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Abstract

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MATHEMATICAL PHYSICS

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ON THE VARIATIONAL PRINCIPLE IN QUANTUM KINETICS

(Presented by Academician L. I. Sedov on 11 X 1967)

As shown in works ([1,2]), Lagrange' s principle can serve as a basis for constructing more complicated models that take the properties of real bodies into account more radically. In principle, any macroscopic system is completely described by the Lagrange function Λ_{micr} of all its microparticles, molecules, electrons, etc. The macroscopic Lagrangian and δW^*, which describe a nonequilibrium system "in a large-structure way," contain much less information than the function Λ_{micr}. There is yet another consideration that reveals the fundamental difference between these two approaches to the study of real bodies. Macroscopically nonequilibrium systems are described by irreversible equations, whereas the evolution equation of each microparticle of the system is reversible. The kinetic method of describing macroscopic systems synthesizes these contradictions. In the present article an attempt is made to trace the process by which irreversibility appears when a system is described by Wigner quantum-mechanical functions in the language of the variational formalism.

Let a macroscopic system occupy a volume V and consist of N identical particles: bosons or fermions. We shall study the asymptotic behavior of this system in time as $N \to \infty$, $V \to \infty$, and N/V tends to a finite value. In kinetics the system may be regarded as a kind of continuous medium without surface forces; the distribution function $f_N(\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{p}_1, \dots, \mathbf{p}_N, t)$ will be considered the density of this medium. In accordance with such an interpretation, f_N must satisfy the continuity equation in the $6N$-dimensional phase space:

$$\frac{\partial f_N}{\partial t} + \sum_{k=1}^{N} \frac{\partial(\dot{\mathbf{q}}_k f_N)}{\partial \mathbf{q}_k} + \sum_{k=1}^{N} \frac{\partial(\dot{\mathbf{p}}_k f_N)}{\partial \mathbf{p}_k} = 0^*. \tag{1}$$

The functions obtained from f_N by definition

$$f_s(\mathbf{q}_1, \dots, \mathbf{q}_s, \mathbf{p}_1, \dots, \mathbf{p}_s) = V^s \int f_N(\mathbf{q}_1, \dots, \mathbf{q}_s, \mathbf{q}_{s+1}, \dots, \mathbf{q}_N, \mathbf{p}_1, \dots,$$

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$$\ldots, \mathbf{p}_s, \mathbf{p}_{s+1}, \ldots, \mathbf{p}_N)\, d\mathbf{q}_{s+1} \ldots d\mathbf{q}_N d\mathbf{p}_{s+1} \ldots d\mathbf{p}_N, \qquad (2)$$

will obviously obey the equations

$$\frac{\partial f_s}{\partial t} + \sum_{k=1}^{s} \frac{\partial \int \dot{\mathbf{q}}_k f_N \, d\mathbf{q}_{s+1} \ldots d\mathbf{q}_N}{d\mathbf{q}_k} + \sum_{k=1}^{s} \frac{\partial \int \dot{\mathbf{p}}_k f_N \, d\mathbf{q}_{s+1} \ldots d\mathbf{p}_N}{\partial \mathbf{p}_k}.$$

The resulting chain will be determined only when it is possible to express $\dot{\mathbf{q}}_i$ and $\dot{\mathbf{p}}_i$ through the density f_N and the dynamical variables $\mathbf{q}_k$ and $\mathbf{p}_k$. Below it is shown how to obtain an equation for the quantum distribution function f_N phenomenologically, bypassing microscopic consideration. For classical systems a similar idea was developed in paper ([3]).

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* Of course, it does not follow *a priori* from anywhere that the quantum distribution function introduced by Wigner obeys an equation of this kind. This is a postulate justified *a posteriori*.

From the Eulerian point of view, the motion of the phase "fluid" is completely determined if, at each instant of time t, in the phase space X there is constructed a field of the $6N$-component "velocity" vector $\mathbf{x}(\dot{q}_{1x}, \ldots, \dot{q}_{Nz}, \dot{p}_{1x}, \ldots, \dot{p}_{Nz})$. If to the $6N$ coordinates one adjoins the time coordinate, then the streamlines of the vector $(\dot{q}_{1x}, \ldots, \dot{q}_{Nz}, p_{1x}, \ldots, p_{Nz}, 1)$ in the resulting $(6N+1)$-dimensional space Y will have the meaning of trajectories of small phase elements. Let us take an arbitrary domain $V \subset Y$ and define on it the functional

$$\begin{aligned} R = \int_V \Bigg\{ \sum_{k=1}^{N} \left(\dot{\mathbf{q}}_k \mathbf{p}_k - \frac{p_k^2}{2m} \right) f_N - \frac{1}{2(2\pi)^6} \sum_{i<k} \int_0^1 d\alpha \int_\infty d\vec{\eta}_i \, d\vec{\eta}_k \, d\vec{\tau}_i \, d\vec{\tau}_k \\ \times \exp\left[i\vec{\tau}_i(\vec{\eta}_i - \mathbf{p}_i) + i\vec{\tau}_k(\vec{\eta}_k - \mathbf{p}_k) \right] \\ \times \left[\Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k - \frac{\alpha\hbar(\vec{\tau}_i - \vec{\tau}_k)}{2} \right| \right) \right. \\ \left. + \Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k + \frac{\alpha\hbar(\vec{\tau}_i - \vec{\tau}_k)}{2} \right| \right) \right] \\ \times f_N(\mathbf{q}_1, \ldots, \mathbf{q}_N, \mathbf{p}_1, \ldots, \vec{\eta}_i, \ldots, \vec{\eta}_k, \ldots, \mathbf{p}_N) \Bigg\} dV. \end{aligned}$$

It is curious to note that if, in integrating over V, all the variables p_{ix}, p_{iy}, p_{iz} $(i = 1, \ldots, n)$ vary from $-\infty$ to $+\infty$, then the expression for R goes over into Hamilton' s action in classical kinetic theory (3). The true velocity field differs from admissible ones by extremal properties. Let us perform an arbitrary deformation of the trajectories of the phase fluid in Y from some class G (it will

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be defined below). This means that a point $\mathbf{x} \in Y$ passes into the point $\mathbf{x}'(\mathbf{x})$. The condition of continuity of the configuration obtained can be expressed by the equality

$$f'_N(\mathbf{q}'_1, \dots, \mathbf{p}'_N) = f_N(\mathbf{q}_1, \dots, \mathbf{p}_N) D(q_{1x}, \dots, p_{Nz}) / D(q'_{1x}, \dots, p'_{Nz}).$$

To find the true velocity field in the domain V, we formulate the principle: only for the actual velocity field will the linear part of the increment of the functional R on the domain V under an arbitrary deformation of Y from the class G, added to the integral δW taken over the surface $V - \Omega$, give zero. We define the class G of admissible deformations by the relations

$$\mathbf{q}'_i - \mathbf{q}_i = \delta \mathbf{q}_i(\mathbf{q}_1, \dots, \mathbf{q}_N, t), \qquad \mathbf{p}'_i - \mathbf{p}_i = \delta \mathbf{p}_i(\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{p}_i, t),$$

$$i = 1, \dots, n, \qquad \delta t = 0.$$

In accordance with the formalism of paper (1), we write δW in the form

$$\int_\Omega \left[n_t \delta T + \sum_{i=1}^{N} \sum_{\nu=1}^{3} \left(n_{q_{i\nu}} \delta Q_{i\nu} + n_{p_{i\nu}} \delta P_{i\nu} \right) \right] d\Omega,$$

where $\delta T, \delta Q_{i\nu}, \delta P_{i\nu}$ are certain functions depending linearly on the vector of the admissible deformation $\delta \mathbf{x}$, but, generally speaking, in a functional way, and independent of the choice of V. From the equality $\delta R + \delta W = 0$ we find the explicit form of these functions:

$$\delta T = \sum_{i=1}^{N} \delta \mathbf{q}_i \mathbf{p}_i f_N, \qquad \delta Q_{i\nu} = \dot{q}_{i\nu} \delta T, \qquad \delta P_{i\nu} = \dot{p}_{i\nu} \delta T + \sum_{\mu=1}^{\infty} \frac{\partial^\mu \delta p_{i\nu}}{\partial p_{ix}^{m_1} \partial p_{iy}^{m_2} \partial p_{iz}^{m_3}} \chi^{i\nu}_{m_1 m_2 m_3},$$

where

$$\begin{aligned} \chi^{i\nu}_{m_1 m_2 m_3} = {} & \frac{(-1)^\mu}{2(2\pi)^3} \sum_{k=1}^{N} \int_0^1 d\alpha \int_\infty d\vec{\eta}_i \, d\vec{\tau} \, \exp\left[i \vec{\tau} (\vec{\eta}_i - \mathbf{p}_i) \right] \, f_N(\vec{\eta}_i, \mathbf{p}_i + {}^\nu \mathbf{p}_k - \vec{\eta}_i) \\ & \times \frac{(\eta_{ix} - p_{ix})^{m_1} (\eta_{iy} - p_{iy})^{m_2} (\eta_{iz} - p_{iz})^{m_3}}{m_1! \, m_2! \, m_3!} \left[\Phi \left(\left| \mathbf{q}_i - \mathbf{q}_k - \frac{\alpha \hbar \vec{\tau}}{2} \right| \right) \right. \\ & \left. + \Phi \left(\left| \mathbf{q}_i - \mathbf{q}_k + \frac{\alpha \hbar \vec{\tau}}{2} \right| \right) \right], \end{aligned}$$

and the equations of motion

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$$\dot{\mathbf{q}}_i = \frac{\mathbf{p}_i}{m}, \quad f_N \dot{\mathbf{p}}_i = -\frac{1}{2(2\pi)^3} \sum_{k=1}^{N} \int_0^1 d\alpha \int_\infty d\vec{\eta}_i \, d\vec{\tau} \, \exp[i\vec{\tau}(\vec{\eta}_i - \vec{p}_i)] f_N(\vec{\eta}_i, \mathbf{p}_i + \mathbf{p}_k - \vec{\eta}_i) \times$$

$$\times \frac{\partial}{\partial \mathbf{q}_i} \left[\Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k - \frac{\alpha\hbar\vec{\tau}}{2} \right| \right) + \Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k + \frac{\alpha\hbar\vec{\tau}}{2} \right| \right) \right].$$

Substituting the expressions for $\dot{\mathbf{q}}_i$ and $\dot{\mathbf{p}}_i$ into equation (1), we obtain

$$\frac{\partial f_N}{\partial t} + \sum_{k=1}^{N} \frac{\mathbf{p}_k}{m} \frac{\partial f_N}{\partial \mathbf{q}_k} - \frac{i}{\hbar} \sum_{i,k} \left[\Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k + \frac{\hbar}{2i} \frac{\partial}{\partial \mathbf{p}_i} \right| \right) - \right.$$

$$\left. -\Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k - \frac{\hbar}{2i} \frac{\partial}{\partial \mathbf{p}_i} \right| \right) \right] f_N = 0.$$

It is interesting to note that the equations of the chain can be obtained without resorting to the definition of the functions f_s by formulas (2): the functions $f_s(\mathbf{q}_1, \dots, \mathbf{q}_s, \mathbf{p}_1, \dots, \mathbf{p}_s)$ $(s = 1, 2, \dots, N-1)$, in turn, can be regarded as density functions of the substance in the corresponding spaces X^s. In accordance with this, during the motion of the phase fluid for f_s the continuity equation must be satisfied,

$$\frac{\partial}{\partial t} f_s + \sum_{k=1}^{s} \operatorname{div}_{q_k} \dot{\mathbf{q}}_k f_s + \sum_{k=1}^{s} \operatorname{div}_{p_k} \dot{\mathbf{p}}_k f_s = 0.$$

To find the trajectories of motion of small phase elements one may formulate a variational principle (analogous to that used above), from which we obtain the equations:

$$\dot{\mathbf{q}}_i = \frac{\mathbf{p}_i}{m}, \quad f_s \dot{\mathbf{p}}_i = -\sum_{k=1}^{s} \frac{1}{2(2\pi)^3} \int_0^1 d\alpha \int_\infty d\vec{\eta}_i \, d\vec{\tau} \, \exp[i\vec{\tau}(\vec{\eta}_i - \vec{p}_i)] f_s(\vec{\eta}_i, \mathbf{p}_i + \mathbf{p}_k - \vec{\eta}_i) \times$$

$$\times \frac{\partial}{\partial \mathbf{q}_i} \left[\Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k - \frac{\alpha\hbar\vec{\tau}}{2} \right| \right) + \Phi\left(\left| \mathbf{q}_i - \mathbf{q}_k + \frac{\alpha\hbar\vec{\tau}}{2} \right| \right) \right] - \sum_{k=1}^{s} \frac{1 - s/N}{2\nu(2\pi)^3} \times$$

$$\times \int_0^1 d\alpha \int_\infty d\vec{\eta}_i \, d\vec{\tau} \, d\mathbf{q}_{s+1} \, d\mathbf{p}_{s+1} \exp[i\vec{\tau}(\vec{\eta}_i - \mathbf{p}_i)] \frac{\partial}{\partial \mathbf{q}_k} \left[\Phi\left(\left| \mathbf{q}_k - \mathbf{q}_{s+1} - \frac{\alpha\hbar\vec{\tau}}{2} \right| \right) + \right.$$

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$$+\Phi\left(\left|\mathbf{q}_k-\mathbf{q}_{s+1}+\frac{\alpha\hbar\vec{\tau}}{2}\right|\right)\Big]\, f_{s+1}(\mathbf{q}_1,\dots,\mathbf{q}_{s+1},\mathbf{p}_1,\dots,\vec{\eta}_i,\dots,\mathbf{p}_{s+1}).$$

Substituting into the continuity equation for f_s the values found for $\dot{\mathbf{q}}_i$ and $\dot{\mathbf{p}}_i$, we obtain the quantum equation for f_s

$$\frac{\partial f_s}{\partial t}+\sum_{i=1}^{s}\frac{\mathbf{p}_i}{m}\frac{\partial f_s}{\partial \mathbf{q}_i}+\frac{i}{\hbar}\sum_{i,k}\left[\Phi\left(\left|\mathbf{q}_i-\mathbf{q}_k-\frac{\hbar}{2i}\frac{\partial}{\partial \mathbf{p}_i}\right|\right)-\right.$$

$$\left.-\Phi\left(\left|\mathbf{q}_i-\mathbf{q}_k+\frac{\hbar}{2i}\frac{\partial}{\partial \mathbf{p}_i}\right|\right)\right] f_s+\frac{i(1-s/N)}{\hbar\nu}\int_\infty d\mathbf{q}_{s+1}\,d\mathbf{p}_{s+1}\times$$

$$\times\left\{\sum_{k=1}^{s}\left[\Phi\left(\left|\mathbf{q}_k-\mathbf{q}_{s+1}-\frac{\hbar}{2i}\frac{\partial}{\partial \mathbf{p}_k}\right|\right)-\Phi\left(\left|\mathbf{q}_k-\mathbf{q}_{s+1}+\frac{\hbar}{2i}\frac{\partial}{\partial \mathbf{p}_k}\right|\right)\right] f_{s+1}\right\}.$$

The property of macroscopic systems to tend irreversibly toward the most probable (equilibrium) state is in contradiction with the reversibility of the chain of kinetic equations. Therefore, the irreversibility of the behavior of a macro-object can be explained kinetically only by consequences arising from the properties of the truncated chain. In order to construct any closed kinetic model, it is necessary to rely on information about the character of the interaction between particles, on statistical hypotheses, and to take into account the degree

deviations of the system from the equilibrium state, etc. It is interesting to note that the variational principle put forward in (1) also makes it possible in kinetic theory to use information of this kind in a rational way. Let us obtain, for example, the quantum kinetic equation for a system with weak interaction (in the "kinetic" regime) in the second approximation with respect to the small parameter ε ($\Phi(|q|)=\varepsilon\Psi(|q|)$). Here we regard the function f_1 as the density of distribution of matter in the 6-dimensional phase space, satisfying the continuity equation
$\partial f_1/\partial t+\dot{q}\,\partial f_1/\partial q+\dot{p}\,\partial f_1/\partial p=0$. In the new situation the velocity field $(\dot{\mathbf{q}},\dot{\mathbf{p}})$ can be obtained from the variational principle

$$\delta\int_{V^{(1)}} L\,dV^{(1)}+\delta W+\int_{V^{(1)}}\delta A\,dV^{(1)}$$

by specifying the Lagrange function L and the coefficients of the linear form, with respect to variations, δA, which is not the complete variation of some function. The essence of the appearance of δA is as follows: when approximate expressions for f_2 are used, it is impossible simultaneously to satisfy the equalities $\delta(f_1 dq_1 dp_1)=0$ and $\delta(f_2 dq_1 dp_1)=0$ (q_2 and p_2 are nonvaried variables). Therefore one has first to vary formally that part $R^{(1)}$ which contains f_2, under

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the condition $\delta(f_2 dq_1 dp_1) = 0$, and only then use the approximate expression for f_2. Let us write down the form of δA for a system of identical particles obeying different statistics in the homogeneous case (it was obtained on the basis of N. N. Bogoliubov' s dynamical method (4)):

$$\delta A = \delta q\, Q^* f_1 = -\frac{2s+1}{2(2\pi)^5 \hbar^4 v i} \int_0^1 d\alpha \int_\infty' d\vec{\eta}\, d\vec{\tau}\, \exp[i\vec{\tau}(\vec{\eta} - \vec{p})] f_1\left(\vec{\eta} + \frac{\vec{\alpha}}{2}\right) f_1\left(\vec{p}_2 - \frac{\vec{\alpha}}{2}\right)$$
$$\times \frac{\partial}{\partial q_1}\left[\Phi\left(\left|\mathbf{q}_1 - \mathbf{q}_2 - \frac{\hbar\alpha\vec{\tau}}{2}\right|\right) + \Phi\left(\left|\mathbf{q}_1 - \mathbf{q}_2 + \frac{\hbar\alpha\vec{\tau}}{2}\right|\right)\right] [v(\vec{\alpha}) \pm v(\vec{\alpha} - \vec{\eta} + \vec{p}_2)]$$
$$\times \left[1 \pm \frac{(2\pi\hbar)^3}{v} f_1\left(\vec{\eta} - \frac{\vec{\alpha}}{2}\right) \pm \frac{(2\pi\hbar)^3}{v} f_1\left(\vec{p}_2 + \frac{\vec{\alpha}}{2}\right)\right]$$
$$\times \left\{\exp\left[\frac{i}{\hbar}\vec{\alpha}(\mathbf{q}_1 - \mathbf{q}_2)\right] \delta_-\left(\frac{\vec{\eta}\vec{\alpha} - \vec{p}_2\vec{\alpha}}{m\hbar}\right) - \exp\left[-\frac{i}{\hbar}\vec{\alpha}(\mathbf{q}_1 - \mathbf{q}_2)\right] \delta_+\left(\frac{\vec{\eta}\vec{\alpha} - \vec{p}_2\vec{\alpha}}{m\hbar}\right)\right\} dq_2 dp_2.$$

In this notation, for systems obeying Bose—Einstein statistics, in the terms having two signs one must take the upper sign; for Fermi systems it is necessary to take the lower sign; s is the spin number. In both cases the dissipative forces compel the phase medium in momentum space to expand on average, ultimately bringing the system to the most probable distribution. Indeed:

$$\frac{d}{dt}\, dp = \mathrm{div}_p\, \dot{\mathbf{p}}\, dp,$$

therefore, averaged over momentum space, the expansion rate of a unit volume is

$$\int f\ \mathrm{div}_p\, \dot{\mathbf{p}}\, dp = \int f\ \mathrm{div}_p\, Q^*\, dp.$$

It is easy to show that this expression can be reduced to the form

$$\frac{d}{dt}\int f \ln f\, dp;$$

it is always greater than zero and is equal to zero in the limiting state of the system. For the general inhomogeneous case, as Pauli noted (5), such an assertion is not valid.

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