

BROWNIAN MOTION AS A MODEL OF THE EVOLUTION OF A NONEQUILIBRIUM SYSTEM

B. Lev

*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine,
14-b, Metrolohichna St., Kyiv 03680, Ukraine*

(Received October 16, 2009)

According to the principles of thermodynamics any system being in contact with the thermal bath passes in the equilibrium state for the relaxation time. The paper presents a model of Brownian motion of the system which allows one to determine its stationary states far from the equilibrium. The stationary distribution function of a nonequilibrium state can be represented by none of the known equilibrium distributions. It is shown at which conditions the equilibrium states are realized, and new stationary states of the nonequilibrium systems are predicted.

Key words: ion implantation, silicon, doping profile, channeling, molecular dynamics, Monte Carlo method.

PACS number(s): 73.21.Fg, 78.67.De

According to the basic principles of thermodynamics an arbitrary macroscopic system in contact with the thermal bath reaches the equilibrium state for the relaxation time. The properties of such a system are determined by its peculiarities and the characteristics of the thermal bath. Its equilibrium state can be completely defined only under ideal conditions [1–3]. The establishment of the equilibrium in a separate system results in both the establishment of the identical thermodynamical parameters equivalent to those of the thermostat and the absence of flows in the system itself. In the case of the nonequilibrium open systems, the flows always exist, and the definition of invariable parameters for such a system seems impossible. Nevertheless, it is possible to define the stationary states for open systems, whose distribution function will be different from the known equilibrium distributions. Such a state can be interpreted as “equilibrium” in the sense of its constancy in time, but the thermodynamical parameters of the system and the environment will be different. To such systems, can refer hot electrons in semiconductors [4], a system of photons on the inhomogeneous scattering where the diffraction coefficient depends on the frequency of photons [5, 6], a system of high-energy particles which is created as a result of the collision of particles on accelerators and a bigger particle in the dusty plasma [7], a system of Brownian particles. Of course, the description of the behavior of Brownian particles has had a long history [8, 9], but it seems interesting and appropriate to study the behavior of such a system under conditions far from equilibrium which can be a model for the description of the nonequilibrium systems. The content of the model consists in the following. A separate Brownian particle is a macroscopic system with many degrees of freedom. This particle (or a system) interacts with the environment (with the thermostat) in two independent ways. The first way consists in the direct influence of the environment on a separate particle (system) via the introduction to or the withdrawal of the energy from a separate system by means of its dissipation into the thermostat or the absorption of the energy from it (the distinctive positive or

negative friction). Another way to change a state of the separate system consists in the direct fluctuation effect of the environment which is reduced to a rapid change of the state of the system. Such a change can occur due to both the influence of the other systems and a change of the characteristics of the thermostat on the presence of many degrees of freedom in it. Both the presence of other systems and the direct effect of the chosen system affect the thermostat. In this sense, the environment where the chosen system is positioned, is not a fixed formation like the thermostat, but affect directly the processes running in the chosen system. It is easy to imagine that a relaxation of the system occurs with respect to the slowest variable which can be the energy. At every time moment a change of the slowest parameter of the system is known, but the effect of the other parameters on its variation will have a random character. This pattern corresponds to the stochastic dynamics of a separate system, and the description of an ensemble of such systems will correspond to the determination of the distribution function of the system. Therefore, there appears a possibility to describe a system of Brownian particles (systems) which can be under nonequilibrium conditions and to find the possible stationary states of such a system. In this sense, we can obtain a possibility to describe the nonequilibrium systems which are far from equilibrium. Each macroscopic system can be considered as a Brownian particle, and its state can be described in terms of the energy of such a particle (system). It is obvious that the state of a separate macroscopic system depends on the environment which plays the role of the thermostat, acts directly, in this interpretation, on the chosen system with fluctuations in their exchange by energy, and is not a fixed invariable structure. For this reason there arises an urgent necessity to develop mathematical approaches to a possible description of such nonequilibrium systems with the purpose of defining their new states with the possibility of foreseeing the plausible stationary states of open systems and conditions of their existence.

In practice, the statistical description is based on the knowledge of only several integrals of motion such as

energy. The latter, as a controlling parameter of the nonequilibrium system seems to be its slowest parameter. In the absence of another information about the nonequilibrium system the determination of a state of the system in terms of energy is attractive, the more so as energy in the frame of equilibrium statistical mechanics is the invariant of the system. Generally, one can assume that this equation which describe the changing energy in the nonequilibrium system has the form equivalent to the nonlinear Langevin equation

$$\frac{d\varepsilon}{dt} = f(\varepsilon) + g(\varepsilon)L(t). \quad (1)$$

The dynamical equation for a change of the energy reminds, in our interpretation, the Langevin equation, but it has a more profound content because it accounts for both the direct action of the environment on a chosen system (the first term of the equation) and the connection of the chosen system with the environment via possible fluctuations of the conditions under which the system is placed (the second term of the equation). The external influence is reduced, in the first turn, to a change of the system's energy which the system obtains from or gives back to the environment. But a change of the state of the system is not defined by only this point. First of all, each parameter of the system varies by the fluctuations corresponding to the possible ones which depend on the energy of the system through the coefficient $g(\varepsilon)$. The ground state of any system is determined within fluctuations whose mean value can be zero, but the correlations are conserved in this case. In addition, an arbitrary system can be in contact with a nonlinear environment, whose behavior is not fully unambiguous. A random migration of the system over various states is a result of both the direct action of the environment and a random action due to the contact of the system with the nonlinear environment, where it is placed. A random influence of the environment can be taken into account only in the form of the correlations between fluctuations at different time moments $\langle L(t)L(t') \rangle = \phi(t - t')$ because the mean value of such fluctuations is equal to zero. The mean value $\langle \dots \rangle$ of the correlations is nonzero only during the time interval of the action. Therefore, the function $\phi\delta(t - t')$ must have a sharp peak as the time interval tends to zero, which corresponds to the condition $\int \phi(\tau)d\tau = \sigma^2$ characterizing a white noise [8]. The energy representation holds also for ordinary Brownian particles, but it was not in use for unknown reasons. It is worth noting that such a representation seems the most expedient for the description of the behavior of nonequilibrium systems. The dynamics of an ordinary Brownian particle is described in terms of velocity v with the help of the Langevin equation:

$$\frac{dv}{dt} = -\gamma v + F(t), \quad (2)$$

where γ is the coefficient of friction, and $F(t)$ is a random force accounting for the irregular action of the environment on a separated particle. The mean over the statistical ensemble $\langle F(t) \rangle = 0$, but $\langle F(t)F(t') \rangle = \phi^2\delta(t - t')$,

which corresponds to the condition for a white noise and thus accounts for the correlations in the movement of particles under the action of a random force. For a Brownian particle, a change of the energy $\varepsilon = \frac{Mv^2}{2}$ can be presented as

$$\frac{d\varepsilon}{dt} = Mv\frac{dv}{dt} = -2\gamma\varepsilon + \sqrt{2M\varepsilon}F(t), \quad (3)$$

which corresponds to the initial equation with $f(\varepsilon) = -2\gamma\varepsilon$, $g(\varepsilon) = \sqrt{\varepsilon}$ and $L(t) = \sqrt{2M}F(t)$. By using a solution of the Langevin equation for velocity [8], one can find that $\langle v(\infty) \rangle = \frac{\phi^2}{2\gamma} = \frac{kT}{M}$ and $\langle \varepsilon \rangle = \frac{kT}{2}$, where T is the temperature of the thermostat, i.e. that of the environment. By solving the equation for a change of the energy, we can also find that $\sqrt{\langle \varepsilon \rangle^2} = \frac{\sigma^2}{4\gamma} \equiv \frac{\phi^2}{4\gamma} 2M = kT$ where many-time correlations of the energy are not taken into account. The obtained relation corresponds to the equilibrium conditions when a system of Brownian particles is in equilibrium with the environment playing the role of the thermostat for them. As seen from the above-presented consideration various representations of the Brownian motion are equivalent, but the energy representation acquires for more general nonequilibrium systems. For this reason, it will be more expedient to consider the definition of the nonequilibrium distribution functions of states from nonlinear Fokker–Planck equation. Such an approach will be suitable for the description of the behavior of the nonequilibrium system on the receipt of the relevant energy from outside, its loss on the direct action of the environment, and the dissipation of energy on a random influence of the environment. In view of possible complex processes which can run in the system itself and under the exchange with the environment, it is necessary to use a more general approach with the nonlinear Langevin equation. Though the Langevin equation differs from the Fokker–Planck equation in form, but they are mathematically equivalent [8]. If we assume that the coefficient $g(\varepsilon)$ depends on energy at the initial time moment, then it is necessary to use the Fokker–Planck equation in the Itó form. If this coefficient depends on energy prior to and after the transition, one uses the Fokker–Planck equation in the Stratonovich form [8]

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \varepsilon} (f(\varepsilon)\rho) + \frac{\sigma^2}{2} \frac{\partial}{\partial \varepsilon} g(\varepsilon) \frac{\partial}{\partial \varepsilon} g(\varepsilon)\rho. \quad (4)$$

In what follows, will be used only the Stratonovich representation, the more so as there exists a direct connection between the two approaches [8, 9]. Both the equations have no particular physical content until a physical process under consideration is specified. In most cases, various possible states of the system depend on both the initial value of the energy and possible subsequent values. The above-presented equation for the nonequilibrium distribution function of the system can be rewritten in the form of the law of conservation for the distribution function

$$\frac{\partial \rho(E, t)}{\partial t} = \frac{\partial J(\rho(\varepsilon, t))}{\partial \varepsilon}, \quad (5)$$

where the probability flow can be represented in the form

$$J = - \left(f(\varepsilon) - \frac{\sigma^2}{2} g(\varepsilon) \frac{\partial}{\partial \varepsilon} g(\varepsilon) \right) \rho + \frac{\sigma^2}{2} g^2(\varepsilon) \frac{\partial}{\partial \varepsilon} \rho. \quad (6)$$

The general stationary solution of the Fokker–Planck equation in the absence of the flow, $J(\rho(\varepsilon, t)) = 0$, looks as

$$\rho_s(\varepsilon) = A \exp \left\{ \int_{\varepsilon_0}^{\varepsilon} \frac{2f(\varepsilon') d\varepsilon'}{\sigma^2 g^2(\varepsilon')} - \ln \frac{g(\varepsilon)}{g(\varepsilon_0)} \right\}. \quad (7)$$

The equilibrium distribution function as a stationary solution under nonlinear properties of the environment can be rewritten in the form $\rho_s(\varepsilon) = A \exp \{-U(\varepsilon)\}$ where

$$U(\varepsilon) = \ln \frac{g(\varepsilon)}{g(\varepsilon_0)} - \int_{\varepsilon_0}^{\varepsilon} \frac{2f(\varepsilon') d\varepsilon'}{\sigma^2 g^2(\varepsilon')}. \quad (8)$$

This distribution function has the extremal value at the energy which can be found from the equation $U'(\tilde{\varepsilon}) = \frac{1}{D(\tilde{\varepsilon})} (D'(\tilde{\varepsilon}) - f(\tilde{\varepsilon}))$ where the symbol ' stands for the derivative with respect to the energy. This equation is completely equivalent to $D'(\tilde{\varepsilon}) = f(\tilde{\varepsilon})$ which determines the conditions of the equilibrium between the diffusion over states of the environment and the dissipation in the system under which the stationary solution is realized and defines completely the energy of a new equilibrium state. The stationary nonequilibrium distribution function under the given conditions can be defined as

$$\rho_s(\varepsilon) = \exp \{-U(\tilde{\varepsilon})\} \exp \{-U''(\tilde{\varepsilon})\varepsilon^2\}, \quad (9)$$

where $-U''(\tilde{\varepsilon}) = \frac{1}{D(\tilde{\varepsilon})} (D''(\tilde{\varepsilon}) - f'(\tilde{\varepsilon}))$. This distribution function has the form of the Gauss distribution. If the dissipation in the system is described by a nonlinear function $f(\varepsilon)$ of energy, and the coefficient of diffusion depends on the system's energy, a number of situations characterized by new equilibrium states of the nonequilibrium system can be realized. We will try to describe some possible cases:

(a) If the coefficient of diffusion is constant $g(\varepsilon) = 1$, the stationary solution can be written in the form

$$\rho(\varepsilon) = A \exp \left(\int_{\varepsilon_0}^{\varepsilon} \frac{f(\varepsilon')}{\sigma^2} d\varepsilon' \right), \quad (10)$$

where ε_0 is the initial value of energy. If the energy of the system is conserved, $f(\varepsilon) = 0$, the stationary distribution function can be transformed into a constant. One can note that the value $\varepsilon = \varepsilon_0$ is not only a limiting point, but also the stationary point of the system in the absence of the dissipation and a random walk over possible energies. The given value of energy is such at which a stationary probability distribution of the system is concentrated according to the conditions of normalization [9]. Only in this case, the distribution function is a microcanonical distribution.

(b) If the coefficient of diffusion is constant, $g(\varepsilon) = 1$, the equation for the nonequilibrium distribution function takes the form of the ordinary diffusion equation, whose solution is $\rho(\varepsilon) = A \frac{1}{\sqrt{4\pi\sigma^2 t}} \exp \left(-\frac{(\varepsilon - \varepsilon_0)^2}{4\sigma^2 t} \right)$. It describes the migration of the system over arbitrary values of energy. The probability decreases, and the distribution function spreads by the law $\langle (\varepsilon - \varepsilon_0)^2 \rangle = 2\sigma^2 t$. This solution describes the evolution of the system in the case where the initial state is represented by the delta-function $\rho(\varepsilon) = \delta(\varepsilon - \varepsilon_0)$. All states of the system are located on the constant energy surface on which the migration of the system occurs. Fluctuations of the environment are absent in this case, and the equilibrium distribution function corresponds to the microcanonical ensemble.

(c) If the coefficient of diffusion depends on the energy, but energy of the system is conserved, $f(\varepsilon) = 0$, the stationary distribution function takes the form

$$\rho_s(\varepsilon) = A \exp \left\{ -\ln \frac{g(\varepsilon)}{g(\varepsilon_0)} \right\} \quad (11)$$

which corresponds to the canonical equilibrium distribution, $\rho(\varepsilon) = A \exp \{-\beta(\varepsilon - \varepsilon_0)\}$, only if $g(\varepsilon) = e^{\beta\varepsilon}$, where β is the reciprocal temperature. Such a distribution can be realized only if the coefficient of diffusion depends specifically on energy: $D(\varepsilon) = \frac{\sigma^2}{2} g^2(\varepsilon) = \frac{\sigma^2}{2} e^{2\beta\varepsilon}$. The physical conditions correspond to the peculiarities of the interaction of the system with the environment and account for the processes of dissipation for such a system through interaction.

The equilibrium relation for fluctuations of the energy can be given in the form [3]

$$\langle \varepsilon^2 \rangle = \frac{\alpha(0)}{\beta} = \frac{\sigma^2}{2} g^2(0), \quad (12)$$

where $\alpha(0)$ is the susceptibility of the system, $\alpha(0) = c_v$ is the heat capacity, and β is the reciprocal temperature. For a nonlinear environment and a nonequilibrium system, a more general representation for the susceptibility of the system depends on the state of the system and, hence, on energy and can be written in the form

$$\alpha(\varepsilon) = \frac{\beta\sigma^2}{2} g^2(\varepsilon), \quad (13)$$

where a possible reaction of the system to the external influence is taken into account. Now, if $g(\varepsilon) = 1$, it is easy to determine the relation between the temperature and the characteristics of noise or fluctuations of the environment, $c_v T = \frac{\beta\sigma^2}{2}$, which characterizes the susceptibility of the system to the environment or the thermostat. The previous equality can be interpreted as the definition of the system's temperature, $T = \frac{\sigma^2}{2\alpha(\varepsilon)} g^2(\varepsilon)$.

(d) Let now a change of the energy of the system be nonzero, $f(\varepsilon) \neq 0$. In view of the dependence of the coefficient of diffusion on energy one can write the equilibrium distribution function as

$$\rho_s(\varepsilon) = A \exp \left\{ -2\beta \left(2\beta - \frac{f'(\tilde{\varepsilon})}{f(\tilde{\varepsilon})} \right) \varepsilon^2 \right\}. \quad (14)$$

The coefficient of diffusion plays the role of a universal characteristic of the environment. The stationary distribution function can be realized now only if the supplied and dissipated energies are in balance. If the system obtains a greater amount of energy than it can dissipate, being in contact with the environment, the stationary distribution function cannot be defined, and a new equilibrium state cannot be realized.

The energy representation can be more illustrative if we wish to understand the conditions of the formation of equilibrium (stationary) states for a nonequilibrium system. For example, let us return to an ordinary system of Brownian particles. The stationary distribution function of Brownian particles can be written in the energy representation as

$$\rho_s(\varepsilon) = A \exp \left\{ -\frac{4\gamma}{\sigma^2} \varepsilon - \ln \sqrt{\varepsilon} \right\} \equiv A \frac{1}{\sqrt{\varepsilon}} \exp(-\beta\varepsilon), \quad (15)$$

where we use the well-known relation $\frac{2\gamma}{\sigma^2} = \beta$. In view of the conditions of normalization $\int \rho_s(\varepsilon) d\varepsilon \equiv \int \rho_s(p) dp$, the equilibrium distribution function can be rewritten in the momentum representation in the well-known form

$$\rho_s(p) = A \exp \left(-\beta \frac{p^2}{2M} \right) = A \exp \left(-\frac{Mv^2}{2kT} \right). \quad (16)$$

The given stationary distribution function reproduces completely the well-known equilibrium Maxwell distribution function for ordinary Brownian particles.

The dependence of the coefficient of diffusion on energy can be determined from the linear Langevin equation, by using the theory of Markov processes and by accounting for the nonequilibrium fluctuations of arbitrary coefficients in the function describing the direct action of the environment $f(\varepsilon)$. Can set $f(\varepsilon) = \gamma\varepsilon - \varepsilon^2$ where the second term accounts for the restriction to the absorption of the energy by the system. The energy absorption parameter can be given, as above, in the form $\gamma_t = \gamma + \xi_t$, where the second term accounts for a random influence of the environment on the given coefficient. In this case the Fokker-Planck equation takes the form [9]

$$\frac{\partial \rho(\varepsilon, t)}{\partial t} = \frac{\partial}{\partial \varepsilon} ((\gamma\varepsilon - \varepsilon^2)\rho(\varepsilon, t)) + \frac{\sigma^2}{2} \frac{\partial^2}{\partial \varepsilon^2} \varepsilon^2 \rho(v, t). \quad (17)$$

The stationary solution of the equation looks as

$$\rho_s(\varepsilon, t) = N \varepsilon^{-(\frac{2\gamma}{\sigma^2} + 1)} \exp \left\{ -\frac{2}{\sigma^2} \varepsilon \right\}, \quad (18)$$

which is not equivalent to the equilibrium distribution function.

Let us consider also the so-called phenomenological Rayleigh model of active friction [11] when the coefficient of friction can be written in terms of the velocity in the form $\gamma = -\gamma_0 + \alpha v^2 \equiv \alpha(v^2) - v_0^2$, $v_0^2 = \frac{\gamma_0}{\alpha}$. This model describes a restriction to the coefficient of friction. It becomes negative if $v^2 < v_0^2$, which corresponds, in our representation, to the absorption of energy by the system from the environment. In this case, the stationary distribution function for velocities can be write as

$$\rho_s(v, t) = N \exp \left\{ -\frac{\alpha}{4D} (v^2 - v_0^2)^2 \right\} \quad (19)$$

In the energy representation at the constant coefficient of diffusion, this formula takes the form

$$\rho_s(\varepsilon, t) = N \exp \left\{ -\frac{\alpha}{4D} (\varepsilon - \varepsilon_0)^2 \right\} \quad (20)$$

which corresponds to the Gauss distribution over the energy of the system. In the limit of a low noise $\frac{D}{\alpha} \rightarrow 0$, the largest probability for the system to have the corresponding energy is close to the limiting value, and a stationary distribution is transformed into the delta-function $\rho_s(\varepsilon, t) = N\delta(\varepsilon - \varepsilon_0)$.

Thus, there has been proposed a model describing the nonequilibrium systems with the purpose of determining new stationary states of such a system which are far from equilibrium. There been obtained the stationary distribution functions of nonequilibrium systems for various mechanisms of absorption and dissipation of energy by a system in contact with a nonlinear environment. New admissible states of a nonequilibrium system are defined and a method for their determination is proposed. The conditions under which an equilibrium distribution is realized in the system are determined. Some simple cases can be experimentally verified. In the first turn, this concerns the system of macroscopic particles in a dusty plasma or a system of Brownian particles with the inhomogeneous coefficient of friction.

-
- [1] K. Huang, *Statistical mechanics* (Wiley, New York, 1987).
 [2] R. Balescu, *Equilibrium and nonequilibrium Statistical Mechanics* (Wiley, New York, 1975).
 [3] L. D. Landau, E. M. Lifshits, *Statistical physics* (Pergamon Press, Oxford, 1983).
 [4] D. N. Zubarev, *Nonequilibrium statistical thermodynamics* (Plenum Press, 1974).
 [5] C. W. Gardiner, P. Zoller, *Quantum noise* (Springer, Berlin, 2000).
 [6] D. F. Wells, G. J. Milburn, *Quantum optics* (Springer,

- Berlin, 1994).
 [7] B. I. Lev, A. G. Zagorodny, *Phys. Lett. A* **376** 1101, (2009).
 [8] N. G. van Kampen, *Stochastic processes in physics and chemistry* (Elsevier, Amsterdam, 1992).
 [9] W. Horsthemke, R. Lefever, *Noise-Induced Transitions* (Springer, Berlin, 1984).
 [10] S. Chandrasekhar, *Rev. Mod. Phys.* **15**, 1 (1943).
 [11] J. W. S. Rayleigh, *The theory of sound* (Dover, New York, 1945).

БРОУНІВСЬКИЙ РУХ ЯК МОДЕЛЬ ЕВОЛЮЦІЇ НЕРІВНОВАЖНОЇ СИСТЕМИ

Б. Лев

*Інститут теоретичної фізики ім. М. М. Боголюбова НАН України,
вул. Метрологічна, 14-б, Київ, 03680, Україна*

Згідно з принципами термодинаміки всяка система, яка перебуває в контакті з термостатом, упродовж часу релаксації переходить у рівноважний стан. У статті представлено модель броунівського руху системи, яка дає змогу означити стаціонарний стан системи задовго до переходу в рівноважний стан. Стаціонарна функція розподілу нерівноважного стану не може бути представлена жодною з відомих рівноважних функцій розподілу. Показано, при яких умовах рівноважні стани реалізуються, та передбачено нові стаціонарні стани нерівноважних систем.