METHOD OF INTEGRALS OVER TRAJECTORIES IN THE HYDROMECHANICS OF SUSPENSIONS

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The apparatus of Feynman integrals over trajectories is used to derive continual conservation equations for suspension phases and to analyze particle diffusion in a fluidized bed.

Construction of the principles of disperse system hydromechanics is fraught with serious difficulties, due to a significant degree to the stochastic nature of these systems and the necessity to develop and give a foundation to special new methods of investigation that combine the traditional methods of mechanics with certain ideas about averaging which are specific for statistical physics. Consequently, searches and the application of new, in principle, and sufficiently constructive approaches are of substantial interest in this rapidly developing region of science. One such approach can be based on the analysis of possible trajectories of the system in its phase space and on the integration procedure using the Wiener probabilistic measure in the space of these trajectories.

The approach mentioned is used below on two different kinds of problems, on deriving the fundamental continual conservation equations for the suspension phases of spherical particles, and on the description of random displacements of one particle. The most sequential of the known solutions of the first problem is related to using the averaging procedure developed in [1, 2] for the local "microscopic" conservation equations in the ensemble of spatial particle configurations given by the instantaneous positions (but not the velocity, acceleration, etc., vectors) of the centers of all particles. As can be shown [3], the use of such an ensemble is actually equivalent to a very limiting assumption that the particle translational motion velocities are proportional to the forces acting on them, i.e., to a known quasistationary "strong friction" approximation. Application of the approach proposed in this paper permits getting rid of the constraint mentioned by extending the fundamental equations to arbitrary situations in which the ensemble of states is defined not only by the set of vectors fixing the location of the centers of the particles, but also their time derivatives.

Analysis of the second problem permits proposing an alternative method of describing the statistical properties of random trajectories of separate particles in ordinary space, and giving a physical interpretation for their displacement as specific realizations of a Brownian motion random process that turns out to be useful for processing appropriate experimental results. As an illustration we examine particle displacement in a fluidized bed.

1. Derivation of Continual Equations. The probability of object passage through a "window" $(a_1, b_1), \ldots, (a_n, b_n)$ at the times $t_1, \ldots, t_n$ for the trajectory peak represented in Fig. 1 (corresponding to a one-dimensional process) is determined by the expression [4]:

$$P_{t_1, \ldots, t_n} = \int\limits_{a_1}^{b_1} \cdots \int\limits_{a_n}^{b_n} P(0 \mid x_1, t_1 - t_0) \cdots P(x_{n-1} \mid x_n, t_n - t_{n-1})\, dx_1 \cdots dx_n. \tag{1}$$

As $n \to \infty$ this expression (1) goes over into an infinite integral over the Feynman trajectories [5], where the differential volume element in the trajectory functional space is the Wiener measure. The probability that the trajectory will belong to a certain class A, as well as the mean of an arbitrary functional $G[x(t)]$, are expressed in terms of Feynman integrals over trajectories thus [5]:

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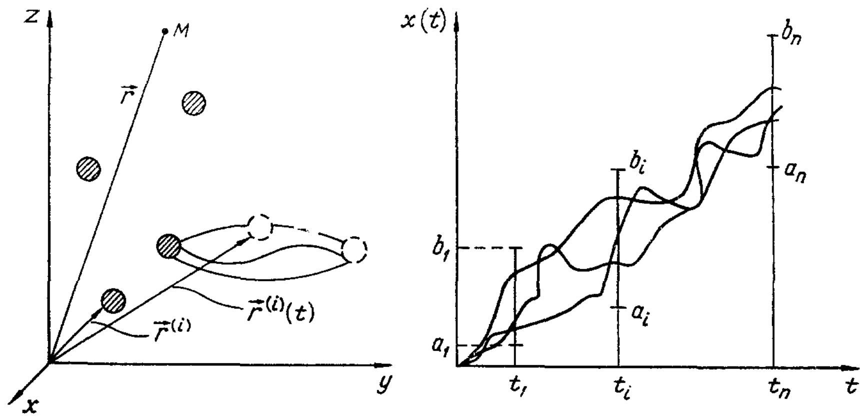

Fig. 1. Random trajectories in one-dimensional phase space.

$$P_A = \int_A P\,[x(t)]\,Dx\,(t), \quad \langle G \rangle = \int_A G\,[x(t)]\,P\,[x(t)]\,Dx\,(t). \tag{2}$$

It is assumed here that the probability density functions P[x(t)] is normalized to unity. The relationships (2) are easily extended to phase trajectories in the space of three or more dimensions.

As in [1, 2], we consider a suspension containing N spherical particles. The state of the particle system is described at any time by a point in the phase space of the coordinates of the particle centers and their time derivatives $\{\mathbf{r}^{(1)}(t), \ldots, \mathbf{r}^{(N)}(t), \dot{\mathbf{r}}^{(1)}(t), \ldots, \dot{\mathbf{r}}^{(N)}(t), \ldots\}$ and its behavior is described by trajectories in this space x(t). The local physical quantities (density, momentum, moment of momentum, different kinds of energy, entropy, etc.) denoted by the common symbol G can be considered as functionals of the trajectories, i.e., $G = G(t, \mathbf{r}, [x(t)])$. The mean value of G for a suspension is in conformity with (2)

$$\langle G \rangle (t, \mathbf{r}) = \int G(t, \mathbf{r}, [x(t)])\,P\,[x(t)]\,Dx\,(t). \tag{3}$$

If the generalized functions

$$\Theta_0(\mathbf{r}, [x(t)]) = \begin{cases} 1, & \mathbf{r} \in V_0\,[x(t)], \\ 0, & \mathbf{r} \in V_1\,[x(t)], \end{cases} \quad \Theta_1(\mathbf{r}, [x(t)]) = 1 - \Theta_0,$$

are introduced, then it is easy to define the means over the phases in an analogous manner [1, 2]:

$$\begin{aligned} \langle \Theta_0 G \rangle (t, \mathbf{r}) &= \int \Theta_0(\mathbf{r}, [x(t)])\,G(t, r, [x(t)])\,P\,[x(t)]\,Dx\,(t), \\ \langle \Theta_1 G \rangle (t, \mathbf{r}) &= \int \Theta_1(\mathbf{r}, [x(t)])\,G(t, r, [x(t)])\,P\,[x(t)]\,Dx\,(t). \end{aligned} \tag{4}$$

Since the integrals over the trajectories possess the properties of Lebesgue integrals, they can be differentiated under the integral sign with respect to the independent variable **r** playing the part of a parameter. If, in addition, the inequality $t \gg \tau$ is satisfied, where τ is the "microscopic" time scale at the level of the individual particles, it can be considered approximately that the operations of differentiation with respect to the time and integration in the functional space of the trajectories will commutate. We then have from (4)

$$\begin{aligned} &\left\langle \frac{\partial}{\partial \mathbf{r}}\,\Theta_0 G \right\rangle = \frac{\partial}{d\mathbf{r}}\,\langle \Theta_0 G \rangle, \quad \left\langle \frac{\partial}{d\mathbf{r}}\,\Theta_1 G \right\rangle = \frac{\partial}{\partial \mathbf{r}}\,\langle \Theta_1 G \rangle, \\ &\left\langle \frac{\partial}{\partial t}\,\Theta_0 G \right\rangle = \frac{\partial}{\partial t}\,\langle \Theta_0 G \rangle, \quad \left\langle \frac{d}{\partial t}\,\Theta_1 G \right\rangle = \frac{\partial}{\partial t}\,\langle \Theta_1 G \rangle. \end{aligned} \tag{5}$$

Writing the Feynman integrals (4) of the left and right sides of the local balance equation

$$\frac{dG}{dt} = -\frac{\partial \mathbf{Q}}{\partial \mathbf{r}},$$

which expresses the rate of change of the quantity G in terms of the divergence of the corresponding flux **Q**, and taking (5) into account, we obtain

$$\left\langle \Theta_0 \frac{dG}{dt} \right\rangle = \frac{\partial}{\partial \mathbf{r}} \langle \mathbf{Q} \rangle - \left\langle \Theta_1 \frac{\partial \mathbf{Q}}{\partial \mathbf{r}} \right\rangle, \quad \left\langle \Theta_1 \frac{dG}{dt} \right\rangle = \left\langle \Theta_1 \left\langle \frac{\partial \mathbf{Q}}{\partial \mathbf{r}} \right\rangle \right\rangle. \tag{6}$$

In principle, the system (6) contains all the continual conservation equations obtained earlier in [1, 2], as well as in [6, 7], and agrees in form. However, no constraints were imposed on the properties of the statistical ensemble of states in the derivation of (6), but just the fact of the existence of the random trajectories x(t), which can be nondifferentiable in the general case, was used. (This latter is important, in principle, since jumplike changes in the particle velocities and their time derivatives during collisions correspond to phase trajectory discontinuities.) Consequently, the system (6) possesses a considerably higher degree of generality than follows from its derivation in [1, 2, 6, 7] which is based on the utilization of just an ensemble of particle configurations at a certain time.

If we go over to the trajectory of a single particle in its coordinate space in the integrals (3) and (4) then, in principle, the so-called problem of a "trial" particle can be formulated, whose solution will permit finding the viscosity and other effective properties of the suspension and will thereby close the system of equations (6).

2. Random Particle Behavior. The dispersed phases in real particle fluxes participate in ordered average motion of this phase, which can be described by solving the appropriate boundary value problem for (6). Moreover, because of random particle interactions and with the pressure and velocity field fluctuations of the dispersion medium that exist in not only turbulent but also laminar flows of disperse mixtures, the individual particles are entrained into chaotic fine-scale motion. Phenomenologically the total particle motion can be represented by using the Langevin equation which has the following form in the one-dimensional case:

$$\frac{dv}{dt} + \beta v = A(t), \qquad A(t) = A_1(t) + A_2(t). \tag{7}$$

The total force in (7) is represented in the form of the sum of two components, the first of which describes the regular action from the average flow of the dispersion medium and the external mass forces while the second characterizes the purely random action on the particle under consideration by the other particles and the random fluctuations of the dispersion medium.

Separation of the total particle motion into regular associated with the large-scale circulation flows and fine-scale chaotic is especially significant for fluidized systems [8]; the Langevin equations method was applied to such systems in [9].

Following [10], we represent the mean value of the regular force acting on a particle by the relationship $A_1 = \eta\beta v$, where the weight factor η takes account of the statistical properties of this force. The physical meaning of the quantity η will be cleared up below. The particle motion described by (7) possesses the Gaussian properties of a Markov process [11] under the usual assumptions about the properties of $A_2(t)$, where the correlation function for the particle velocity with the expression for A_1 taken into account is represented in the form

$$R_{vv'}(t, t') = \langle v^2 \rangle (1-\eta)^2 \exp[-\beta(1-\eta)|t-t'|]. \tag{8}$$

The rms particle bias can be expressed by standard means in terms of the second variational product of the characteristic functional of the process, which in the most general case may be written as follows for a Gaussian process [5]:

$$\Phi[k(t)] = \exp[i \int k(t) F(t)\, dt] \exp\left[-\frac{1}{2} \iint k(t) k(t') R_{xx'}(t, t')\, dt dt'\right], \tag{9}$$

where $R_{xx'}(t, t')$ is the correlation function for the particle coordinate for which we obtain, on the basis of (8),

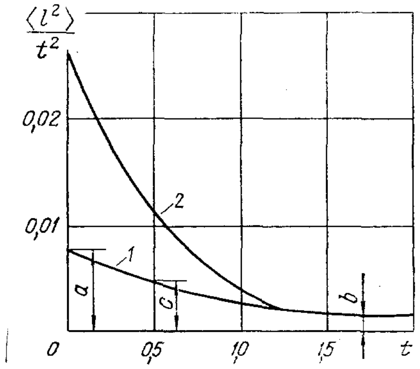

Fig. 2

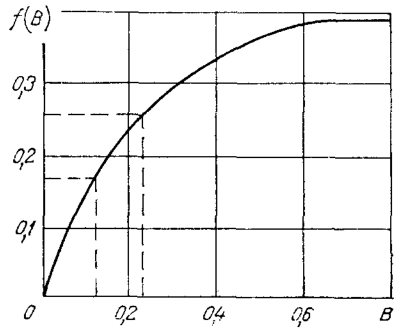

Fig. 3

Fig. 2. Time dependence of $\langle l^2\rangle/t^2$ calculated from the experimental data in [16]: 1, 2) w = 1.19 and 1.62 m/sec; t, sec; $\langle l^2\rangle/t^2$, m^2/sec^2.

Fig. 3. Dependence of the left side of (17) on B.

$$R_{xx'}(\tau, s) = \int_0^\tau\int_0^s R_{vv'}(t, t')\,dt\,dt' = \frac{\langle v^2\rangle(1-\eta)}{\beta}\left[\tau - \frac{\varphi(\tau)}{\beta(1-\eta)} + s - \frac{\varphi(s)}{\beta(1-\eta)} - |\tau - s| + \frac{\varphi(\tau - s)}{\beta(1-\eta)}\right], \quad \varphi(\tau) = 1 - \exp[-\beta(1-\eta)/\tau]. \tag{10}$$

Omitting the details of calculating the variational derivative, we arrive at the result

$$\langle x^2\rangle = -\left.\frac{\delta^2\Phi}{\delta k(s)\,\delta k(\tau)}\right|_{k=0,\ s=\tau=t} = F^2 + R_{xx'}|_{s=\tau=t} = \langle v\rangle^2\eta^2t^2 + 2\frac{\langle v^2\rangle(1-\eta)}{\beta}\left[t - \frac{\varphi(t)}{\beta(1-\eta)}\right]. \tag{11}$$

Only a stationary random process was actually considered in the calculations and the representations (9) and (10) as well as the expression $F^2 = \langle v\rangle^2\eta^2t^2$ for a regular contribution to $\langle x^2\rangle$ corresponding to the representation used above for A_1 and describing particle drift with mean velocity $\langle v\rangle$ were taken into account. The quantity $D = \langle v^2\rangle/\beta$ in (11) has the meaning of an effective particle diffusion factor.

The result (11) allows interpretation on the basis of a representation of Brownian vector motion proposed in [12] for the description of random trajectories of biological (live) objects. If the particle displacement is represented as the successive imposition of M separate elementary shifts (ranges) then the latter can be separated into M' "vector" (directional) and M" "Brownian" (chaotic) ranges, where M = M' + M". The fraction $\eta = M'/M$ as $M \to \infty$ is the degree of vectorization of the random motion. Since vectorization of the ranges is also a random process, the direct observation of vector ranges is difficult.

For a continual description of particle diffusion in a disperse flow the degree of vectorization η can be considered as a certain order parameter. Indeed, the flow can be considered a typical dissipative structure characterized by a macroscopic time scale T and an internal microscopic scale τ associated with the fine-scale chaotic motion within the macroscopic fluctuations in concentration of a dispersed medium. The relationship (11) is asymptotically correct for $t \gtrsim T \gg \tau$. The process will be explicitly nonstationary in an analysis of diffusion in the time intervals $t \gtrsim \tau$. In this case a local (in time) order parameter $\eta(t)$ can be introduced and the operator form of the diffusion coefficient

$$D = D^\infty + \frac{D^{(0)} - D^{(\infty)}}{1 + \tau d/dt}, \tag{12}$$

corresponding to the description of the process in a relaxation approximation [14] can be used. Here $D^{(0)}$ and $D^{(\infty)}$ are diffusion coefficients for completely chaotic ($\eta = 0$) and strictly directional ($\eta = 1$) particle motion.

Let us note that for $\eta = 0$ the relationship (11) goes over into the known Ornstein formula, which is transformed into the classical Einstein formula as $t \to \infty$.

3. Example: Particle Diffusion in a Fluidized Bed. The vector component of the displacement for a particle in a fluidized bed is due to particle entrainment in regular circula-

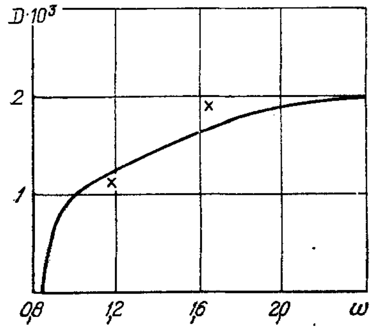

Fig. 4. Dependence of the particle diffusion coefficient in a fluidized bed on the fluidization rate; points are experiment in [16]; curve is theory in [17]. D in m^2/sec and w in m/sec.

tion motion, and the Brownian component is due to its fine-scale fluctuations. The relationship (11) was relied upon in the problem under consideration in [15].

The fundamental characteristics of the motion, the order parameter, the diffusion coefficient, and the drift velocity, can be found by using (11) in the experimental dependences of $\langle x^2\rangle/t$ on the time. The appropriate computational procedure for the case when the direction of the vector ranges is known, is described in [12]. Here we consider processing test data in the general case when this direction is unknown, in the example of results in [16] where motion trajectories were investigated for a labelled radioactive particle in a cylindrical fluidized bed for two fluidization regimes. The tests in [16] reduced to determining the radial r and vertical z coordinates of the particles at equal time intervals (0.5 sec and 0.25 sec for 1.19 and 1.62 m/sec fluidization rate values, respectively). For such a two-dimensional particle displacement (11) can be rewritten in the form $[B = \beta^{-1}(1-\eta)^{-1}]$

$$\langle l^2 \rangle = \langle r^2 + z^2 \rangle = \frac{D}{B}\,\frac{\eta^2}{1-\eta}\,t^2 + 4D(1-\eta)\left[t - B\left(1-\exp\left(-\frac{t}{B}\right)\right)\right]. \tag{13}$$

It is convenient to process the data to determine the characteristics of the motion by using the dependence $\langle l^2\rangle/t^2$, whose left side is determined experimentally by measured particle coordinates after fixed time intervals Δt

$$\frac{\langle l_j^2 \rangle}{t_j^2} = \frac{1}{(n-j)(j\Delta t)^2}\sum_{i=1}^{n-j}\left[(r_{i+j}-r_i)^2 + (z_{i+j}-z_i)^2\right], \tag{14}$$

where j = 1, 2, ..., n is the number of measurements. The dependences (14) are presented in Fig. 2 for tests in [16]. To find the parameters D, B, and η in (13), a system of equations should be compiled that considers the behavior of the quantity $\langle l^2\rangle/t^2$ as $t \to 0$ and $t \to \infty$, as well as the value of this quantity at a certain arbitrary time (for instance, t = 0.5 sec). We then arrive at the equations

$$\begin{gathered}\lim_{t\to 0}\frac{\langle l^2\rangle}{t^2} = \frac{D}{B}(1-\eta)\left[\left(\frac{\eta}{1-\eta}\right)^2 + 2\right] = a,\\ \lim_{t\to\infty}\frac{\langle l^2\rangle}{t^2} = \frac{D}{B}\,\frac{\eta^2}{1-\eta} = b,\\ \left.\frac{\langle l^2\rangle}{t^2}\right|_{t=0.5} = \frac{D}{B}(1-\eta)\left[\left(\frac{\eta}{1-\eta}\right)^2 + 4\left(2B - 4B^2 + 4B^2\exp\left[-\frac{1}{2B}\right]\right)\right] = c.\end{gathered} \tag{15}$$

Having determined a, b, and c from dependences (14) represented in Fig. 2, it is easy to find D, B, and η from system (15). We have

$$\eta = \frac{\sqrt{2b}\,(\sqrt{a-b}-\sqrt{2b})}{a-3b}, \quad D = \frac{(a-b)B}{2(1-\eta)}, \tag{16}$$

where B is the solution of the transcendental equation

$$2B - 4B^2 + 4B^2\exp\left[-\frac{1}{2B}\right] = \frac{c-b}{2(a-b)} \tag{17}$$

and can be determined graphically [the dependence of the left side of (17) on B is shown in Fig. 3].

Values of the particle diffusion coefficient for two regimes of conducting the tests in [16] are displayed by the points in Fig. 4. Here the theoretical dependence of the diffusion coefficient on the fluidization rate, computed for the conditions of the experiment in [16] on the basis of the model in [17] is presented. As is seen, there is a fair agreement between the data of theory and experiment. On one hand, this indicates adequacy of the representation and methodology of processing experiments developed in this paper and, on the other hand, the adequacy of the theory of fine-scale mixing in fluidized systems proposed in [17].

NOTATION

A, random force; $B = \beta^{-1}(1-\eta)^{-1}$; a, b, c, experimentally determined quantities in (15)-(17); D, diffusion coefficient; F, function in (9) and a scalar in (11); G, an average physical quantity; k(t), a trajectory in wave space; l, complete displacement; M, number of paths; N, number of particles; P, probability density; Q, flux of the quantity G; R, correlation function; $\mathbf{r}^{(i)}$, radius vector of the center of the i-th particle; r, z, radial and axial coordinates; T, macroscopic time scale; t, time; V_0, V_1, parts of space occupied by the disperse medium and the particles, respectively; v, particle velocity; w, fluidization rate; x(t), trajectory in phase space; β, resistance factor; η, degree of vectorization of the motion; Θ_0, Θ_1, generalized functions introduced in V_0 and V_1; τ, microscopic time scale; φ, a quantity introduced in (10).

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