USING OF NUMERICAL MODELING FOR VERIFICATION OF THE FUNCTIONAL HYPOTHESIS

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One-dimensional harmonic oscillator in a quasi-equilibrium medium which consists of non-interacting harmonic oscillators has been considered. Kinetic equation for this Brownian particle has been derived on the basis of the Bogolyubov functional hypothesis. Solution of the kinetic equation was numerically compared with an exact solution obtained by Bogolyubov. The results of this comparison are presented in a simple graphic form.

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1. INTRODUCTION

This work is devoted to justification of applicability domain of the Bogolyubov functional hypothesis and his reduced description method (RDM) on the basis of an exact solvable model. The RDM (which is based on the functional hypothesis) is one of basic approaches to investigation of nonequilibrium processes, therefore the interest in its verification has become clear.

The kinetics of a one-dimensional harmonic oscillator in a quasi-equilibrium medium which consists of non-interacting harmonic oscillators is investigated in this work. The interaction between the oscillator and the environment is supposed to be weak. This model was considered in the paper of Bogolyubov [1], where he has found its exact solution in a very complex form.

The state of the aforesaid system is completely described by the distribution function $\rho(x_0, X, t)$, where x_0 are phase variables of the oscillator and X are phase variables of the medium. The quasi-equilibrium environment is described by the equilibrium thermodynamic parameters, which in general can depend on time because of a reverse influence of the oscillator on the medium. The energy of the medium $E_m(t)$ is selected as such parameter.

We consider simplification in description of the system when its state is determined by the distribution function of energy of the oscillator $w(E,t)$ and by the energy of the medium $E_m(t)$. According to the functional hypothesis the distribution function of the system at long times has the structure $\rho(x_0, X, w(t), E_m(t))$. We have derived an integral equation for the distribution $\rho(x_0, X, w, E_m)$, and also a system of kinetic equations

$$\dot{w}(E,t) = L(E, w(t), E_m(t)),$$

$$\dot{E}_m(t) = L_m(w(t), E_m(t)).$$

The mentioned values were calculated in a perturbation theory in small interaction between the Brownian oscillator and the medium.

The analytical results obtained for $w(E,t)$ by the RDM are numerically compared with the Bogolyubov exact solution.

2. THE KINETIC EQUATION OF BOGOLUBOV'S MODEL IN THE REDUCED DESCRIPTION METHOD

The Hamiltonian for our model is the following

$$H = H_b + H_m + H_{bm}, \tag{1}$$

where the subscript b refers to the Brownian harmonic oscillator with a frequency ω_0

$$H_b = \frac{1}{2}(p_0^2 + \omega_0^2 q_0^2), \tag{2}$$

the subscript m refers to the medium consisting of a big number of harmonic oscillators with frequencies ω_a

$$H_m = \frac{1}{2}\sum_{a=1}^{N}(p_a^2 + \omega_a^2 q_a^2). \tag{3}$$

The Hamiltonian of interaction H_{bm} is given by

$$H_{bm} = \sum_{a=1}^{N}\alpha_a q_a q_0, \tag{4}$$

where α_a are the small values ($\alpha_a \sim \varepsilon$, $\varepsilon \ll 1$).

Let the initial (when $t = 0$) phase variables of the Brownian oscillator are q_0^0, p_0^0; and phase variables of the medium $\{q_a, p_a\}$ are canonical distributed random variables:

$$w_b = e^{\frac{F - H_b}{T}} \tag{5}$$

(here and further T stands for kT).

The Liouville equation for the distribution function of the system is the following

$$\rho(x_0, X, t) = \mathbf{L}\rho(x_0, X, t), \tag{6}$$

where

$$\mathbf{L} = \mathbf{L}_b + \mathbf{L}_m + \mathbf{L}_{bm} = \mathbf{L}_0 + \mathbf{L}_{bm},$$

$$\mathbf{L}_m = -p_0\frac{\partial}{\partial q_0} + \omega_0^2 q_0\frac{\partial}{\partial p_0},$$

$$\mathbf{L}_b = -\sum_{a=1}^{N} p_a\frac{\partial}{\partial q_a} + \sum_{a=1}^{N}\omega_a^2 q_a\frac{\partial}{\partial p_a},$$

$$\mathbf{L}_{bm} = \sum_{a=1}^{N}\alpha_a q_a\frac{\partial}{\partial p_0} + \sum_{a=1}^{N}\alpha_a q_0\frac{\partial}{\partial p_a} \tag{7}$$

and

$$x_0 \equiv (p_0, q_0),\ x_a \equiv (p_a, q_a),\ X \equiv (x_1, \ldots, x_n). \quad (8)$$

The distribution function $\rho(x_0, X, t)$ satisfies the normalization condition

$$\int dx_0 dX \rho(x_0, X, t) = 1. \quad (9)$$

The formal solution of the Liouville equation can be written as

$$\rho(x_0, X, t) = e^{\mathbf{L}t} \rho_0(x_0, X), \quad (10)$$

where

$$\rho_0(x_0, X) = \rho(x_0, X, 0).$$

We will consider a kinetic stage of the evolution, when the simplification in the description of the system state takes place and it is determined by the distribution function $w(E,t)$ of the Brownian oscillator energy and by the medium energy $E_m(t)$. It means that at time, considerably larger that time τ_0, according to a functional hypothesis, $\rho(x_0, X, t)$ should have the following structure

$$\rho(x_0, X, t) \xrightarrow[t \gg \tau_0]{} \rho(x_0, X, w(t), E_m(t)), \quad (11)$$

where reduced description parameters $w(E,t)$, and $E_m(t)$ are defined by relations

$$\int dx_0 dX \rho(x_0, X, t) \delta(E - H_s) \xrightarrow[t \gg \tau_0]{} w(E,t),$$
$$\int dx_0 dX \rho(x_0, X, t) H_m \xrightarrow[t \gg \tau_0]{} E_m(t). \quad (12)$$

The Liouville equation (6) at times $t \gg \tau_0$ takes the form

$$\dot{\rho}(x_0, X, w(t), E_m(t)) = \mathbf{L}\rho(x_0, X, w(t), E_m(t)). \quad (13)$$

This equation and definitions Eqs.(14) lead to the following equation for $w(E,t)$

$$\dot{w}(E,t) = L(E, w(t), E_m(t)),\ (t \gg \tau_0), \quad (14)$$

where

$$L(E, w, E_m) \equiv$$
$$\equiv \frac{\partial}{\partial E} \int dx_0 dX \rho(x_0, X, w, E_m) \delta(E - H_s) \sum_{a=1}^{N} \alpha_a q_a p_0 \ . (15)$$

The kinetic equation for $E_m(t)$ is given by the formula

$$\dot{E}_m(t) = L_m(w(t), E_m(t)),\ (t \gg \tau_0), \quad (16)$$

where

$$L_m(w, E_m) \equiv .$$
$$\equiv -\int dx_0 dX \rho(x_0, X, w, E_m) \sum_{a=1}^{N} \alpha_a q_0 p_a. \quad (17)$$

The Liouville equation at the reduced description Eq.(13) can be written due to Eqs. (14), (16) in the form

$$\mathbf{L}\rho(x_0, X, w, E_m) = \int dE \frac{\delta \rho(x_0, X, w, E_m)}{\delta w(E)} L(E, w, E_m)$$
$$+ \frac{\partial \rho(x_0, X, w, E_b)}{\partial E_b} L_b(w, E_b). \quad (18)$$

For this equation we use the following boundary condition of the complete correlation

$$e^{\mathbf{L}_0 \tau} \rho(x_0, X, w, E_m) \xrightarrow[t \gg \tau_0]{} e^{\mathbf{L}_0 \tau} \rho_q(x_0, X, w, E_m),$$
$$\rho_q(w, E_m) \equiv \frac{\omega_0}{2\pi} w(H_b) w_m(E_m). \quad (19)$$

By an usual way [2,3] Eq. (18) with condition (19) give the following integral equation for distribution function $\rho(w, E_m)$

$$\rho(w, E_m) = \rho_q(w, E_m) + \int_0^{+\infty} d\tau e^{\mathbf{L}_0 \tau} \{ \mathbf{L}_{bm} \rho(w, E_m)$$
$$- \int dE \frac{\delta \rho(w, E_m)}{\delta w(E)} L(E, w, E_m) - \frac{\partial \rho(w, E_m)}{\partial E_m} L_m(w, E_m) \} . . (20)$$

We solve this Eq. (20) for $\rho(x_0, X, w, E_m)$ with expressions Eqs. (15), (17) for $L(E, w, E_m)$ and $L_m(w, E_m)$ by iterations in a perturbation theory in interaction constant ε.

The results of the calculations up to second order in ε are the following

$$\rho^{(0)} = \rho_q(w, E_m);\ L^{(1)} = 0,\ L_m^{(1)} = 0;$$
$$\rho^{(1)} = \frac{\omega_0}{2\pi} w_b \int_0^{\infty} d\tau e^{\tau \mathbf{L}_0} \sum_{a=1}^{N} \alpha_a \left\{ q_a p_0 \frac{\partial w(E)}{\partial E} \right.$$
$$\left. - q_0 p_a \frac{1}{T} w(E) \right\}_{E \to H_b},\ L_m^{(2)} = 0. \quad (21)$$

The formula for $\rho^{(1)}$ gives kinetic equation for $w(E,t)$

$$\dot{w}(E,t) = \frac{\pi}{2} T I(\omega_0) \frac{\partial}{\partial E} \left\{ E \left(\frac{\partial}{\partial E} + \frac{1}{T} \right) w(E,t) \right\}, \quad (22)$$

where

$$I(\omega) = \sum_{a=1}^{N} \frac{\alpha_a^2}{\omega_a^2} \delta(\omega - \omega_a). \quad (23)$$

So, we have obtained the necessary kinetic equation on the basis of the RDM. In the considered approximation the dependence of the medium energy $E_m(t)$ on time is absent.

3. NUMERICAL COMPARISON OF THE RESULTS OF DIFFERENT APPROACHES

Bogolyubov has obtained the exact expression for distribution function of the Brownian oscillator $\rho_b(q_0, p_0, t)$ in thermodynamic limit (when $N \to \infty$) in form

$$\rho_b(q_0, p_0, t) = \Phi(q_0 - q^*(t), p_0 - p^*(t), t), \quad (24)$$

where

$$q^*(t) = q_0^0 v'(t) + p_0^0 v(t),$$
$$p^*(t) = q_0^0 v''(t) + p_0^0 v'(t), \quad (25)$$

and

$$\Phi(\xi, \eta, t) = \frac{1}{2\pi\sqrt{AC - B^2}} \exp\left\{ \frac{C\xi^2 - 2B\xi\eta + A\eta^2}{2(B^2 - AC)} \right\}. \quad (26)$$

The functions $A(t)$, $B(t)$, $C(t)$ are coefficients of the quadratic form

$$A(t)\lambda^2 + 2B(t)\lambda\mu + B(t)\mu^2$$

$$= T\int_0^\infty d\omega I(\omega)\left|\int_0^t d\tau\{\lambda\nu(\tau) + \mu\nu'(\tau)\}e^{-i\omega\tau}\right|^2 . \qquad (27)$$

Here function $\nu(t)$ is the solution of the following differential equation

$$\nu''(t) + \omega_0^2\nu(t) = \int_0^t d\tau\, Q(t-\tau)\nu'(\tau) , \qquad (28)$$

with initial conditions $\nu(0) = 0$, $\nu'(0) = 1$, where

$$Q(t) = \int_0^\infty d\omega I(\omega)(1-\cos\omega t). \qquad (29)$$

The comparison of the exact solution and the result of the RDM consists in analysis of the difference between exact distribution of energy

$$P(E,t) = \int_{(H_b<E)} dq_0 dp_0 \rho_b(q_0, p_0, t)$$

$$= \int_{-\sqrt{2E}}^{\sqrt{2E}} dp_0 \int_{-q(E,p_0)}^{q(E,p_0)} dq_0 \rho_b(q_0, p_0, t) ,$$

$$q(E, p_0) = \frac{\sqrt{2E - p_0^2}}{\omega_0} \qquad (30)$$

and distribution

$$P_0(E,t) = \int_0^E dE' w(E',t) \qquad (31)$$

calculated on the basis of the RDM.

Kinetic equation (22) for distribution function $w(E,t)$ is solved by us numerically in dimensionless form

$$\frac{\partial w(\tilde{E},\tilde{t})}{\partial\tilde{t}} = \frac{\pi}{2}\frac{\partial}{\partial\tilde{E}}\left\{\tilde{E}\left(\frac{\partial}{\partial\tilde{E}} + 1\right)w(\tilde{E},\tilde{t})\right\},$$

$$\tilde{E} = \frac{E}{T},\ \tilde{t} = t\lambda^2 ,\ \lambda \equiv I(\omega_0) , \qquad (32)$$

with the following boundary conditions

$$w(\tilde{E},\tilde{t}) \to e^{-\tilde{E}} ,\ \tilde{t} \to +\infty ;$$

$$w(\tilde{E},\tilde{t}) \to \delta(\tilde{E} - \tilde{E}_0) ,\ \tilde{t} \to 0 ;$$

$$w(\tilde{E},\tilde{t}) \to 0 ,\ \tilde{E} \to +\infty. \qquad (33)$$

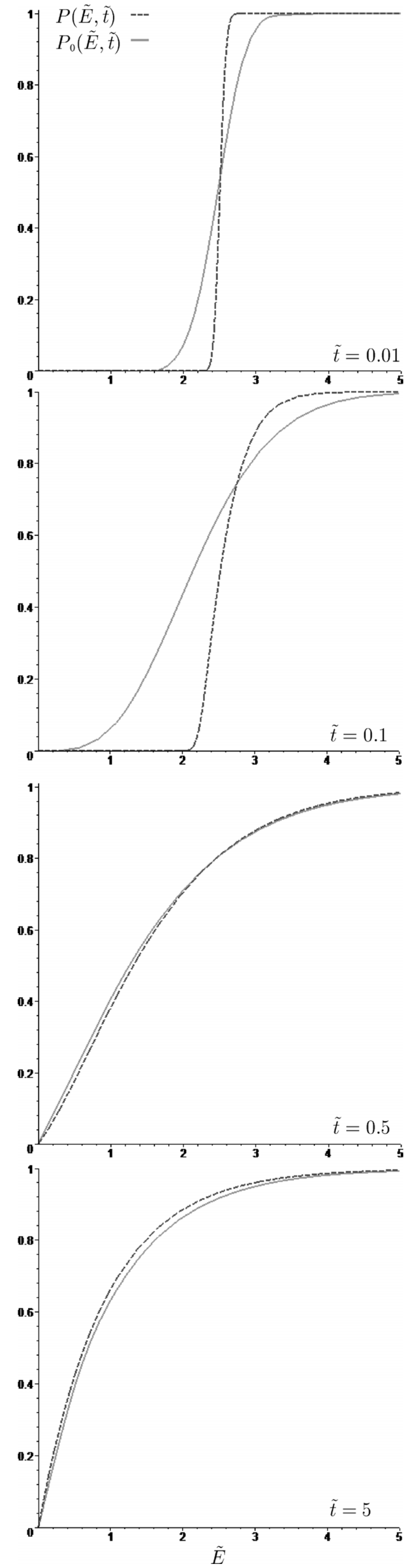
The differential equation (30) has a form of the second Newton's law with a complex dissipative force and is numerically integrated too.

The results of a graphical comparison of the distributions $P_0(E,t)$ and $P(E,t)$ at different times are shown in the figure. The parameters of this experiment are

$$\lambda = 0.006, \quad \tilde{E}_0 = 2.5, \quad \omega_0 = 0.001\, s^{-1}.$$

First two graphics show essential distinctions between the distributions at initial time, but their further evolution (when $t \gg 0.5\lambda^{-2}$) is almost identical and they approach to the equilibrium distribution.

Thus, we have performed the comparison of exact and approximate solutions and have displayed their closeness at long times.



Comparison of the distributions $P(E,t)$ and $P_0(E,t)$ at different times. Dotted line shows the exact solution, solid line shows the result of the reduced description method

4. CONCLUSION

We have numerically compared solution of the approximate kinetic equation, which is obtained with the help of functional hypothesis, with the exact solution. It was shown that at long times the RDM leads to energy distributions which are close to one another.

In the next paper we plan to compare the Bogolyubov exact result with consequences of the kinetic equation of the third order approximation in interaction.

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ИСПОЛЬЗОВАНИЕ ЧИСЛЕННОГО МОДЕЛИРОВАНИЯ ДЛЯ ПРОВЕРКИ ФУНКЦИОНАЛЬНОЙ ГИПОТЕЗЫ

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Рассмотрен одномерный гармонический осциллятор в квазиравновесной среде, которая состоит из невзаимодействующих гармонических осцилляторов. На основе функциональной гипотезы Боголюбова получено кинетическое уравнение для этой броуновской частицы. Решение кинетического уравнения численно сравнено с точным решением, полученным Боголюбовым. Результаты сравнения представлены в простой графической форме.

ВИКОРИСТАННЯ ЧИСЕЛЬНОГО МОДЕЛЮВАННЯ ДЛЯ ПЕРЕВІРКИ ФУНКЦІОНАЛЬНОЇ ГІПОТЕЗИ

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Розглянуто одновимірний гармонічний осцилятор у квазірівноважному середовищі, яке складається з гармонічних осциляторів, що не взаємодіють. На основі функціональної гіпотези Боголюбова одержано кінетичне рівняння для цієї броунівської частинки. Розв'язок кінетичного рівняння чисельно порівняно з точним розв'язком, одержаним Боголюбовим. Підсумки порівняння представлені в простій графічній формі.