The Brownian motion in statistically equilibrium correlated systems: numerical simulation

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In this work we present the new results of numerical investigation of mass-transfer processes in correlated systems within the wide range of parameters, corresponding to the conditions of experiments in laboratory dusty plasmas. The diffusion is the main mass-transfer process, which defines the energetic losses (dissipation) in the system and its dynamical characteristics. In case of small deviations of the considered homogeneous system from the statistical equilibrium, its diffusion coefficient D can be derived from the time dependences of the mass-transfer evolution functions $D_{GK}(t)$ and $D_m(t)$: $D \equiv \lim_{t\to\infty} D_{GK}(t)$ and $D \equiv \lim_{t\to\infty} D_m(t)$, respectively, where $D_{GK}(t) = \int_0^t \langle V_x(0)V_x(t')\rangle dt'$, $D_m(t) = <(x)^2>/(2t)$. Here $<V_x(0)V_x(t)>$ is an autocorrelation function of the grains' velocities, t is the time, $V = V_x(t) \equiv dx_j/dt$ is the velocity of j-th particle in the certain direction **x**, $x = x_j(t)$ is the displacement of the j-th particle along one coordinate, and the brackets $< >$ denote the ensemble and time averaging (the averaging over all time intervals with the duration t). [1-4]. To describe the Brownian motion, the Langevin system of equations with the random force F_{ran} is usually used [2-4]. In this case, the displacement of a j-th grain along the chosen coordinate $x = x_j(t)$ for the time t in a homogeneous quasi-equilibrium medium under an action of some potential force F_p is described by the solution of the following system of differential equations [2-4]:

$$M\frac{d^2x}{dt^2} = -Mv_{fr}\frac{dx}{dt} + F_p + F_{ran}\,. \qquad (1)$$

The cases of non-interacting particles ($F_p = 0$) and a single Brownian particle in the linear harmonic trap ($F_p = -M\omega_c^2 x$) were considered in [2, 4-7]. Nevertheless, these cases, as well as the other existing analytical approaches, don't imply the description of the transition from the ballistic to the diffusive regime for the system of *interacting* grains (with the nonzero interparticle interaction potential φ), and the role of the number of these grains $N_p \neq 1$ in their Brownian motion [1-4, 7-10].

To describe the motion of interacting particles in a liquid ($D \neq 0$), we need to take into account the dependence of the force F_p in the system (1) from the fluctuations of electrical field

δE, which are induced by the thermal motion of grains with a charge Q. To the first approximation this force can be introduced as $F_p = -Q\delta E$ and described by the equation

$$\partial F_p / \partial t = -2M\omega_c^2 V - \sigma F_p, \qquad (2)$$

where σ is the characteristic frequency of fluctuations of the electric field caused by the thermal motion of interacting particles, which is defined by their mobility coefficient. The solution of equations (1) and (2) gives for $V = V_x(t)$

$$M\frac{d^2V}{dt^2} = -M(\nu_{fr} + \sigma)\frac{dV}{dt} - M(2\omega_c^2 + \nu_{fr}\sigma)V + \sigma F_{ran} + \frac{dF_{ran}}{dt}. \qquad (3)$$

Further, assuming $\langle F_{ran}\ V_x(0)\rangle = 0$ [3, 4] and the boundary conditions $\langle x^2\ (t=0)\rangle = 0$; $\left.\frac{d\langle x^2\rangle}{dt}\right|_{t=0} = 0$; $\langle V_o V\rangle\big|_{t=0} = T/M$; $\int_0^\infty \langle V_o V\rangle dt = D$, we get the solution

$$\langle x^2(t)\rangle = 2C_1\left(\frac{t}{\gamma-\omega_1} - \frac{1-\exp(-(\gamma-\omega_1)t)}{(\gamma-\omega_1)^2}\right) + 2C_2\left(\frac{t}{\gamma+\omega_1} - \frac{1-\exp(-(\gamma+\omega_1)t)}{(\gamma+\omega_1)^2}\right), \qquad (4)$$

where $\gamma = (\sigma+\nu_{fr})/2$, $\omega_1 = (\gamma^2 - \{2\omega_c^2+\sigma\nu_{fr}\})^{1/2}$, $(C_1+C_2)=T/M$, and $(C_1/\{\gamma-\omega_1\}+C_2/\{\gamma+\omega_1\})=D$. Using the relationship (4), we can obtain the both mass-transfer evolution functions as $D_{GK}(t) = \frac{1}{2}\frac{d\langle x^2\rangle}{dt}$ and $D_m(t) = \langle(x)^2\rangle/(2t)$. In case $\sigma = 0$, $\omega_c \neq 0$ this solution for $D_{GK}(t)$ and $D_m(t)$ transforms in the known relationships for the harmonic oscillator ($D = 0$); and when $\sigma = 0$ and $\omega_c = 0$, it fully corresponds the case of non-interacting grains, where $D = D_o$. The value of σ can be obtained from the Eqs. (1) and (3) after averaging and some simple mathematical manipulations:

$$\sigma = \frac{b\omega_c^2 DM/T}{1 - DM\nu_{fr}/T}, \qquad (5)$$

For the numerical simulation we used the Langevin molecular dynamics method, based on the solution of the system of N_p ordinary differential equations of motion (where N_p is the number of particles in the calculation cell), taking into account the Langevin force F_{ran} and the forces of pair interparticle interaction F_{int}. The simulation technique is detailed in [8]. The simulations were made for the Yukawa systems with the screening parameters $\kappa \equiv r_p/\lambda = 1 \div 4$ (where $r_p = (N_p/S)^{1/2}$, S is the square of the simulated cell for two-dimensional systems, and $r_p = (N_p/V)^{1/3}$, V is the volume of the simulated cell for three-dimensional systems, respectively).

The calculations were carried out for the homogeneous three-dimensional system and for the two-dimensional system simulating the extensive dust layer; the periodical boundary conditions were used. In the first case the number of independent particles N_p in the central cell

was varied from 250 to 686; accordingly, the potential of the interparticle interaction was cut on the distance $r_{cut} \sim 4r_p$ - $8r_p$. For the simulation of the extensive dust layer the number of independent particles in the central cell N_p was varied from 256 to 4096. Dependent on the number of particles, the cut-off length r_{cut} varied from $5r_p$ to $25r_p$. The main calculations were performed for $N_p = 1024$ independent particles with the cut-off length of potential $r_{cut} = 12r_p$.

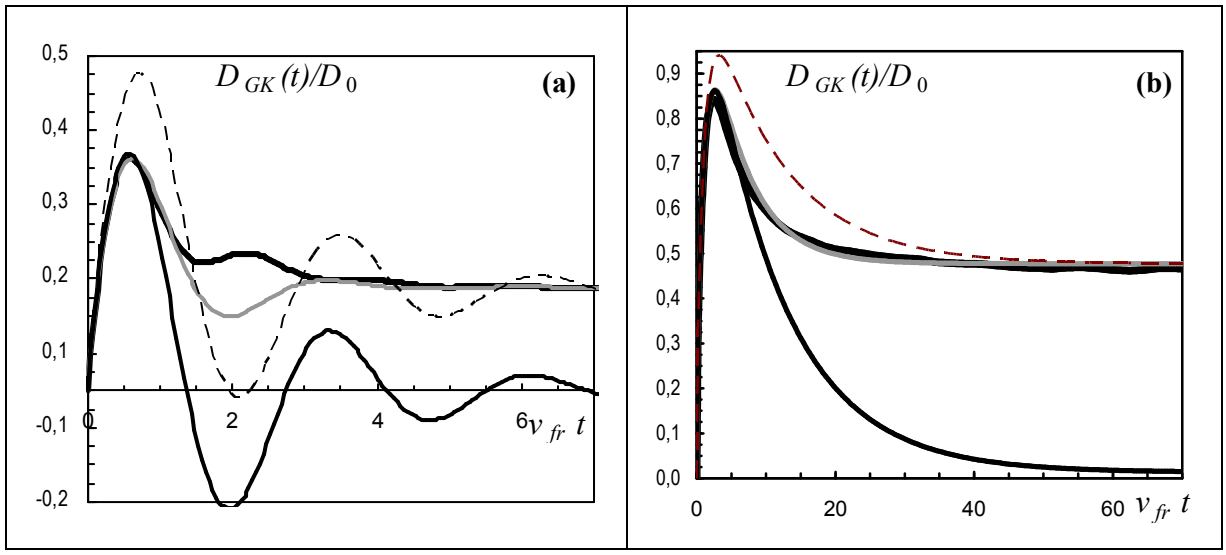

Fig.1. The functions $D_{GK}(\nu_{fr}\, t)/D_o$ for the numerical experiments in 2D–structures, κ =2 (bold black lines) and parameters ξ =1, Γ^*= 45 (**a**) and ξ =0.125, Γ^*=10 (**b**). The gray lines denote the proposed analytical approximations; the fine black lines – the case of the harmonic oscillator (σ =0, D = 0), the dotted line – the solution (4) at σ =0 and $D \neq 0$.

It is easy to see that the analytical curves describe the evolution of mass-transfer functions pretty well, including the dynamics of the transition between the ballistic and diffusive regimes, in contrast to the harmonic approximation, which fits well on short observation times only (see Figs 1(a), 1(b)). The same figures 1(a), 1(b) show the functions $D_{GK}(\nu_{fr}t)$, obtained by solving Eq. (4) with $\sigma = 0$ and $D \neq 0$, which give only approximate qualitative/quantitative picture of evolution of the grains motion to the diffusive regime. Nevertheless, we should note that the proposed approximation (4) even with $\sigma \neq 0$ (5) doesn't include the possibility of development of additional high-frequency oscillations in correlated systems with $\Gamma^* >$ 2-3. These oscillations can be easily observed at low friction $\xi_c > 8^{-1/2}$, and their formation can result from the emerging of longitudinal and transverse modes in low-dissipative media [11]. Note also that the oscillations in these systems ($\xi_c > 8^{-1/2}$) practically don't show up in the behavior of functions $D_m(t)$, see Fig. 2.

The best agreement with the analytical model was observed for the strongly dissipative systems ($\xi_c < 8^{-1/2}$). In case of strongly correlated structures with the low friction ($\xi_c > 8^{-1/2}$), the more detailed quantitative analysis of the behavior of mass-transfer evolution functions should be done, taking into account the spatial dependence of fluctuations of the electrical field.

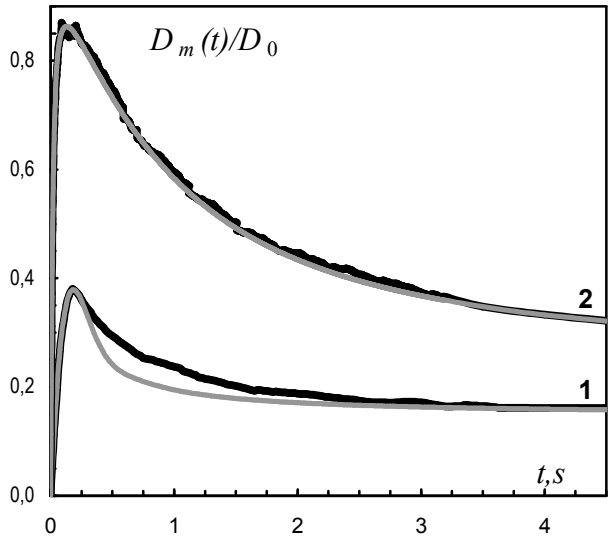

Fig.2. The functions $D_m(t)/D_0$ for the numerical experiments in 3D – structures (bold black lines), $\Gamma^* = 80$, $\kappa = 3$ with the parameters $\xi = 0.4$, $\nu_{fr} = 10\ s^{-1}$ (**1**) and $\xi = 0.04$, $\nu_{fr} = 100\ s^{-1}$ (**2**). The gray lines denote the proposed analytical approximations.

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