

If we admit that the action functional is twice differentiable, we can write

$$(4.6) \quad \delta J = \delta^1 J + \delta^2 J + \beta(\delta\psi)^2,$$

where now

$$(4.7) \quad J = J(\psi, \partial\psi, \delta\psi, \delta^2\psi),$$

$$(4.8) \quad \lim_{\delta\psi \rightarrow 0} \beta = 0,$$

$$(4.9) \quad \delta^1 J = \varepsilon \left. \frac{d}{d\varepsilon} J \right|_{\varepsilon=0} = \int_{t_1}^{t_2} dt \int_{\mathcal{D}} dV(\mathbf{x}) \left( \frac{\partial l}{\partial \psi_i} \delta\psi_i + \frac{\partial l}{\partial (\partial_\alpha \psi_i)} \delta(\partial_\alpha \psi_i) \right),$$

$$(4.10) \quad \delta^2 J = \frac{\varepsilon^2}{2} \left. \frac{d^2}{d\varepsilon^2} J \right|_{\varepsilon=0} \\ = \frac{1}{2} \int_{t_1}^{t_2} dt \int_{\mathcal{D}} dV(\mathbf{x}) \left( \frac{\partial^2 l}{\partial \psi_i \partial \psi_j} \delta\psi_i \delta\psi_j + 2 \frac{\partial^2 l}{\partial \psi_i \partial (\partial_\alpha \psi_j)} \delta\psi_i \delta(\partial_\alpha \psi_j) \right. \\ \left. + \frac{\partial^2 l}{\partial (\partial_\alpha \psi_i) \partial (\partial_\beta \psi_j)} \delta(\partial_\alpha \psi_i) \delta(\partial_\beta \psi_j) \right).$$

In the calculus of variations the study of the second variation is called the accessory extremal problem and is considered as the variational problem per se. One can attach to every differential equation its variational equation. The variational equations of the Euler–Lagrange Equations (1.4) are the Jacobi equations

$$(4.11) \quad \Omega_i = d_t \frac{\partial \Omega}{\partial (\partial_t \eta_i)} + \sum_{\alpha=1}^3 d_\alpha \frac{\partial \Omega}{\partial (\partial_\alpha \eta_i)} - \frac{\partial \Omega}{\partial \eta_i} = 0, \quad i = 1, \dots, N.$$

The kernel  $\Omega$  has the form

$$(4.12) \quad 2\Omega(\mathbf{x}, t; \psi, \partial\psi; \eta, \partial\eta) = \sum_{i,j=1}^N \frac{\partial^2 l}{\partial \psi_i \partial \psi_j} \eta_i \eta_j + \sum_{\alpha=0}^3 \frac{2\partial^2 l}{\partial \psi_i \partial (\partial_\alpha \psi_j)} \eta_i \partial_\alpha \eta_j \\ + \sum_{\alpha,\beta=0}^3 \frac{\partial^2 l}{\partial (\partial_\alpha \psi_i) \partial (\partial_\beta \psi_j)} \partial_\alpha \eta_i \partial_\beta \eta_j.$$

Here  $x^0 = t$ ,  $x^1 = x$ ,  $x^2 = y$ ,  $x^3 = z$ . The variations  $\eta_i(\mathbf{x}, t)$  are the solutions of the Jacobi equations.

Making use of the Euler formula for the homogeneous function of the second degree and of the Jacobi equations (4.11), one can obtain the non-homogeneous balance equations [2]

$$(4.13) \quad \partial_t s + \text{div} \mathbf{J} = \sigma,$$

where density  $s$ , flux  $\mathbf{J}$  and production rate density  $\sigma$  are given by the following formulae:

density

$$(4.14) \quad s = \sum_{i=1}^N \frac{\partial \Omega}{\partial (\partial_t \eta_i)} \eta_i,$$

flux

$$(4.15) \quad J_\alpha = \sum_{i=1}^N \frac{\partial \Omega}{\partial (\partial_\alpha \eta_i)} \eta_i,$$

production rate density

$$(4.16) \quad \sigma = 2\Omega, \quad (\epsilon)$$

or, equivalently,

$$(4.17) \quad s = \mathcal{D}_i \frac{\partial I}{\partial(\partial_t \psi_i)},$$

$$J = \mathcal{D}_i \frac{\partial I}{\partial(\partial_\alpha \psi_i)},$$

where

$$(4.18) \quad \mathcal{D}_i = \eta_i \left( \eta_j \frac{\partial}{\partial \psi_j} + \partial_t \eta_j \frac{\partial}{\partial(\partial_t \psi_j)} + \partial_\beta \eta_j \frac{\partial}{\partial(\partial_\beta \psi_j)} \right), \quad \beta = 1, 2, 3.$$

ANTHONY [2] calls the quantity  $s$  “entropy” if the perturbation  $\eta$  are assumed in the form

$$(4.19) \quad \eta = iA\psi, \quad \eta^* = -iA\psi^*,$$

which is due to the gauge invariance of the Lagrangian.

For our Lagrange density (3.14) and the gauge transformation (1.10) of the function  $\psi$  and Eq. (1.11) of the function  $\psi^*$ , the kernel  $\Omega$  has the following form

$$(4.20) \quad \Omega = \frac{i\tilde{\hbar}}{2} (\eta^* \partial_t \eta - \eta \partial_t \eta^*) - \frac{\tilde{\hbar}^2}{2m} \partial_\alpha \eta \partial_\alpha \eta^* - U(\mathbf{x}) \eta \eta^* - L(\psi, \psi^*) \eta \eta^* - N,$$

$\alpha = 1, 2, 3,$

where

$$(4.21) \quad N = \left( \psi \frac{\partial L}{\partial \psi} + \psi^* \frac{\partial L}{\partial \psi^*} + \psi \psi^* \frac{\partial^2 L}{\partial \psi \partial \psi^*} \right) \eta \eta^*$$

$$+ \frac{1}{2} \left[ \psi^* \left( \psi \frac{\partial^2 L}{\partial \psi^2} + 2 \frac{\partial L}{\partial \psi} \right) \eta^2 + \psi \left( \psi^* \frac{\partial^2 L}{\partial \psi^{*2}} + 2 \frac{\partial L}{\partial \psi^*} \right) \eta^{*2} \right].$$

It is obtained from Eqs. (4.14) and (4.15) that

$$(4.22) \quad s = 0,$$

$$(4.23) \quad J_\alpha = -\frac{\tilde{\hbar}^2}{2m} (\eta \partial_\alpha \eta^* + \eta^* \partial_\alpha \eta), \quad \alpha = 1, 2, 3.$$

The balance equation (4.13) gives the following condition for the potential  $L(\psi, \psi^*)$

$$(4.24) \quad \psi^* \frac{\partial L}{\partial \psi^*} + \psi \frac{\partial L}{\partial \psi} + \psi^2 \frac{\partial^2 L}{\partial \psi^2} + \psi^{*2} \frac{\partial^2 L}{\partial \psi^{*2}} - 2\psi \psi^* \frac{\partial^2 L}{\partial \psi \partial \psi^*} = 0$$

or

$$(4.25) \quad \left( \psi \frac{\partial}{\partial \psi} - \psi^* \frac{\partial}{\partial \psi^*} \right)^2 L = 0.$$

Thus, as it follows from Eq. (3.16), Eq. (4.25) gives us no new information about  $L(\psi, \psi^*)$ .

It is worth mentioning that the non-vanishing density  $s$ , following from Eq. (4.14), in ANTHONY'S paper [2] is due to the "divergent" term

$$(4.26) \quad \frac{T_0}{2\psi\psi^*} \ln\left(\frac{\psi\psi^*}{T_0}\right) \partial_t(\psi\psi^*),$$

in his Lagrangian for the heat conduction. The non-homogeneous balance equation (4.13) gives the Fourier heat conductivity equation

$$(4.27) \quad c \partial_t T - \lambda^{\alpha\beta} \partial_\alpha \partial_\beta T = 0,$$

the already known Euler-Lagrange equation. The quantities  $s$ ,  $J_\alpha$  and  $\sigma$  written in the variables  $(\varphi, T)$  equal zero from the very beginning. A very similar situation can be observed also in our case. Equation (4.13) with  $\eta$  and  $\eta^*$  defined by Eq. (4.19) gives in fact the following equation

$$(4.28) \quad \psi^* \left( -i\tilde{h} \partial_t \psi - \frac{\tilde{h}^2}{2m} \partial_\alpha \partial_\alpha \psi + U(\mathbf{x})\psi + G(\psi, \psi^*)\psi \right) \\ + \psi \left( i\tilde{h} \partial_t \psi^* - \frac{\tilde{h}^2}{2m} \partial_\alpha \partial_\alpha \psi^* + U(\mathbf{x})\psi^* + G(\psi, \psi^*)\psi^* \right) \\ - \psi\psi^* \left( \psi \frac{\partial}{\partial \psi} - \psi^* \frac{\partial}{\partial \psi^*} \right)^2 L(\psi, \psi^*) = 0.$$

We already know that all three terms equal zero because of the Euler-Lagrange equations and on the basis of the condition (3.16), respectively. It is easy to see, however, that one can rearrange Eq. (4.28) to Anthony's "entropy" balance equation (4.13) with

$$(4.29) \quad s = -i\tilde{h} \ln\left(\frac{\psi^*}{\psi}\right), \\ J_\alpha = \frac{\tilde{h}^2}{2m} \frac{1}{\psi\psi^*} (\psi^* \partial_\alpha \psi + \psi \partial_\alpha \psi^*), \\ \sigma = \frac{\tilde{h}^2}{2m} \frac{1}{(\psi\psi^*)^2} (\psi^{*2} \partial_\alpha \psi \partial_\alpha \psi + \psi^2 \partial_\alpha \psi^* \partial_\alpha \psi^*) - 2(U(\mathbf{x}) + G(\psi, \psi^*)),$$

or, in the old system of variables,

$$(4.30) \quad s = 2mDS(\mathbf{x}, t), \\ J_\alpha = mDu_\alpha(\mathbf{x}, t) = -2mD^2 \partial_\alpha R(\mathbf{x}, t), \\ \sigma = -\frac{m}{2} (\mathbf{v}^2 - \mathbf{u}^2) - U(\mathbf{x}) - G(\psi, \psi^*) = -2mD^2((\nabla S)^2 - (\nabla R)^2) - U - G.$$

We have found that the potential  $G(\psi, \psi^*)$ , (compare Eqs. (3.9), (3.12) and (3.16)) admissible from the Lagrange formalism point of view had a form

$$(4.31) \quad G(\psi\psi^*) = \frac{\tilde{h}}{2\tau} \ln(\psi\psi^*)$$

and that the term

$$(4.32) \quad i \ln\left(\frac{\psi^*}{\psi}\right)$$

in our potential (2.19) should vanish. This means that the peculiar velocity

$$(4.33) \quad \mathbf{v}(\mathbf{x}, t) = \frac{i\hbar}{2m} \nabla \ln \left( \frac{\psi^*}{\psi} \right),$$

vanishes too. This situation corresponds to the stationary case,  $\varrho = \varrho(\mathbf{x})$  which is characteristic for the dissipative structures (compare the discussion in [7] and [9]). It follows from Eqs. (2.11)<sub>1</sub> and (2.19) that the potential  $S(\mathbf{x}, t)$  can be represented as

$$(4.34) \quad S = C(t).$$

If we accept that

$$(4.35) \quad \begin{aligned} C(t) &= 2Ft/\hbar, \\ U(\mathbf{x}, t) &= U_0(\mathbf{x}), \end{aligned}$$

then our wave function has the form of a stationary solution

$$(4.36) \quad \begin{aligned} \psi(\mathbf{x}, t) &= \phi(\mathbf{x}) e^{-\frac{iFt}{\hbar}}, \\ \phi^2(\mathbf{x}) &= \frac{\varrho(\mathbf{x})}{\varrho_0}, \end{aligned}$$

and our Schrödinger-like equation takes the following form

$$(4.37) \quad D\Delta\phi = \frac{\phi \ln \phi}{\tau} + \frac{1}{\hbar} (U_0 - F)\phi.$$

Let us have a look at the notion of the entropy from the phenomenological point of view. With the measurable function  $p(\mathbf{x})$ , called density, such that

$$(4.38) \quad \int_{R^3} p(\mathbf{x}) dV(\mathbf{x}) = 1,$$

is connected the statistical entropy of the density  $p(\mathbf{x})$  defined as follows [17]

$$(4.39) \quad \mathcal{S}(p) = \int_{R^3} d\mathcal{S}(p(\mathbf{x})),$$

where

$$(4.40) \quad d\mathcal{S}(p(\mathbf{x})) = p_0 \eta \left( \frac{p(\mathbf{x})}{p_0} \right) dV(\mathbf{x}),$$

and

$$(4.41) \quad \eta(a) = \begin{cases} -ka \ln a & \text{for } a > 0, \\ 0 & \text{for } a = 0. \end{cases}$$

Because of the correspondence

$$(4.42) \quad \frac{p(\mathbf{x})}{p_0} = \frac{\varrho(\mathbf{x})}{\varrho_0},$$

we can rewrite Eq. (4.39) as

$$(4.43) \quad \mathcal{S}(\varrho) = -k \int_{R^3} \varrho(\mathbf{x}) \ln \left( \frac{\varrho(\mathbf{x})}{\varrho_0} \right) dV(\mathbf{x}) = -k \langle \ln \left( \frac{\varrho(\mathbf{x})}{\varrho_0} \right) \rangle.$$

We use here the following notation for the mean value of a function  $f(\mathbf{x})$  as

$$(4.44) \quad \langle f(\mathbf{x}) \rangle = \int_{R^3} f(\mathbf{x}) \varrho(\mathbf{x}) dV(\mathbf{x}).$$

The rate of the mean value is given by the formula

$$(4.45) \quad \frac{d\langle f \rangle}{dt} = \int_{R^3} \left( \frac{\partial f}{\partial t} \varrho + f \frac{\partial \varrho}{\partial t} \right) dV(\mathbf{x}) = \left\langle \frac{\partial f}{\partial t} + \mathbf{v} \nabla f \right\rangle,$$

where we have made use of the continuity equation (2.17).

It is obtained for  $f = k \ln(\varrho/\varrho_0)$  that

$$(4.46) \quad \frac{d\mathcal{S}(\varrho)}{dt} = k \int_{R^3} \varrho \nabla \mathbf{v} dV(\mathbf{x}) = 2kD \langle \Delta S \rangle.$$

In the stationary case  $\partial_t \varrho = 0$ , and if we make use of Eq. (2.17) once again, we obtain that

$$(4.47) \quad \left. \frac{d\mathcal{S}}{dt} \right|_{st} = \frac{1}{D} \int_{R^3} \mathbf{u} \mathbf{v} dV(\mathbf{x}).$$

It follows that one can hardly interpret Eq. (4.30) as being directly connected with the entropy. It is seen, on the other hand, that Eqs. (4.13) and (4.34) give

$$(4.48) \quad \partial_t S = D \Delta R - D((\nabla S)^2 - (\nabla R)^2) - \frac{U+G}{2Dm}.$$

This is a very important result from the methodological point of view. We see that studying the second variation enables to find the proper form of the Lagrangian. This fact is already recognized in the inverse problem of the calculus of variations.

## 5. Conclusions

In the paper we tried to incorporate the process of diffusion of crystal lattice defects described by the nonlinear equation of motion into Lagrange formalism. The approach has been only partially successful: the obtained Lagrangian merely describes the stationary distributions of defects.

It was hoped that the form of the equation of motion would be a full success. It was the nonlinear Schrödinger-like equation and it was known that for the Schrödinger equation the Lagrangian exists. Why then did our procedure fail? To answer this question, one has to find the interpretation of the variable  $\varphi(\mathbf{x}, t)$  in the papers of ANTHONY [2–5]. It is seen, especially from the paper [5], that one can interpret  $\varphi$  as the parameter describing the distance from the equilibrium state. In our case we also have a quantity which describes

the departure from the equilibrium — this is the drift velocity  $\mathbf{b}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t)$ . But the parameter  $\varphi$  has one more meaning: it embodies explicitly the influence of all parameters not included into the main equation of motion, environment inclusively. In this sense it "closes" the system. The idea is to incorporate the irreversible (dissipative) processes into the Lagrange formalism. The dissipation takes place in an enormous number of ways, but we can always say that it occurs as the transfer of the energy from the one to other degrees of freedom of the system. It follows that the definition of the regarded system is very important. The process is irreversible if there is no way to restore both the system and its *environment* to their respective initial states [18]. That is why the environment in the wide sense should be included into future investigations.

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### Appendix

THEOREM [11]. *The set of  $N$  functions*

$$I_k \equiv \sum_{i=1}^N \sum_{\alpha, \beta=0}^3 (A_{ki}^{\alpha\beta}(\mathbf{x}, \psi, \partial\psi) \partial_\alpha \partial_\beta \psi^i + B_k(\mathbf{x}, \psi, \partial\psi)), \quad k = 1, \dots, N,$$

is then and only then self-adjoint when the following identities are fulfilled:

$$(A.1) \quad A_{[ki]}^{\alpha\beta} \Big|_{\mathbf{x}, \psi, \partial\psi} \equiv 0,$$

$$(A.2) \quad \frac{\partial A_{ij}^{\alpha\beta}}{\partial(\partial_\gamma \psi^k)} \Big|_{(ik) \mathbf{x}, \psi, \partial\psi} \equiv \frac{\partial A_{ik}^{\alpha\gamma}}{\partial(\partial_\beta \psi^j)} \Big|_{(\alpha\beta)},$$

$$(A.3) \quad \left( \frac{\partial^2 A_{ij}^{\alpha\beta}}{\partial(\partial_\mu \psi^k) \partial(\partial_\nu \psi^l)} \Big|_{(\mu\nu) [ik] \mathbf{x}, \psi, \partial\psi} \right) \equiv \left( \frac{\partial^2 A_{ki}^{\mu\nu}}{\partial(\partial_\alpha \psi^i) \partial(\partial_\beta \psi^j)} \Big|_{(\alpha\beta) [ik]} \right),$$

$$(A.4) \quad \frac{\partial B_i}{\partial(\partial_\alpha \psi^k)} \Big|_{(ik) \mathbf{x}, \psi, \partial\psi} \equiv \left( \frac{\partial}{\partial x_{ex}^\beta} + \partial_\beta \psi^j \frac{\partial}{\partial \psi^j} \right) A_{ik}^{\alpha\beta},$$

$$(A.5) \quad 2 \frac{\partial B_i}{\partial \psi^k} \Big|_{[ik] \mathbf{x}, \psi, \partial\psi} \equiv \left( \frac{\partial}{\partial x_{ex}^\alpha} + \partial_\alpha \psi^j \frac{\partial}{\partial \psi^j} \right) \frac{\partial B_i}{\partial(\partial_\alpha \psi^k)} \Big|_{[ik]}.$$

Here  $\psi_i$ ,  $i = 1, \dots, N$  are functions of independent variables  $x^\alpha$ ,  $\alpha = 0, 1, 2, 3$ , ( $x^0 = t$ ,  $x^1 = x$ ,  $x^2 = y$ ,  $x^3 = z$ ). By  $\partial/\partial x_{ex}^\beta$  the explicit differentiation is understood.

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