International Journal of Theoretical Physics, Vol. 24, No. 6, 1985

Nonlinear Diffusion and Nelson–Brown Movement

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Received January 2, 1985

The nonlinear diffusion process, which can be described as the Nelson–Brown motion, is considered. The obtained equation becomes the classical linear diffusion equation for small relaxation times, and for long relaxation times it is transferred into the Schrödinger-like equation. The possible nonequilibrium stationary states are discussed.

1. INTRODUCTION

The influence of an external field acting on a point defect is described in the classical formulation of the diffusion theory by the Stokes relation

$$\mathbf{F}=\zeta\mathbf{b} \tag{1}$$

which connects the force $\mathbf{F}$ acting on a point defect with its mean velocity $\mathbf{b}$. The coefficient $1/\zeta$ is called the mobility of the defect. The Stokes relation, from the Newtonian mechanics point of view, is an approximation in which the inertial effects are neglected. Thus there seems to be a need of formulating a theory that fuses the collective description of atoms' behavior, manifesting itself in the existence of the diffusion flux, with the Newtonian dynamics of a single atom.

The clue is the Schrödinger equation

$$i\hbar\partial_t\psi=-\hbar^2\,\Delta\psi/2m+U\psi \tag{2}$$

where $\hbar=h/2\pi$ is the reduced Planck constant. The above equation joins together the direct information about the dynamics of a material point in R^3 (its mass m, potential of external forces U) with information about the "condensation" degree of subsets of R^3 with results of space localization tests of this material point. One can imagine these subsets as "clouds" of differential density.

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0020-7748/85/0600-0533$04.50/0

The diffusion process also has to do with "clouds," but this time with real clouds of particles taking part in the diffusion.

On the other hand there exists a method called stochastic quantization, used to derive equation (2) by means of the diffusion Markov process (Nelson, 1966). It is well known that the Markov process can sometimes approximate well a movement of a particle taking part in a diffusion process (Girhman and Skorokhod, 1968; Stepunovitch and Ulitzkij, 1978). This theoretical situation suggests that equation (2) obtained in such a manner describes rather a certain nonlinear diffusion process than quantum phenomena (cf. Mielnik and Tengstrand, 1983). In this case there should be introduced, instead of the reduced Planck constant $\hbar$, a certain parameter $\hbar$ which, for real physical processes, should not reach the value of $\hbar$. The parameter $\hbar$ is given in the form (e.g., Ghirardi et al., 1978)

$$\hbar = m\sigma^2 \tag{3}$$

where m is the mass of an atom and σ^2 is the variance parameter of the stochastic variable of the Markov diffusion process.

It is shown in this paper that the stochastic quantization method allows us, in the presence of a special form of an external field, to construct a nonlinear equation of the form (2) but with the constant $\hbar$ instead of $\hbar$,

$$\hbar = 2Dm \tag{4}$$

where D is the diffusion coefficient and

$$U \to V = V(\psi, \mathbf{x}, t) = U(\mathbf{x}, t) + \hbar V_0(\psi)/2\tau \tag{5}$$

where τ is a constant having the dimension of time and meaning of a relaxation time. The equation obtained,

$$i\hbar\partial_t\psi = -\hbar^2 \Delta\psi/2m + V\psi \tag{6}$$

becomes equivalent to the classical equation of linear diffusion, i.e., it is based on the relation (1) for very small relaxation times ($\tau \to 0$) and transforms into the equation

$$i\hbar\partial_t\psi = -\hbar^2 \Delta\psi/2m + U\psi \tag{7}$$

for processes with very long relaxation times ($\tau \to \infty$). Thus equation (6) describes the nonlinear diffusion processes for finite relaxation times. The existence of an equation with such properties brings closer the answer to the question at the end of the paper of Mielnik and Tengstrand (1983): "What precisely is the Nelson scheme? Is it only a formal art? Or, perhaps, an emerging fragment of a yet undiscovered theory?."

2. DIFFUSION AS STOCHASTIC PROCESS

It is well known (Flynn, 1972; Christian, 1975) that diffusion can be regarded in many cases as a random motion of a particle. Such an approach is justified for crystal solid bodies if one considers:

2.1. Thermally Activated Point Defects (Flynn, 1972)

Atoms in crystal lattice, excited by thermal energy, vibrate around their averaged in time positions. Certain types of the fluctuations can cause the displacements of atoms into interstitial positions where they can find new equilibrium positions. These interstitial atoms are called thermally activated point defects. Then, with the help of the fluctuations, they can migrate into new interstitial positions. However, the mean number of atoms moving in various directions is equal, so finally we can observe a chaotic movement and mixture of atoms but without any of their macroscopic flux. The thermally activated defects exist in equilibrium crystal structure in nonzero absolute temperature.

2.2. Self-Diffusion Phenomenon (Christian, 1975; Smirnov, 1982)

If a chemical element creating a crystalline substance is a mixture of isotopes [which occurs to most elements (Scholz, 1968)] there is still the possibility that there exists a nonzero gradient of one of the isotopes concentration in the otherwise perfect body. Diffusion forced by the described situation is called a self-diffusion (of an isotope). Atom displacements in the macroscopic self-diffusion process are equivalent to random walk. Let us remark that in this case the so-called vacancy mechanism is the main mechanism of diffusion, which means that the elementary act of diffusion consists in exchanging the atom and vacancy positions: atom moves replacing sequentially empty crystal lattice nodes.

2.3. Chemical Diffusion with Small Concentrations (Christian, 1975; Smirnov, 1982)

The case of a chemical diffusion (called also mutual diffusion) takes place in alloys which are not in an equilibrium state with respect to the distribution of different constituents. If in an alloy the atoms of one element are in the interstitial positions of another element crystal lattice, then the chemical diffusion can be regarded as a random walk. It follows from the fact that in such alloys the inserted atoms (so-called extra matter) are much smaller than the matrix atoms. Moreover, their concentration is usually small too and therefore we can neglect their interactions. In this case diffusion has the thermally activated interstitial random walk character and sequential jumps of atoms from one interstitial position into another can be regarded as independent random events.

The diffusion process is described in a macroscale by the function $n = n(\mathbf{x}, t)$, called a volume concentration of a matter taking part in the diffusion ($[n] = \mathrm{cm}^{-3}$). We are not interested in the influence of the boundary of a body, so we restrict our discussion to the infinite body identified with the R^3 space of positions of diffusing particles. At every instant of time $t \geq 0$ a finite but very large number of particles takes part in a diffusion process, i.e.,

$$\forall t \geq 0 \qquad N(t) = \int_{R^3} n(\mathbf{x}, t)\, dV(\mathbf{x}) < \infty \tag{8}$$

We consider the case of identical but distinguishable particles (remaining in the frames of the classical mechanics) with negligible interactions only. The last approximation is often made, for example for small concentrations of diffusing atoms in crystalline body (see, e.g., Smirnov, 1982).

We call a discrete $N(t)$-element subset of the space R^3 defined as positions of all diffusing particles at an instant of time $t \geq 0$ a microstate Ω_t.

We denote by $dp_t(\mathbf{x})$ the probability of observing at instant t a diffusing particle in a neighborhood of a point $\mathbf{x}$ with a volume $dV(\mathbf{x})$, and by $p(\mathbf{x}, t)$ the density of this probability, i.e.,

$$dp_t(\mathbf{x}) = p(\mathbf{x}, t)\, dV(\mathbf{x}) \tag{9}$$

It follows from the assumptions about the absence of interactions and identity of particles from a microstate Ω_t that the microstate can be identified with a $N(t)$-element statistical ensemble for a statistical variable $\mathbf{x}(t)$ defined as a position of a certain atom at an instant of time $t \geq 0$. Consequently, the probability $dp_t(\mathbf{x})$ can be calculated from the formula (Klimontovitch, 1982)

$$dp_t(\mathbf{x}) = \lim_{N(t)\to\infty} n(\mathbf{x}, t)\, dV(\mathbf{x})/N(t) \tag{10}$$

and the approximation is the better the greater $N(t)$ is. From equations (9) and (10) follows

$$p(\mathbf{x}, t) = n(\mathbf{x}, t)/N(t) \tag{11}$$

A mathematical model which relatively well describes a random walk of a diffusing particle in the presence of an external force field is the so-called diffusion Markov process (Girhman and Skorokhod, 1968; Stepunovitch and Ulitzkij, 1978). In our paper we constrain ourselves considering the diffusion Markov process defined by the stochastic Ito equation of a form

$$d\mathbf{x} = \mathbf{b}(\mathbf{x}, t)\, dt + d\mathbf{W}(t) \tag{12}$$

where $\mathbf{W}=\mathbf{W}(t)$ is a Wiener process in R^3. This means that $\mathbf{W}$ is the uniform Gaussian process with independent increments for which

$$\mathbf{W}(0)=\mathbf{0}, \qquad E[\mathbf{W}(t)]=\mathbf{0}$$
$$E[\mathbf{W}(t)\otimes\mathbf{W}(t)]=\sigma^2 tI, \qquad t\geq 0, \sigma^2>0 \tag{13}$$

where E is the expectation value operator and I is a unit matrix. It follows that

$$E_{\mathbf{x}(t)}[d\mathbf{x}(t)]=\mathbf{b}(\mathbf{x}, t)\,dt \tag{14}$$
$$E_{\mathbf{x}(t)}[(d\mathbf{x}(t)-\mathbf{b}(\mathbf{x}, t)\,dt)\otimes(d\mathbf{x}(t)-\mathbf{b}(\mathbf{x}, t)\,dt)]=\sigma^2\,dtI$$

where $E_{\mathbf{x}(t)}$ is a conditional expectation value operator. Equation (14) means that solution $\mathbf{x}(t)$, $t\geq 0$, of the stochastic Ito equation (12) is a random process in R^3, stochastically uniform and isotropic. The components $x_i(t)$, $i=1,2,3$, for $t\geq 0$ in the orthonormal Cartesian coordinate system in R^3 are incorrelated random variables.

The probability $P(\mathbf{x}(t)\in\mathcal{P})$ that there exists a trajectory of the Ito equation which cuts a set $\mathcal{P}\subset R^3$ at the time instant t and in the position $\mathbf{x}(t)$ is of the form

$$P(\mathbf{x}(t)\in\mathcal{P})=\int_{\mathcal{P}} p(\mathbf{x}, t)\,dV(\mathbf{x}) \tag{15}$$

where the probability density fulfils the Fokker–Planck equation (Ghiradi et al., 1978):

$$\partial_t p=\tfrac{1}{2}\sigma^2\,\Delta p-\operatorname{div}(p\mathbf{b}) \tag{16}$$

According to our assumptions, the probability density $p(\mathbf{x}, t)$ is connected with the volume concentration $n(\mathbf{x}, t)$ of the diffusing particles with the help of equation (11). Thus the condition (8) is equivalent to the probabilistic measure normalization condition

$$P(\mathbf{x}(t)\in R^3)=1 \tag{17}$$

When the proper assumptions about the function $\mathbf{b}(\mathbf{x}, t)$ are made, the solution of the equation (12), with the initial condition $\mathbf{x}(0)=\mathbf{x}_0\in R^3$, exists, it is continuous and unique defined with the probability 1 (Nelson, 1967; Girhman and Skorokhod, 1968). In many very important cases the solution $\mathbf{x}(t)$ is not differentiable and we need a substitute for the derivative (Nelson, 1966).

Let $f=f(\mathbf{x}, t)$ be a smooth vector or scalar function. By D_+ and D_- we denote the operators of stochastic differentiation along the trajectory

$\mathbf{x}(t)$, $t \geq 0$, of the Ito equation, which are by definition

$$\begin{aligned} D_+ f(\mathbf{x}(t), t) &= \lim_{h \to 0_+} E_{\mathbf{x}(t)}[\{f(\mathbf{x}(t+h), t+h) - f(\mathbf{x}(t), t)\}/h] \\ D_- f(\mathbf{x}(t), t) &= \lim_{h \to 0_-} E_{\mathbf{x}(t)}[\{f(\mathbf{x}(t), t) - f(\mathbf{x}(t-h), t-h)\}/h] \end{aligned} \tag{18}$$

Thus

$$\begin{aligned} D_+ &= \partial_t + \mathbf{b}(\mathbf{x}, t) \cdot \nabla + (\sigma^2/2)\Delta \\ D_- &= \partial_t + \mathbf{b}_*(\mathbf{x}, t) \cdot \nabla - (\sigma^2/2)\Delta \end{aligned} \tag{19}$$

where we denote

$$\mathbf{b}_*(\mathbf{x}, t) = \mathbf{b}(\mathbf{x}, t) - \sigma^2 \frac{\nabla p(\mathbf{x}, t)}{p(\mathbf{x}, t)} \tag{20}$$

We have for the trajectory of the Ito equation

$$\begin{aligned} D_+ \mathbf{x}(t) &= \mathbf{b}(\mathbf{x}(t), t) \\ D_- \mathbf{x}(t) &= \mathbf{b}_*(\mathbf{x}(t), t) \end{aligned} \tag{21}$$

The operators D_+ and D_- represent the future and past of the diffusion Markov process, respectively. Particularly, at every instant of time t there exist two mean velocities of the wandering particle: (i) velocity $\mathbf{b}_*$ with which the particle arrives at the point $\mathbf{x}$; (ii) velocity $\mathbf{b}$ with which the particle starts from the point $\mathbf{x}$.

We introduce the notation

$$\begin{aligned} \mathbf{v}(\mathbf{x}, t) &= [\mathbf{b}_*(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t)]/2 \\ \mathbf{u}(\mathbf{x}, t) &= [\mathbf{b}_*(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}, t)]/2 \end{aligned} \tag{22}$$

In this case

$$\mathbf{u} = -\sigma^2 \frac{\nabla p}{2p} \tag{23}$$

and

$$\mathbf{u} = \mathbf{v} - \mathbf{b} \tag{24}$$

In the literature concerning the diffusion theory, the velocity $\mathbf{b}(\mathbf{x}, t)$ is called the mean velocity, while the velocity $\mathbf{b}_*(\mathbf{x}, t)$ is not considered at all. In the mixture theory velocities analogous to $\mathbf{v}(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$ are discussed. They are called peculiar and diffusion velocities, respectively (Truesdell, 1969). In the literature referring to the stochastic quantization theory (e.g., Nelson, 1967), not the vector $\mathbf{u}(\mathbf{x}, t)$ is regarded but $-\mathbf{u}(\mathbf{x}, t)$, which is called the osmotic velocity. In our paper we use the terminology taken from the mixture theory.

One can relate to the stochastic Ito equation (12) an operator of the mean second derivative (Nelson, 1966; Nelson, 1967; Ghirardi et al., 1978)

$$A\mathbf{x}(t)=\tfrac{1}{2}(D_+D_-+D_-D_+)(\mathbf{x}(t)) \tag{25}$$

This operator is invariant with respect to the symmetry operation $t\to -t$. It follows from equations (19), (22), and (25) that along the trajectory of the Ito equation

$$A\mathbf{x}(t)=\mathbf{a}(\mathbf{x}(t), t) \tag{26}$$

where

$$\mathbf{a}=\partial_t\mathbf{v}+(\mathbf{v}\cdot\nabla)\mathbf{v}-(\mathbf{u}\cdot\nabla)\mathbf{u}+\tfrac{1}{2}\sigma^2\,\Delta \boldsymbol{u} \tag{27}$$

We call the field $\mathbf{a}(\mathbf{x}, t), \mathbf{x}\in R^3$, $t\geq 0$, the peculiar acceleration field of the diffusion Markov process.

3. MACROSCOPIC INTERPRETATION OF THE FOKKER–PLANCK EQUATION

It is assumed in the classical formulation of the diffusion theory that the mean velocity $\mathbf{b}(\mathbf{x}, t)$ is defined by the force $\mathbf{F}(\mathbf{x}, t)$ acting on the diffusing particle, according to the Stokes relation (1). Let us consider the case when

$$\mathbf{F}=\mathbf{F}(\mathbf{x})=-\nabla U_0(\mathbf{x}) \tag{28}$$

It follows from the Fokker–Planck equation (16) that a stationary probability distribution $p=p(\mathbf{x})$ such that

$$\lim_{|\mathbf{x}|\to\infty} p(\mathbf{x})=0 \tag{29}$$

is of the form (Haken, 1978)

$$p(\mathbf{x})=C\exp[-2U_0(\mathbf{x})/\zeta\sigma^2] \tag{30}$$

For the distribution $p(\mathbf{x})$ there should be the Boltzmann distribution, i.e., in order to describe a thermodynamical equilibrium state in the external field with the potential $U_0(\mathbf{x})$ and at the absolute temperature T, it should be

$$2/\zeta\sigma^2=1/kT \tag{31}$$

or, equivalently,

$$\sigma^2=2D \tag{32}$$

where

$$D = kT/\zeta \tag{33}$$

and k is the Boltzmann constant. Equation (33) is called the Einstein relation. It connects the self-diffusion coefficient D with the mobility of a diffusing particle $1/\zeta$. The diffusion coefficient of the form (33) can be also used as the chemical diffusion coefficient in ideal solutions (Smirnov, 1982). Our generalization consists in assuming that the relation (32) between the variance parameter σ^2 and the diffusion coefficient D is valid for an arbitrary diffusion process, which can be regarded as the random walk of a particle described by the Ito equation (12). In particular we use the relation (32) also in the case when the Stokes relation (1) does not hold any more.

Equations (11) and (32) allow us to write down the Fokker-Planck equation (16) in the form

$$\partial_t n = D\,\Delta n - \operatorname{div}(n\mathbf{b}) + \beta(t)n \tag{34}$$

where $\beta(t)$, $t \geq 0$, is the rate of the change of the total number of the diffusing particles

$$\beta(t) = \dot{N}(t)/N(t) \tag{35}$$

The function β describes, e.g., in the case of a chemical diffusion in an infinite body, the change of a number of diffusing particles caused by the increase or decay of gas inclusions by gas diffusion in metals.

Equation (34) is the diffusion equation with sources for isotropic bodies with respect to the diffusion phenomenon in the case of crystal bodies—for crystals with cubic lattices. The influence of the external field on the diffusion process is described by the function $\mathbf{b} = \mathbf{b}(\mathbf{x}, t)$. The coefficient D is understood as a certain phenomenological coefficient. Its particular form for every type of diffusion process can be determined from model microstructural considerations or from the experiment. If we consider a model in which diffusion is caused by thermofluctuations of interstitial atoms and a jump from one position into another follows when the energetic barrier is overcome, the diffusion coefficient D can be determined by the empirical Arrhenius formula

$$D = D(T) = D_0 \exp(-E_a/kT) \tag{36}$$

where the coefficients D_0 and E_a do not depend on the temperature T. In the chemical diffusion with the interstitial mechanism in the binary alloys with a cubic lattice and with a small concentration of interstitial atoms (process of the type 2.3) one can neglect interactions of diffusing particles and then (Smirnov, 1982)

$$D_0 = A_0 a^2/\tau_0 \tag{37}$$

Here a is a constant of a cubic lattice, A_0 is a coefficient depending on the geometrical properties of the interstitial distribution, and τ_0 is a constant with a dimension of time and of a value of the frequency vibrations of atoms in the interstitial positions, i.e., 10^{-13} sec. One can take approximately $D_0 = 10^{-2} \div 10^0$ cm^2/sec. E_a is the activation energy of the diffusion process defined as the elastic energy of a matrix necessary to expand the atoms of a crystal lattice by the interstitial atoms at zero absolute temperature. For the majority of metals $E_a/kT_m = 17 \div 19$, where T_m is the melting temperature (Bockstein, 1984).

Recapitulating, if the diffusion coefficient can be determined by the Einstein relation (33) the requirement of the Fokker–Planck equation (16) with the conditions (28) and (29) to define the Boltzmann probability distribution is equivalent to the identification of the Fokker–Planck and diffusion equations. In our paper we hold the requirement of equivalence of the Fokker–Planck equation (16) and the diffusion equation (34) with σ^2 defined by (32) but with D not of the form (33). This means that in a stationary case the Fokker–Planck equation defines the non-Boltzmann (nonequilibrium) probability distributions $p(\mathbf{x})$ of the form (30) and (32) when the Stokes relation is valid.

4. DIFFUSION AS THE NELSON–BROWN MOVEMENT

According to statements in the previous section let us consider the diffusion process which is described by the evolution equation of the mass density of the form [cf. equation (34)]

$$\partial_t \rho = D\Delta\rho - \operatorname{div}(\rho\mathbf{b}) + \beta(t)\rho \tag{38}$$

We denote [cf. equations (8) and (35)]

$$\begin{gathered} M(t) = \int_{R^3} \rho(\mathbf{x}, t)\, dV(\mathbf{x}) = M_0 \exp\left[\int_0^t \beta(s)\, ds\right] \\ \rho(\mathbf{x}, t) = mn(\mathbf{x}, t) \end{gathered} \tag{39}$$

where $n(\mathbf{x}, t)$ is the volume concentration of point defects with mass m, and $M_0 = M(0)$ is the total initial mass of the diffusing defects.

If we take into account that [cf. equations (11) and (39)]

$$p(\mathbf{x}, t) = \rho(\mathbf{x}, t)/M(t) \tag{40}$$

and [cf. equations (20), (22), (23), (24), and (32)]

$$\mathbf{u}(\mathbf{x}, t) = -D\nabla p(\mathbf{x}, t)/p(\mathbf{x}, t) = -D\nabla \ln[p(\mathbf{x}, t)/p_0] \tag{41}$$

where p_0 is an arbitrary constant with the dimension of $p(\mathbf{x}, t)$, we can rewrite equation (38) in the form of the continuity equation

$$\partial_t p + \operatorname{div}(p\mathbf{v}) = 0 \tag{42}$$

Let us consider the situation when the Stokes relation (1) is not valid, i.e., when the force $\mathbf{K}(\mathbf{x}, t)$ of the form[2]

$$\mathbf{K}(\mathbf{x}, t) = -\zeta\mathbf{b}(\mathbf{x}, t) + \mathbf{F}(\mathbf{x}, t) \tag{43}$$

does not vanish identically. The coefficient ζ appearing above is a certain friction coefficient describing the interaction of diffusing matter with a body, but we do not assume that the Einstein relation (33) obliges. We assume that the force $\mathbf{K}(\mathbf{x}, t)$ is the total force acting on a diffusing particle in the presence of an external field. Imitating the stochastic quantization method (Nelson, 1966; Nelson, 1967; Ghirardi et al., 1978; Yasue, 1978; Nishioka, 1983) we postulate the following relation between the anholonomic field of peculiar accelerations $\mathbf{a}(\mathbf{x}, t)$ $[\mathbf{a}(\mathbf{x}, t) \neq \ddot{\mathbf{x}}(t)]$ of a diffusing particle with the mass m and the field $\mathbf{K}(\mathbf{x}, t)$ of forces acting on that particle,

$$m\mathbf{a}(\mathbf{x}, t) = \mathbf{K}(\mathbf{x}, t) \tag{44}$$

where $\mathbf{a}(\mathbf{x}, t)$, $\mathbf{x} \in R^3$, $t \geqslant 0$, is defined by equations (27) and (32)

$$\mathbf{a} = \partial_t\mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} - (\mathbf{u} \cdot \nabla)\mathbf{u} + D\Delta\mathbf{u} \tag{45}$$

The dynamical condition defined by equations (43), (44), and (45) is called the Nelson relation.

If we take into account the fact that $\mathbf{u}$ is a potential field [equation (41)] and make use of the equations

$$\Delta\mathbf{u} = \nabla \operatorname{div} \mathbf{u} - \operatorname{rot} \operatorname{rot} \mathbf{u}, \qquad \nabla\mathbf{u}^2 = 2\mathbf{u}\nabla\mathbf{u}$$

the condition (44) can be rewritten in the form of the following evolution equation of the peculiar velocity vector $\mathbf{v}(\mathbf{x}, t)$

$$\partial_t\mathbf{v} = -(\mathbf{v} - \mathbf{u})/\tau - \nabla[D \operatorname{div} \mathbf{u} + (\mathbf{v}^2 - \mathbf{u}^2)/2] + \mathbf{F}/m \tag{46}$$

where τ is a constant with a dimension of time and by definition

$$\tau = m/\zeta \tag{47}$$

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[2] The stochastic quantization method deals with one particle only. The particle has a mass m and moves without friction. That is the reason why $\mathbf{F}(\mathbf{x}, t)$ is considered as the total force (Nelson, 1966; Nelson, 1967; Ghirardi et al., 1978). Other forms of forces are discussed too (Yasue, 1978; Nishioka, 1983).

In statistical physics the constant τ is called the kinetic relaxation time and it is shown that if

$$\tau_* = dt = t - t_0 > 0 \tag{48}$$

is the length of the physically infinitely small interval of time which defines the scale of time for observations of the diffusion process, then for

$$\tau \ll \tau_* \tag{49}$$

the Stokes formula (1) can be accepted and the diffusion process can be considered as a quasistatic process, i.e., as a sequence of equilibrium states (Klimontovitch, 1982). It follows from equations (46) and (47) that τ has similar meaning, because the limit $\tau \to 0$ with $\zeta = \text{const}$ gives

$$\mathbf{b} = \mathbf{v} - \mathbf{u} = \mathbf{F}/\zeta \tag{50}$$

which together with equations (33) and (38) means the classical description of the diffusion phenomenon. If

$$\tau \geq \tau_* \tag{51}$$

the use of the Stokes relation is not justified (Klimontovitch, 1982). In that case we propose the description of the diffusion process based on the Nelson relation (43)–(45). This means that diffusion is described by the equations (40)–(42) and (46) or equivalently by (38) and (46), where the relation (24) is assumed and [cf. equations (40) and (41)]

$$\begin{gathered} \mathbf{u}(\mathbf{x}, t) = -D\nabla \rho(\mathbf{x}, t)/\rho(\mathbf{x}, t) = -D\nabla \ln[\rho(\mathbf{x}, t)/\rho_0] \\ \rho_0 = p_0 M_0 \end{gathered} \tag{52}$$

That system of equations is equivalent to equations (16), (24), (32), (41), and (46) and characterizes completely the Markov process (Ghirardi et al., 1978). The Markov process defined in such a manner is called (Mielnik and Tengstrand, 1983) the Nelson–Brown movement of the diffusing particle.

We note that the continuity equation (42) is linear with respect to the variables p and $\mathbf{j} = p\mathbf{v}$. This means that if the pairs p_i, $\mathbf{j}_i$, $i = 1, 2$, are the solutions then also the pair p, $\mathbf{j}$ given by definition as

$$p = p_1 + p_2, \qquad \mathbf{j} = p\mathbf{v} = p_1\mathbf{v}_1 + p_2\mathbf{v}_2 \tag{53}$$

is a solution. We want to stress following (Ghirardi et al., 1978) that, on the contrary, the dynamical Nelson relation (46) does not have this property.

It is seen that the Nelson relation is responsible for the fact that the description of the Nelson–Brown movement depends on the evolution of the mean quantities of that movement. This means, from the point of view of the diffusion process, that the Nelson relation puts certain constraints on the microstates of the diffusing matter which counteract the quite chaotic movement caused by the absence of interactions of diffusing particles. As a physical explanation of the existence of these constraints one can propose, for example, the so-called deformational interaction of diffusing particles phenomenon, which is observed, e.g, in the diffusion of hydrogen (Maximov and Pankratov, 1975) in metals. Those foreign atoms occupy in metals interstitial positions and the diffusion process is of the type 2.3. The interstitials deform a lattice by pushing aside the surrounding matrix atoms. They in turn displace the next atoms, and so on. Finally, a long-range displacement field appears, which vanishes as r^{-2}. So, even in very small concentrations, the diffusing atoms interact through the created displacement field and can develop a certain ordering in the diffusing atoms distribution. The existence of that substructure depends strongly on temperature. We come back to the problem of the connection of the Nelson relation with the ordering of microstates in the fifth part of the paper.

5. ANALOGY WITH QUANTUM MECHANICS AND DISSIPATIVE STRUCTURES

Following the lines of the stochastic quantization method (Nelson, 1966; Nelson, 1967; Ghirardi, 1978; Yasue, 1978; Nishioka, 1983) we consider the Nelson–Brown movement in the case when the peculiar velocity $\mathbf{v}(\mathbf{x}, t)$ and external force $\mathbf{F}(\mathbf{x}, t)$ are potential fields, i.e.,

$$\mathbf{v}(\mathbf{x}, t) = 2D\nabla S(\mathbf{x}, t) \tag{54}$$

$$\mathbf{F}(\mathbf{x}, t) = -\nabla U(\mathbf{x}, t) \tag{55}$$

We know that the field $\mathbf{u}(\mathbf{x}, t)$ has a similar representation [cf. equation (41)]

$$\mathbf{u}(\mathbf{x}, t) = -2D\nabla R(\mathbf{x}, t) \tag{56}$$

where

$$R(\mathbf{x}, t) = \ln[p(\mathbf{x}, t)/p_0]/2 \tag{57}$$

It follows that equations (42) and (46) take the form

$$\partial_t R = -D\Delta S - 2D\nabla R \cdot \nabla S \tag{58}$$

$$\partial_t S = D\Delta R - D[(\nabla S)^2 - (\nabla R)^2] - V/2Dm \tag{59}$$

where

$$V = U + 2Dm[R + S + C(t)]/\tau \tag{60}$$

and $C_1(t) = -C(t)/2Dm$ is an integration constant of equation (54)[3].

If we put

$$\psi(\mathbf{x}, t) = \exp(R + iS) \tag{61}$$

then equations (58) and (59) read

$$i\hbar\partial_t\psi = -\hbar^2\,\Delta\psi/2m + V\psi \tag{62}$$

where

$$V = U + \hbar[\ln|\psi|^2 + i\ln(\psi^*/\psi) + C(t)]/2\tau \tag{63}$$

and $\hbar$ is given by (4). In these new notations equations (54) and (56) take the forms

$$\mathbf{u}(\mathbf{x}, t) = -\hbar(\nabla \ln|\psi|^2)/2m \tag{64}$$

$$\mathbf{v}(\mathbf{x}, t) = i\hbar[\nabla \ln(\psi^*/\psi)]/2m \tag{65}$$

Equation (62) is a new phenomenological representation of a system of equations (42), (41), and (46) and defines with the help of equations (64) and (65) fields $\mathbf{u}(\mathbf{x}, t)$ and $\mathbf{v}(\mathbf{x}, t)$ of the Nelson–Brown motion describing a diffusion process.

When $\tau \to \infty$ then equation (62) takes the form of the Schrödinger-like equation

$$i\hbar\partial_t\psi = -\hbar^2\Delta\psi/2m + U\psi \tag{66}$$

However, it is not the Schrödinger equation, because in limits of the validity of the Arrhenius formula (36) the parameter $\hbar$ cannot reach the value of the reduced Planck constant $\hbar = h/2\pi$. It can be easily shown that the temperatures calculated from equation (4) and the Arrhenius formula (36) with the assumption $\hbar = \hbar$ for experimental data of D_0 and E_a for various metals (e.g., Bihr et al., 1978; Rein et al., 1978; Maier et al., 1979) are much greater than the melting temperatures!

In what follows we restrict our considerations to $0 \le \tau < \infty$ because the case $\tau = \infty$ is not typical for the diffusion phenomena.

We note that although equation (62) is not an equation of the quantum mechanics, it can still describe certain quantum effects because the probability of a transition of an interstitial to the next site depends on the mass of a diffusing particle. This is, for example, possible as a result of influence of certain quantum effects and can be included in calculations of the diffusion coefficient D (Maximov and Pankratov, 1975; Franklin, 1975). Quantum effects are especially considerable at low temperatures, at which the Arrhenius formula is not valid and the problem of the value of the quantity $\hbar$ appears once more. We leave that problem open, because it is

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[3] The constant $C(t)$ can be always put equal to zero by a proper choice of $S(\mathbf{x}, t)$.

out of the scope of our paper: our aim is to describe macroscopic and not quantum effects. To this end we represent equations (62) and (63) without microscopic quantities, i.e., in the forms

$$i\partial_t\psi = -D\Delta\psi + V/\hbar \tag{67}$$

$$V/\hbar = U/\hbar + [\ln|\psi|^2 + i\ln(\psi^*/\psi) + C(t)]/2\tau \tag{68}$$

where $\hbar$ is interpreted as a certain material constant with a dimension of action ($[\hbar] = \mathrm{g\,cm^2\,sec^{-1}}$). The constant $\hbar$ together with the diffusion coefficient D ($[D] = \mathrm{cm^2\,sec^{-1}}$) and relaxation time τ ($[\tau] = \mathrm{sec}$) characterize the properties of a body with diffusion. The interpretation of equation (40) remains unchanged: it describes the restriction of equation (67) to the case of negligible interactions of diffusing particles. Thus the function (15) is the probability that the diffusing particle is inside the set $\mathscr{P}$ at the instant t. With such an interpretation of equation (67) the random walk of a diffusing particle with mass m can be considered as the Nelson-Brown movement if the condition

$$m = \hbar/2D \tag{69}$$

is fulfilled.

The nonlinearity[4] of the considered diffusion process with respect to ρ and the stochastic character of its microscopic mechanism suggest that equation (67) can be used to describe diffusion in states far from equilibrium (Gumiński, 1983). From this point of view the stationary solutions of (67) are particularly interesting, i.e., solutions of the form

$$\psi(\mathbf{x}, t) = \phi(\mathbf{x})\exp(-iFt/\hbar) \tag{70}$$

where F is a constant with a dimension of energy. Namely, the far-from-equilibrium stationary mass distributions are characteristic for so-called dissipative structures (Belintzev, 1983; Ebeling, 1976). For $p(\mathbf{x}, t)$ of the form (40) such stationary solutions are possible if $M(t) = M_0 = \mathrm{const}$ and

$$\begin{aligned} &p(\mathbf{x}) = \phi^2(\mathbf{x})p_0 \\ &\phi^2(\mathbf{x}) = \rho(\mathbf{x})/\rho_0, \qquad \rho_0 = p_0 M_0 \end{aligned} \tag{71}$$

If we put (70) into (67) and accept that

$$C(t) = 2Ft/\hbar, \qquad U(\mathbf{x}, t) = U_0(\mathbf{x}) \tag{72}$$

we obtain

$$D\Delta\phi = \phi\ln\phi/\tau + (1/\hbar)(U_0(\mathbf{x}) - F)\phi \tag{73}$$

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[4] Anthony (1983) has shown that the Schrödinger and diffusion equations cannot be equivalent to each other. This result is valid only for the linear diffusion equation.

We note that in a stationary case the peculiar velocity $\mathbf{v} = \mathbf{0}$ [cf. (65)] which together with (24) give $\mathbf{b} = -\mathbf{u}$. It follows from equation (52), $\beta(t) \equiv 0$, and the above considerations that the diffusion equation (38) is fulfilled identically for an arbitrary density distribution $\rho(\mathbf{x})$. This means that equation (73) describes those properties of the stationary distributions of diffusing matter which follow from the Nelson relation (43)–(45) only. Let us consider the case when external forces are absent, i.e., when

$$U_0 - F = E_0 = \text{const} \tag{74}$$

If we denote by

$$\hat{\phi}(\mathbf{r}) = \phi(\mathbf{r}L)\exp(E_0\tau/\hbar) \tag{75}$$

where $\mathbf{r} = \mathbf{x}/L$, $L = (D\tau)^{1/2}$, the equation (73) can be rewritten in the form independent, evidently, of the parameters

$$\Delta_\mathbf{r}\hat{\phi}(\mathbf{r}) = \hat{\phi}(\mathbf{r}) \ln \hat{\phi}(\mathbf{r}) \tag{76}$$

The above equation defines stationary distributions of diffusing mass

$$\rho(\mathbf{x}) = \rho_\tau \phi^2(\mathbf{x}/L) \tag{77}$$

where

$$\rho_\tau = \rho_0 \exp(-2E_0\tau/\hbar) \tag{78}$$

to which corresponds the probability distribution

$$p(\mathbf{x}) = p_\tau \phi^2(\mathbf{x}/L) \tag{79}$$

with

$$p_\tau = \rho_\tau / M \tag{80}$$

It is seen that although the function $\hat{\phi}(\mathbf{r}) \equiv 1$ for $\mathbf{r} \in R^3$ is a solution of equation (76), it does not fulfil the condition on probability measure normalization on R^3. For that reason we assume that to the solution $\hat{\phi}(\mathbf{r}) \equiv 1$ corresponds the following mass distribution:

$$\rho(\mathbf{x}) = \begin{cases} \rho_\tau & \text{for } \mathbf{x} \in \Omega(\rho) \\ 0 & \text{for } \mathbf{x} \in R^3 \backslash \Omega(\rho) \end{cases} \tag{81}$$

where $\Omega(\rho) \subset R^3$ is a certain region with $\operatorname{vol}\Omega(\rho) < \infty$. Because uniform distribution of mass M_0 concentrated in $\Omega(\rho)$ is given as

$$\rho_\tau = M_0 / V \tag{82}$$

where $V = \operatorname{vol}\Omega(\rho)$ we have that

$$E_0 = \hbar \ln(p_0 V)/2\tau \tag{83}$$

with $p_0 = \rho_0/M_0$. To the mass distribution (82) corresponds the probability distribution

$$p_\tau = \begin{cases} 1/V & \text{for } \mathbf{x} \in \Omega(\rho) \\ 0 & \text{for } \mathbf{x} \in R^3 \backslash \Omega(\rho) \end{cases} \tag{84}$$

We introduce statistical entropy as a measure of indetermination of a statistical description of stationary states of a dissipative process and defined as follows (Ciesielski, 1971):

$$S(p) = \int_{R^3} dS(p(\mathbf{x})) \tag{85}$$

where

$$dS(p(\mathbf{x})) = p_0 \eta(p(\mathbf{x})/p_0)\, dV(\mathbf{x}) \tag{86}$$

and

$$\eta(w) = \begin{cases} -kw \ln w & \text{for } w > 0 \\ 0 & \text{for } w = 0 \end{cases} \tag{87}$$

Let $\Omega \subset R^3$, $0 < V = \operatorname{vol} \Omega < \infty$ be a certain region and $p(\mathbf{x})$ be a probability distribution on R^3 for which

$$\Omega(\rho) = \{\mathbf{x} \in R^3 \colon p(\mathbf{x}) > 0\} = \Omega \tag{88}$$

where $p(\mathbf{x}) = \rho(\mathbf{x})/M_0$. It follows that

$$\int_\Omega p(\mathbf{x})\, dV(\mathbf{x}) = 1 \tag{89}$$

and then (Ciesielski, 1971; Klimontovitch, 1982)

$$S(p(\mathbf{x})) \le S(p_\tau) = k \ln(p_0 V) \tag{90}$$

where p_τ is the probability given by equation (84). The equality in (90) is attainable for sufficiently smooth distributions $p(\mathbf{x})$ only if $p(\mathbf{x}) = p_\tau$. It can be shown that for the probability distributions $p(\mathbf{x})$ on R^3 defined by (71) with $\rho(\mathbf{x})$ of the form

$$\rho(\mathbf{x}) = \begin{cases} M_0 \hat{\phi}^2(\mathbf{x}/L)/V_0 & \text{for } \mathbf{x} \in \Omega \\ 0 & \text{for } \mathbf{x} \in R^3 \backslash \Omega \end{cases} \tag{91}$$

where $\hat{\phi}(\mathbf{r})$ is a solution of equation (76) in Ω, E_0 of the form (83) and when conditions (88) and (89) are fulfilled then the condition $\nabla\rho(\mathbf{x}) \neq \mathbf{0}$ for almost all $\mathbf{x} \in R^3$ implies that

$$S(p(\mathbf{x})) < S(p_\tau) \tag{92}$$

The inequality (92) is formulated for one particle of a microstate. Our assumption that the interactions of diffusing particles are absent has a mathematical picture in the additivity property of the functional $S(p)$: it allows, if one joins the independent systems into one system, to transfer the inequality (92) on a whole microstate (Ebeling, 1976).

Decrement (increment) of the measure of indetermination of a statistical description is usually interpreted as an increment (decrement) of the ordering level of microstates corresponding to the considered measure, e.g., the level of $S(p_\tau) = k \ln(p_0 V)$ in (92). Distribution p_τ of the form (84) can be considered as describing chaotic and space equilibrium distribution of diffusing particles in Ω [e.g., Brownian particles (Reif, 1965)]. The nonvanishing density gradient which implies the inequality (92) causes the appearance of a space ordering at a microlevel. It is a characteristic picture for a special case of dissipative structures called Turing dissipative structures. The existence of such structures is experimentally confirmed. They can appear as a result of perturbations destroying the stability of uniform equilibrium of matter distributions and have the lower symmetry than the original one (Belintzev, 1983). We have already mentioned the observed ordering microstates in stationary states caused by the deformational interactions of diffusing particles. The inequality (92) allows for precision when the Nelson relation can be discussed as a phenomenologically equivalent to the considered phenomenon: namely, when it appears in the stationary nonequilibrium states. As an example one can give a situation when a part of matrix atoms is replaced by foreign atoms and the geometric equivalence of interstitials is different from their energetic equivalence (Smirnov, 1979).

A complete description of the effects of deformational interaction in the context of the Nelson relation needs an extension of our approach to the field description of the whole body with diffusion. This is, however, out of the scope of our paper and will be discussed elsewhere.

We want to express that in order to interpret equation (76) as an equation describing dissipative structures, we have to introduce a bounded region. Otherwise a system cannot be regarded as thermodynamically open and the dissipative structures cannot appear (see, e.g., Ebeling, 1976).

6. INFLUENCE OF RELAXATION TIME ON DIFFUSION PROCESS

Let us consider a stationary state of a diffusing matter with an ascribed characteristic energy $\theta > 0$. For example, $\theta = kT$ when we have to deal with an equilibrium state. We have, for certain dimensionless parameters $\alpha =$

$\alpha(\hbar, \tau, \theta) > 0$ and $\beta = \beta(m, \hbar, D) > 0$,

$$\theta \doteq \alpha\hbar/\tau, \qquad \hbar = \beta m D \tag{93}$$

It follows from (47) and (93) that

$$D = \theta/\alpha\beta\zeta \tag{94}$$

If we regard the diffusion process as the Nelson-Brown movement, then $\beta = 2$ and

$$D = \theta/2\alpha\zeta \tag{95}$$

When the diffusion coefficient D depends on the relaxation time, then $\alpha = \alpha(\tau)$, and

$$D = D(\Lambda_\tau) = k\Lambda_\tau/\zeta \tag{96}$$

where

$$\Lambda_\tau = \theta/[2k\alpha(t)] \tag{97}$$

We assume that

$$\lim_{\substack{\tau \to 0 \\ \zeta = \text{const}}} \alpha(\tau) = \alpha(0) = 1/2 \tag{98}$$

because then

$$\lim_{\substack{\tau \to 0 \\ \zeta = \text{const}}} D(\Lambda_\tau) = D(\Lambda_0) = k\Lambda_0/\zeta \tag{99}$$

where

$$\Lambda_0 = \theta/k \tag{100}$$

and

$$D(\Lambda_0) = \theta/\zeta \tag{101}$$

For equilibrium states, i.e., when $\theta = kT$, equation (101) reproduces the Einstein relation (33) and when

$$\theta = \zeta D_0 \exp(-E_a/kT) \tag{102}$$

$D(\Lambda_0)$ is in line with the Arrhenius formula (36). It is easy to see that if we put $D = D(\Lambda_\tau)$ for $0 < \tau < \infty$ then the considerations from Sections 4 and 5 of our paper remain without change. In a limit when $\tau \to 0$ and $\zeta = \text{const}$, the classical diffusion equation has the form (38) with $D = D(\Lambda_0)$

and **b** defined by (1). The limit $\tau \to \infty$ needs the additional assumption that there exists a limit of $D(\Lambda_\tau)$

$$D_\infty = \lim_{\substack{\tau \to \infty \\ m = \text{const}}} D(\Lambda_\tau) > 0 \tag{103}$$

We obtain in this case the equation (66) but with $\hbar = \hbar_\infty = 2mD_\infty$. Making use of equations (47), (69), and (96) we can rewrite equation (73) in the following form:

$$\tau D(\Lambda_\tau)\,\Delta\phi = \phi \ln \phi + (U_0 - F)\phi/(2k\Lambda_\tau), \qquad \tau > 0 \tag{104}$$

It is seen from (99) that

$$\lim_{\substack{\tau \to 0 \\ \zeta = \text{const}}} \tau D(\Lambda_\tau) = 0 \tag{105}$$

and the corresponding asymptotic solution of equation (104) reads

$$\phi_0(\mathbf{x}) = \exp\{-[U_0(\mathbf{x}) - F]/2k\Lambda_0\} \tag{106}$$

This solution defines the probability distribution $q_0(\mathbf{x})$ of a form [cf. equation (71)]

$$\begin{gathered} q_0(\mathbf{x}) = p_0\phi_0^2(\mathbf{x}) = C \exp[-U_0(\mathbf{x})/k\Lambda_0] \\ C = p_0 \exp(F/k\Lambda_0) \end{gathered} \tag{107}$$

It follows from the probabilistic measure normalization condition that it should be

$$\begin{gathered} F = k\Lambda_0 \ln Z \\ Z = p_0 \int_{R^3} \exp[-U_0(\mathbf{x})/k\Lambda_0]\, dV(\mathbf{x}) \end{gathered} \tag{108}$$

or, equivalently,

$$F = E - \Lambda_0 S(q_0) \tag{109}$$

where E is a mean energy

$$E = \int_{R^3} U_0(\mathbf{x}) q_0(\mathbf{x})\, dV(\mathbf{x}) \tag{110}$$

Here $S(q_0)$ is a statistical entropy (85).

If $\theta = kT$, then $\Lambda_0 = T$, $q_0(\mathbf{x})$ is the Boltzmann distribution and the statistical entropy $S(q_0)$ can be identified with the thermodynamic entropy (Ebeling, 1976). In this case the constant F can be recognized as a free energy on one particle of a microstate in a thermodynamical equilibrium.

If θ is given by equation (102) then $q_0(\mathbf{x})$ is the same as the probability distribution $p(\mathbf{x})$ defined by equations (30), (32), and (36).

It is seen that in the limit where $\tau \to 0$ and $\zeta = \text{const}$, equation (104) reproduces the probability distributions discussed in Section 3.

We mentioned in Section 5 the possibility of describing the Turing structures with the help of equation (76). Characteristic dimensions of those structures are defined by such macroscopic parameters as diffusion coefficients and kinetics times (Belintzev, 1983), that is, in our case the characteristic length

$$l \sim (D\tau)^{1/2} \tag{111}$$

Let us consider a case when a stationary distribution of diffusing matter has a certain characteristic dimension l, such that for a certain dimensionless parameter $A = A(l, \tau, D) > 0$

$$D = Al^2/\tau \tag{112}$$

We have by definition

$$w = l/\tau \tag{113}$$

$$K = mw^2/2 \tag{114}$$

It follows from equations (47), (69), (93), (113), and (114) that

$$K = \theta/4A\alpha \tag{115}$$

In order to find a value of the parameter A when $\tau \to 0$, consider the case (49) where the Stokes relation (1) is valid and a model of the dynamics of the diffusion process microstates can be based on the Langevin equation (Nelson, 1967; Klimontovitch, 1982)

$$\tau\ddot{\mathbf{z}} = -\dot{\mathbf{z}} + \mathbf{b}(\mathbf{z}, t) + d\mathbf{W}(t) \tag{116}$$

where τ is defined by equation (47) and $\mathbf{W}(t)$ is a Wiener process. It can be shown that for a properly smooth function $\mathbf{b}(\mathbf{z}, t)$, the solution $\mathbf{z} = \mathbf{z}(\tau, t)$, $t \geq 0$, of the above equation with the initial conditions

$$\mathbf{z}(\tau, 0) = \mathbf{x}_0, \qquad \dot{\mathbf{z}}(\tau, 0) = \mathbf{w}_0 \tag{117}$$

has a limit with probability 1,

$$\lim_{\tau \to 0} \mathbf{z}(\tau, t) = \mathbf{x}(t) \tag{118}$$

uniformly on every interval $[a, b] \subset [0, \infty)$ and for every $\mathbf{w}_0 \in R^3$. Here $\mathbf{x}(t)$ is a solution of the stochastic Ito equation (12) with an initial condition $\mathbf{x}(0) = \mathbf{x}_0$. The result remains the same if the initial velocity $\mathbf{w}_0$ is a Gaussian random variable with a mean value zero and a variance $\sigma^2/2\tau$. The interaction of diffusing particles with a body is described in equation (116) by a friction parameter ζ and variance parameter σ^2. Parameter σ^2 can be calculated from a condition that for

$$\mathbf{F}=\zeta\mathbf{b}=\mathbf{0} \tag{119}$$

and for $t\to\infty$ the mean kinetic energy of our system is equal to the characteristic kinetic energy K given by (114) of a stationary diffusion process with the condition (49). The velocity $\mathbf{w}(t)=\mathbf{z}(\tau, t)$ defined by equations (116), (117), and (119) is a random velocity and (Nelson, 1967)

$$\begin{gathered} E[\mathbf{w}(t)]=\mathbf{w}_0\exp(-t/\tau) \\ E[\mathbf{w}'(t)\otimes\mathbf{w}'(t)]=\sigma^2[(1-\exp(-t/\tau)]I/2\tau \end{gathered} \tag{120}$$

where $\mathbf{w}'(t)=\mathbf{w}(t)-E[\mathbf{w}(t)]$. It follows that

$$\begin{gathered} \lim_{t\to\infty} E[\mathbf{w}(t)]=0 \\ \lim_{t\to\infty} E[m\|\mathbf{w}(t)\|^2/2]=3\zeta\sigma^2/4=K \end{gathered} \tag{121}$$

for $\tau\ll\tau_*$. In this case [cf. equations (32), (98), (99), (115), and (121)]

$$\sigma^2/2=D(\Lambda_\tau)\approx D(\Lambda_0) \qquad \text{for } \tau\ll\tau_* \tag{122}$$

and

$$K\approx\theta/2A \qquad \text{for } \tau\ll\tau_* \tag{123}$$

which give

$$\lim_{\substack{\tau\to 0\\ \zeta=\text{const}}} A[l, \tau, D(\Lambda_\tau)]=1/3 \tag{124}$$

It follows from equations (105), (112), and (124) that the characteristic length depends on the relaxation time τ and

$$\begin{gathered} \lim_{\substack{\tau\to 0\\ \zeta=\text{const}}} l(\tau)=l(0)=0 \\ \lim_{\substack{\tau\to 0\\ \zeta=\text{const}}} l^2(\tau)/\tau=3D(\Lambda_0)=3\theta/\zeta \end{gathered} \tag{125}$$

We see that [cf. equation (111)] $l(\tau)=0^*(\sqrt{\tau})$.

Summarizing, the conditions (95)-(99) define such a form of dependence of the diffusion coefficient on the relaxation time τ which is an extension of the formulas considered in the classical description of the diffusion process running by the states close to the thermodynamic equilibrium. Consequently, if the relaxation time τ is not negligible [the inequality

(51)] it influences not only the character of microstates dynamics (Nelson instead of Stokes relation) but also the macroscopic properties of a body with diffusion [$D = D(\Lambda_\tau)$]. That diffusion process makes possible the existence of nonequilibrium stationary structures of diffusing matter with a certain characteristic dimension l depending on the relaxation time τ according to the relation (125). Thus the diffusion phenomenon described above can be characterized by a set of dimensional quantities

$$m, \qquad l(\tau), \qquad \tau, \qquad \hbar(\tau) \tag{126}$$

where $\hbar(\tau) = 2mD(\Lambda_\tau)$.

7. ON THE METHOD, ITS RESULTS, AND POSSIBLE GENERALIZATION

The semiheuristic method used in our paper has not of course, from the phenomenological point of view, a satisfactory proof of efficiency. It serves rather to show the place at which we have to escape from the classical description of a diffusion process if we want to represent it as the Nelson–Brown movement and to show the possible consequences for a phenomenological theory. A key role is played by such a formulation of the Nelson relation which can be treated as a generalization of the Stokes relation. The fact that the Nelson relation is based on the notion of the peculiar acceleration of a diffusing particle allows us to introduce to the phenomenological theory a parameter from a microscale: the mass m of a diffusing atom. Consequently, the variable describing the process was changed: instead of the mass density $\rho(\mathbf{x})$ we have used the density of the probability of localization of a diffusing atom $p(\mathbf{x})$. Restriction to the case when

$$p(\mathbf{x}, t) = \rho(\mathbf{x}, t)/M(t)$$

allowed us to transfer many relations and interpretations to the area out of the limits of the classical description of diffusion and offered facilities to formulate interpretation rules for equation (67) [cf. (92)].

In reality, the probability density $p(\mathbf{x}, t)$ was regarded as a kind of a hidden, or as it is called in the continuum theory, internal variable, i.e., a variable describing the internal state of a material (e.g., Sidoroff, 1975). From this point of view equation (67) introduces such a new complex internal variable $\psi(\mathbf{x}, t)$ that

$$p(\mathbf{x}, t)/p_0 = \psi(\mathbf{x}, t)\psi^*(\mathbf{x}, t)$$

The discussion given in Section 5 showed that this internal variable was connected with the existence of stationary states of diffusing matter far from the thermodynamically equilibrium states. The case of equation (76) discussed in a bounded region suggests that the Nelson–Brown movement can be connected with the theory of dissipative structures. Such an approach requires the generalization of the theory of the Nelson–Brown movement because many new problems appear as, for example, the time of staying of the Markovian particle in that region and its behavior at the boundary. It would be crucial, from the point of view of the dissipative structures theory, to extend the presented theory to a case of two (or more) chemically reacting and diffusing components of a body (e.g, Belintzev, 1983). It seems to be possible if one relates our interpretation of the stochastic quantization method to the proposition of describing in its frames the mixed quantum states, as it is discussed in the paper of Ghirardi et al. (1978).

ACKNOWLEDGMENTS

The authors are indebted to Professor K.-H. Anthony for his interest and for valuable discussions. We are grateful to Deutsche Forschungsgemeinschaft (A.T.) and to Alexander von Humboldt Stiftung (R.K.) for support and to our colleagues from the Department of Theoretical Physics for their hospitality during our stay at the University of Paderborn where the paper was partially done.

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