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A FUNCTIONAL RANDOM-WALK MODEL OF THE MANY-PARTICLE SYSTEM

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ABSTRACT

By Fourier-transforming the author's recently proposed state functional formalism for the BBGKY hierarchy, a new perspective of non-equilibrium statistical mechanics is given: the basic equation is formally very close to the Fokker-Planck equation and may readily be modified to a universal master equation (with irreversibility) by a slight change. Hence the problem reduces to one of a generalized random-walk such that the stochastic quantity to be considered is the particle-number density in the one-body phase space. A general solution is formulated for the weak interaction case.

1. Introduction

Recently the functional formalism of classical non-equilibrium statistical mechanics was proposed by the author[1] to search for general closed-form solutions for distribution functions governed by the BBGKY hierarchy for the infinitely-many-particle system with a finite average density. There the state functional, which embraces all distribution functions in itself as the coefficients of the functional Taylor expansion (except for the numerical factors), was introduced. It is governed by a single second-order functional-differential equation. This formalism originates with Bogoliubov[2] but a basic modification was necessary for a meaningful functional calculus to be performed within the formalism. Be that as it may, it would be quite inconvenient if the state functional is too fine-grained to represent a real irreversible process, even if the solution could be numerically pursued. In fact, on the basis of the exact dynamics, i.e., the Liouville equation or its equivalent, we can hardly expect all possible arbitrary states to develop into a unique, steady (e.g. equilibruim) state. This is obvious, if we remember the time-reversibility of the equation as well as the fact that the entropy in Gibbs's sense is conserved so that the maximum entropy is never achieved, starting from a state of lower entropy. In order to establish an entropy-productive non-equilibruim statistical mechanics, some modification of the basic equation, comparable with coarse-graining procedure, seems to be unavoidable in our state functional formalism also.

The first aim of this paper is to find the best irreversible perspective for the evolution of the state functional[3]. We first notice that the Fourire-transformed basic equation in the cylinder functional approach (established in Sec. 2) has a structure very close to the Fokker-Planck equation which describes a Markov stochastic process, but retaining the time-reversibility as a natural consequence of its equivalence to the BBGKY hierarchy (in the limit when the number of particles tends to infinity). The best method of modifying the equation into a real Fokker-Planck equation at the expense of losing the time-reversibility is described in Sec. 3. As a result, our problem reduces to nothing but the problem of a generalized random-walk played within the special function space equivalent to a certain Riemannian space by the so-called stochastic particle-number density function in the one-body phase space. The mathematical procedure of such a modification is unique in the sense that any other Markov process expected to simulate non-equilibrium statistical mechanics is not closer to the dynamical process than the present one; but it seems somewhat difficult to re-express the procedure in simple conventional physical words, such as coarse-graining.

As the paper's second object, the general method is applied to the case of a gas or a weakly interacting plasma in Sec. 4. In this case the equivalent Riemannian space reduces approximately to a Euclidean space, so that the complexity in calculation is reduced. The closed-form general solution of the initial-value problem is formulated in terms of a repeated multiple integral; which can in practice be conveniently solved by the Monte Carlo quadrature. Since in our theory the accuracy of calculation

is increased simply by increasing the multiplicity M of cylinder functional but not by changing (or deepening) the formulation in a complicated way and, moreover, since there is no difficulty in principle in applying the theory to the strong interaction case, the proposed approach seems to have the proper advantage which is not found in other analytical approaches to the BBGKY hierarchy or the Liouville equation which exploit the more or less sophisticated series expansion in a small parameter,[2,4,5] which may not necessarily be convergent.

Another type of statistical-dynamical research, which may be also called a functional approach, has been developed by considering the evolution of the probability on an ensemble of the events, a member of which evolves strictly according to some dynamics such as the Vlasov equation, the Langevin equation, etc.[6,7] Of course, this research is different in principle from ours; except for the case of taking the Klimontovich equation[8] as the dynamics, when the characteristic functional equation is formally equivalent to the BBGKY hierarchy, as was verified by Nakayama and Dawson[6]. However, it will be seen (in Sec. 3) that if the Vlasov equation is taken as the dynamics, there is a somewhat close relation between this ensemble mechanics and the presented perspective of our formalism.

The discussion is restricted to a single-component system for simplicity. Extension to a multi-component system is straightforward[1].

2. Fourier-transformed State Functional Formalism

According to the previous paper[1], if the s-body generic distribution function is denoted by F_s, the state functional is defined as

$$\psi(y, t) = 1 + \sum_{s=1}^{\infty} \frac{i^s}{s!} \int_X \cdots \int_X F_s(x_1, \cdots, x_s, t) y(x_1) \cdots y(x_s) dx_1 \cdots dx_s \quad , \quad (2.1)$$

where $i = \sqrt{-1}$, X is the entire one-body phase space, $x_1, \cdots x_s \in X$, t is the time variable and $y(x)$ is a real-valued function. Once the state functional is introduced, the BBGKY hierarchy for the infinitely-many-particle system with a finite average density is completely replaced by the following single basic equation with functional differentiation:

$$\frac{\partial \psi}{\partial t} = i \int_X y(x) [H_1(x); \frac{\delta \psi}{i \delta y(x)}] dx - \frac{1}{2} \int_X \int_X \{y(x)y(x') - iny(x) - iny(x')\}$$
$$\times [\phi(|q - q'|); \frac{\delta^2 \psi}{i^2 \delta y(x) \delta y(x')}] dx dx' \quad (2.2)$$

where $H_1(x)$ is the one-body Hamiltonian, [;] the Poisson bracket, n the average number density and $\phi(|q - q'|)$ the interaction potential between particles in which q denotes the displacement vector in the physical space. The operator $\delta/\delta y(x)$ denotes a functional derivative.[9,10] ψ should be subject to the following two associative conditions[1]:

$$\psi(0, t) = 1 \; ; \quad (2.3)$$

$$\lim_{V \to \infty} \int_X \frac{\delta \psi}{i \delta y(x)} dx/V = \psi \; , \quad (2.4)$$

where V is the volume containing the entire system. Both conditions emerge from the form of (2.1) on using the definition of F_s.

Here we introduce a kind of cylinder functional approach to functionals. If $\{s_j(x)\}$ is an orthonormal function set in X, we can calculate $a_j = \int_X s_j(x)y(x)dx$ to define a new function:

$$y^M(x) = \sum_{j=1}^{M} a_j s_j(x) \ . \tag{2. 5}$$

We call $\psi(y^M)$ the cylinder functional $\psi^M(y)$, which is still a functional of y through the definition of a_j, though it can essentially be considered a function of M variables $\{a_j\}$. Then ψ is understood as ψ^M in the limit $M \to \infty$ if it is convergent (for example with respect to the "maximum" norm). If ψ is replaced by ψ^M, the basic equations (2. 2) - (2. 4) become more feasible to treat, since then we have the relation

$$\frac{\delta}{\delta y(x)} = \sum_{j=1}^{M} \frac{\delta a_j}{\delta y(x)} \frac{\partial}{\delta a_j} = \sum_{j=1}^{M} s_j(x) \frac{\partial}{\partial a_j} \tag{2. 6}$$

and thus, (2. 2) becomes just a partial differential equation. From a practical point of view we always consider ψ^M first, assuming that the converging sequence $\{\psi^M\}$ of state cylinder functionals exists. Then we can introduce a new functional $\rho^M(x,t)$ as the Fourier component of ψ^M; namely we have

$$\psi^M(y, t) = \int_{A^M} \rho^M(z, t) \exp\{i \int y^M(x) z^M(x) dx\} \delta z^M \ . \tag{2. 7}$$

where

$$\int_{A^M} \delta z^M \equiv \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{j=1}^{M} db_j / (2\pi)^{1/2} \tag{2. 8}$$

and $z^M(x) = \sum b_j s_j(x)$. For simplicity we omit all the superscript M hereafter, unless necessary for clarity, keeping in mind that every functional is a cylinder functional.

As a result of the transformation (2. 7), the basic equation (2. 2) transforms to the following equation for ρ :

$$\frac{\partial \rho}{\partial t} = -\int_X \frac{\delta}{\delta z(x)}\{Qz(x)\rho\}dx + \frac{1}{2}\int_X\int_X \frac{\delta^2}{\delta z(x)\delta z(x')}\{[\phi(|q - q'|);$$

$$z(x)z(x')]\rho\}dxdx' , \qquad (2. 9)$$

and Q denotes the nonlinear operator such that

$$Qz(x) = [H_1(x); z(x)] + n\int_X dx'[\phi(|q - q'|); z(x)z(x')] . \qquad (2.10)$$

It is noted[1] that $\partial z/\partial t = Qz$ is nothing but the self-consistent Vlasov equation and therefore Q may be called the Vlasov operator. Corresponding to (2. 3) and (2. 4), we have the conditions:

$$\int_A \rho\delta z = 1 ; \qquad (2. 11)$$

$$\int_A \rho\{\lim_{V\to\infty} \int_X z(x)dx/V - 1\}\exp\{i\int_X y(x)z(x)dx\}\delta z = 0 . \qquad (2. 12)$$

From (2. 12) ρ should vanish for all $z(x)$ unless $z(x)$ is such that

$$\lim_{V\to\infty} \int_X z(x)dx/V = 1 , \qquad (2. 13)$$

which defines a hyperplane in R^M. We may call this the hyperplane A_1. The restriction (2. 12) is conservative in time, since the conservation of (2. 4) was proved by the previous paper.[1] Therefore, without any inconsistency we have only to consider the basic equation (2. 9) always in this hyperplane rather than R^M. Accordingly A in (2. 7) and (2. 11) may be read as A_1 on the understanding that $\int_{A_1}\delta z$ indicates the volume integral over A_1. The time-invariance of the condition (2. 11) is evident by virtue of (2. 9).

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hierarchy or the Liouville equation in the limit $N = nV \to \infty$ (n: finite), any dynamical property of the particle system is preserved in our formalism. It is easy to verify the time-reversibility of the basic equation (2. 9): if $\rho(z(q,p), t)$ is a solution, then $\rho(z(q,-p), -t)$ becomes another solution, p denoting the momentum part of the vector x. Also it is possible to derive the conservation laws of mass, momentum, angular momentum and energy directly on the basis of (2. 9). In this case, on comparing (2. 1) with the series expression of (2. 7) in powers of λ, we first have

$$F_1(x) = \int_{A_1} \rho(\cdot, t)z(x)\delta z \ , \qquad (2. 14)$$

$$F_2(x, x') = \int_{A_1} \rho(z, t)z(x)z(x')\delta z \qquad (2. 15)$$

and then can proceed with examining the time-evolution of each physical quantity related with ρ through the above relations.

As a representative example let us examine the momentum case. From (2. 14) and (2. 9), we calculate

$$\frac{\partial}{\partial t}\int_X npF_1(x)dx = n\int_{A_1}\frac{\partial \rho}{\partial t}\int_X pz(x)dx\delta z$$

$$= n\int_{A_1}\int_X pQz(x)\rho dx\delta z$$

where use was made of partial integration, keeping in mind that $|\rho| \to 0$ at infinity ($\int_X z^2 dx = \infty$) in A_1 in order for $\int_{A_1}|\rho|\delta z$ to exist. As is easily seen, there is no effect of the term with a second-order functional-derivative in (2. 9) in this case, since the integral over X in the left-hand side is not a functional higher-order than linear in z. A further calculation gives

$$\frac{\partial}{\partial t}\int_X npF_1 dx = n\int_{A_1}\rho\{\int_X p[H_1;\ z(x)]dx + n\int_X\int_X p[\phi;\ z(x)z(x')]dxdx'\}\delta z$$

$$= n\int_{A_1}\rho\{-\int_X \frac{\partial H_1}{\partial q} z(x)dx - n\int_X\int_X (\frac{\partial\phi}{\partial q} + \frac{\partial\phi}{\partial q'})z(x)z(x')dxdx'\}\delta z\ . \qquad (2.\ 16)$$

Here the boundary condition on $z(x)$ was taken into account: $z(x) \to 0$ for $|p| \to \infty$ and on the boundary of the configuration space. The second term in the curly bracket vanishes because $\partial\phi/\partial q = -\partial\phi/\partial q'$. (This illustrates that the sum of internal forces vanishes due to the action-reaction law.) The first term also vanishes if there is no external force ($\partial H_1/\partial q = 0$). Otherwise it expresses the total external force. Therefore we can see in (2. 16) the generalized conservation law of momentum. It is needless to say that total momentum $\int_X npF_1 dx$ is infinite in the limit $N = nV \to \infty$ but it can be meaningful if we consider the average momentum per particle or per unit volume. The other conservation laws are quite similarly examined, except for the energy case in which care should be taken of the fact that the effect of the term with a second order functional-derivative in (2. 9) appears for the part of the interaction energy including the expression (2. 15), which is a quadratic functional in z.

Finally we add a comment on the other functional formalism equivalent to the BBGKY hierarchy by Nakayama and Dawson.[6] In this formalism the characteristic functional plays a main role of describing the state according to the theory of Hopf[10] for turbulence mechanics. There the evolution of an ensemble is considered, all members of which are microscopic states evolving according to the Klimontovich equation[8] starting with various initial positions and momenta of particles given in the one-body phase space. The basic equation, i.e. the Hopf equation for this ensemble is somewhat different from (2. 2); in particular it is remarkable that it has

no term with a coefficient quadratic in $y(x)$. Correspondingly the characteristic functional itself is different from the state functional (2. 1). A difficulty with this formalism, however, stems from the fact that every solution of the Klimontovich equation does not represent a microscopic state. Hence all solutions of the Hopf equation are not realistic, even if they satisfy the general conditions on the characteristic functional. For the solution to be realistic, the members of the ensemble should be restricted to Klimontovich's special class of singular functions in terms of superposed delta functions.[8] This limits the class of allowed characteristic functionals severely, and it would not be easy to formulate this restriction in a simple manner. Another disadvantage may be seen in the difficulty in finding an appropriate simple-form initial characteristic functional which can be used in practice; for the state functional it is easy, as described in ref. 1 and will be shown in the next section.

3. Master Equation Approach

The basic equation (2. 9) is very close in form to the Fokker-Planck equation which describes a Markov stochastic process. The first term of the right-hand side is the analogue of the so-called friction term and the second resembles the diffusion term. However, there is a difference in principle between (2. 9) and the Fokker-Planck equation; the former is time-reversible as was mentioned already, but the latter is time-irreversible. This reflects the fact that the coefficient function $[\phi;\ z(x)z(x')]$ inside the second-order derivative is not positive-definite. This similarity and difference may contain a key to solving the noted historical question: how to bridge the microscopic reversibility and the

macroscopic irreversibility in the system evolution in a general way.

Now if the coefficient function is considered as the sum of the positive-definite and negative-definite parts at each local point in A_1, the former plays a role of creating an irreversible process, while the latter that of destroying it or creating an anti-irreversible process so that both roles may offset each other to cause the reversible process exactly. So, in order to extract a purely irreversible process from the dynamical process, evidently it is necessary and sufficient to retain only the former part of the coefficient function, so that (2. 9) reduces to a real Fokker-Planck equation. This would be the simplest universal way of introducing the positive time-arrow in the system evolution. There is no further assumption in this procedure, such as weak interaction, diluteness, etc. Therefore its application will be free from any such restriction on physical conditions. Let the Fokker-Planck equation thus obtained be written as

$$\frac{\partial \tilde{\rho}}{\partial t} = - \int_X \frac{\delta}{\delta z(x)} \{Q z(x) \tilde{\rho}\} dx + \frac{1}{2} \int_X \int_X \frac{\delta^2}{\delta z(x) \delta z(x')} \{P[\phi;\ z(x)z(x')] \tilde{\rho}\} dx dx' \ , \tag{3. 1}$$

where the symbol ρ has been replaced by $\tilde{\rho}$ to distinguish its approximate nature due to the above procedure and P is the operator on the coefficient function to make it positive-definite in the way just described. There can still be many ways of constructing a Markov process starting from (2. 9); for example, $P[\phi;\ z(x)z(x')]$ plus any nonnegative function can also be positive-definite. But it would be natural that (3. 1) is the most approximate to (2. 9) among them, since in this modification the first term is invariant and the second term was <u>minimumly</u> changed to make a real diffusion term. Then, the difference $|\rho - \tilde{\rho}|$ would be minimum as a whole. Thus (3. 1) may be called the master equation in the sense that it masters

the irreversible system evolution which is the most loyal to the basic dynamical rule.

By the property of the Fokker-Planck equation it is possible to interpret $\tilde{\rho}$ as the probability density in the space A_1. The condition (2. 11) plays an important role for this interpreration; that is

$$\int_{A_1} \tilde{\rho} \delta z = 1 \ . \qquad (3.\ 2)$$

If the diffusion term is neglected in (3. 1), it can be found that the equation governs the time-evolution of the probability on an ensemble of the trajectories in the space A_1 which develop from various initial values according to the Vlasov equation: $\partial z/\partial t = Qz$. This fact is obvious from the perfect analogy with the Hopf equation in turbulence mechanics,[10] if we go back to the equation for the characteristic functional $\tilde{\Psi}$ which corresponds to $\tilde{\rho}$ (defined in the same way as (2. 7)). In this case, we really deal with nothing but a so-called turbulent field which is basically governed by the Vlasov equation instead of the Navier-Stokes equation. Here we find a complete coincidence with the other statistical-dynamical research based on the Vlasov equation mentioned in Introduction.[6,7] If the diffusion term in (3. 1) is included, the coincidence breaks down and the motion (expressed by z) is affected by some <u>internal</u> random force implied by $P[\phi;\ z(x)z(x')]$, as is well expected from the Langevin equation for Brownian motion; so that <u>what we may call a turbulence</u> will be more irregular and more random. For this case there is the analogy with the Novikov equation in the turbulence mechanics with random force action[11] (though there is a slight difference in situation in that the random force in the Novikov equation is not internal but externally given independently of the field z). From all these facts, it is quite reasonable to interpret $z(x)$ as the <u>stochastic</u> particle-number density in X normalized

in the sense of (2.13). Obviously $z(x)$ is not a macroscopic observable (as is also known from the relations (2. 14) and (2. 15), nor is it a microscopic density such as considered by Klimontovich[8] since it can be a regular function; but may be understood as a fictitious, mathematical working field with an intermediate property.

Let us examine if (3. 1) is consistent with the conservation laws in spite of its modification by P. It is known from the discussion of the previous section that the term with the second-order functional-derivative in the basic equation has no effect on the conservation laws escept for conservation of energy. Accordingly it is evident that the conservation laws of mass, momentum and angular momentum hold also for (3. 1). For the energy case, however, we have

$$\frac{\partial}{\partial t}\left(\int_X nH_1(x)\tilde{F}_1(x)dx + \int_X\int_X \frac{n^2}{2}\phi(q-q')\tilde{F}_2(x,x')dxdx'\right)$$
$$= \frac{n^2}{2}\int_{A_1}\int_X\int_X \phi P[\phi;\, z(x)z(x')]dxdx'\tilde{\rho}\delta z \,, \qquad (3.\ 3)$$

which can not vanish in general. The right-hand side is $O(n^2\lambda^2)$ (λ: representative order of magnitude of ϕ), but the error will accumulate with time. Therefore it is necessary to correct this error in our master equation some way. This can be made by confining the space for z into a manifold in which the conservation of energy is strictly insured. Indeed, since the total energy found on the left-hand side of (3. 3) is rewritten in terms of (2. 14) and (2. 15) as

$$\int_{A_1}\tilde{\rho}\left\{\int_X nH_1 z(x)dx + \int_X\int_X \frac{n^2}{2}\phi z(x)z(x')dxdx'\right\}\delta z \,,$$

we can impose the condition on z:

$$\int_X nH_1 z(x)dx + \int_X\int_X \frac{n^2}{2}\phi z(x)z(x')dxdx' = \text{const.} \qquad (3.\ 4)$$

to guarantee the constancy of the total energy. Equation (3. 4) prescribes a subset of A_1, which may be called a quadratic hypersurface.

It is thus essential that our basic equation (3. 1) should be redefined in such a Riemannian space as prescribed by (3. 4). There is no special difficulty in dealing with the Fokker-Planck equation in a Riemannian space.[12] As is well known, a Fokker-Planck equation governs a generalized Brownian motion and hence we may imagine from our equation a generalized Brownian motion or random walk in the Riemannian space.

It is known that there is a unique steady state of $\tilde{\rho}$, and $\tilde{\rho}$ tends asymptotically to this state irrespectively of any initial condition.[13] It is unfortunate that we cannot at present have any explicit form of the steady-state solution to be compared with the equilibrium canonical distribution for the Gibbs ensemble. However, some similarity in situation may be expected. Namely, the final asymptotic state is the state in which all Brownian particles have fully diffused over the whole Riemannian space ≡ the quadratic hypersurface (3. 4) that corresponds to the constant-energy shell in the grand (6N-dimensional) phase space; and then every point in that space is realizable with some measure irrespective of an initial state, just like a grand phase point in the energy shell in the equilibrium state. We note that in our theory, the concept

of entropy is not necessary to conclude the one-directional evolution of the system, since we have already the uniquely given asymptotic state.

The initial condition imposed on $\tilde{\rho}$ is easily formulated, if the initial correlations among particles are neglected. Namely, on starting from the initial state functional[1]

$$\psi = \exp\{i\int_X y(x)F_o(x)dx\} \tag{3. 5}$$

where $F_o(x)$ is the given initial one-body distribution function, we have

$$\rho = \delta[\, z(x) - F_o(x)\,] \tag{3. 6}$$

by means of the relation (2. 7). (See ref. 1 for the delta functional $\delta[\ ]$.) Naturally, here we rewrites ρ as $\tilde{\rho}$. This means that our random walk begins from the single point in the Riemannian space which is given as $F_o(x)$. Then, the total of the Brownian trajectories beginning from this point provide all the physical information of the irreversible system evolution. Indeed, as is known from comparing (2. 1) and (2. 7), all $\tilde{F}_s$ (the symbol $\tilde{F}_s$ means the approximation to F_s in the sense of our master equation approach) are given as the s-th order correlation function of the stochastic field $z(x)$;

$$\tilde{F}_s(x_1, \cdots, x_s, t) = \int z(x_1)\cdots z(x_s)\tilde{\rho}(z, t)\delta z \tag{3. 7}$$

where the integration is taken over the Riemannian space in A_1; and all physical quantities are related to $\tilde{F}_s$. It may be further noted that since the fluctuation of a macroscopic quantity is closely related to the behavior of F_2^2, an observable macroscopic turbulence should be related through $\tilde{F}_2$ (in (3. 7)) with the turbulence in z which is strong enough to have a correlation

length over a macroscopic scale. This is an interesting situation which opens a new way of statistically pursuing a turbulence in plasma.

In order to compute ρ in (3. 7) for a given M, it is necessary to solve the Fokker-Planck equation with many variables. A practically useful formula for solving the Fokker-Planck equation is presented in the next section for the simple case where the Riemannian space can be approximated by a Euclidean space. This formula tells us how to follow the generalized random walk with the aid of a high-speed computer to constitute the solution of our initial-value problem. It will turn out that the principle of the calculation is nothing but the Monte Carlo quadrature. This method of solution is in principle available also to the (not simple but) general case, for which we should consider the random walk on the Riemannian space. Indeed, since such a Riemannian space is always approximated by the tangential hyperplane locally, the infinitesimal random-walk motion around the tangential point can be followed by quite the same way as given for the simple case, and continuation of this process would complete a chain of random walk on the hypersurface.

Finally, it is interesting to point out that a new hierarchy similar to the BBGKY hierarchy can be obtained from our master equation. Let us multiply (3. 1) by $z(x)$ and integrate it with respect to δz over the Riemannian space, taking into account (2. 10), (2. 14) and (2. 15). Then, we have

$$\frac{\partial \tilde{F}_1}{\partial t} = [H_1; \tilde{F}_1] + n\int_X dx'[\phi; \tilde{F}_2] \qquad (3.\ 8)$$

in the limit $M \to \infty$. Here use was made of partial integration with respect to δz and the closure property of $\{s_j(x)\}$. This is formally the same as the first equation of the BBGKY hierarchy. However, if we multiply (3. 1) by $z(x)z(x')$ and integrate it to obtain the second equation which governs $\tilde{F}_2$, we find easily that the equation obtained is not the same as the second equation of the BBGKY hierarchy because now the second term of (3. 1) comes into play to give an effect of the modification due to the operator P. The same is true for the higher-order equations of the hierarchy. Thus, $\tilde{F}_2$, $\tilde{F}_3$, $\cdots$cannot be time-reversible, so that $\tilde{F}_1$ is also time-irreversible. This is an essential difference between (3. 8) and the corresponding equation for F_1. From the viewpoint of the new hierarchy, it is no puzzle that the proper irreversible approximation to $\tilde{F}_2$ in (3. 8) as seen in Born and Green's[14] work gives rise to the Boltzmann equation with irreversibility. One may see a coarse-grained aspect[15] of $\tilde{F}_1$ from this fact, but we will come back to this matter in the final subsection of Sec. 4.

4. Application to the Weak Interaction Case

By the weak interaction case we mean the case where the total interaction energy between particles is far less than the whole energy of the system, such as the case of a gas or sometimes a plasma. In this case, the Riemannian space reduces to the fixed hyperplane in A_1 which satisfies

$$n\int_X H_1(x)z(x)dx/V = e \quad (e: \text{const.}). \tag{4. 1}$$

This constitutes a subspace of A_1, which we may call B. Our problem thus reduces to solving in general the master equation (3. 1) in B. Here we give the explicit formulation of the operator $\bar{P}$ and next describe the practical program of how to calculate a physical quantity on the basis of our functional random-walk model with the use of a high-speed computer in mind.

(i) Euclidean coordinates in B

To represent a point in B in terms of a set of the Euclidean coordinates, we derive an orthonormal function set in B, starting from $\{s_j(x)\}$. The limiting process $V \to \infty$ is put off until we arrive at the final formula.

Now in the representation: $z(x) = \sum b_j s_j(x)$, (2. 13) defining A_1 is given as

$$\sum_j b_j \int_X s_j(x)dx/V = 1 \ . \tag{4. 2}$$

To find a rotation of R^M such that one of the basic vectors becomes a normal to the hyperplane A_1, the transformation matrix (t_{ij}) such that

$$b_j = \sum_k b_k^{(1)} t_{kj} \quad \text{or} \quad b_k^{(1)} = \sum_j t_{kj} b_j \tag{4. 3}$$

is introduced. $\{b_k^{(1)}\}$ are the new coordinates and the normal coordinate to A_1 is taken as $b_1^{(1)}$. If we put $b_k^{(1)} = 0$ except for $k = 1$ and $b_1^{(1)} = 1$, then (4. 3) gives

$$t_{1j} = \frac{[\sum_k \{\int_X s_k(x)dx/V\}^2]^{1/2}}{\int_X s_j(x)dx/V} \ , \tag{4. 4}$$

since $\{b_j\}$ in this case are nothing but the direction cosines of a normal to A_1. This fixes a part of elements of the matrix (t_{ij}). The other elements, however, can be arbitrarily given except under the condition that (t_{ij}) should be an orthogonal matrix; this arbitrariness corresponds to the freedom of space rotation within A_1.

In the new coordinate system the hyperplane can be expressed by $b_1^{(1)} = b_{1o}^{(1)}$ (a certain const.) This constant, which is the distance between the hyperplane and the origin of R^M, is found by the substitution of (4. 3) into (4. 2) together with $b_k^{(1)} = 0$ except for $k = 1$. Namely

$$b_{1o}^{(1)} = 1/\{\sum_j t_{1j} \int_X s_j(x)dx/V\}$$

$$\text{or } 1/[\sum_j \{\int_X s_j(x)dx/V\}^2]^{1/2}. \qquad (4.\ 5)$$

Thus, a function in A_1 can be expressed as

$$z(x) = \sum_{j\geq 2} b_j^{(1)} s_j^{(1)}(x) + c_1(x) \qquad (4.\ 6)$$

where

$$s_j^{(1)}(x) = \sum_k t_{jk} s_k(x) , \qquad (4.\ 7)$$

$$c_1(x) = b_{1o}^{(1)} s_1^{(1)}(x) . \qquad (4.\ 8)$$

In quite a similar way, we can find a rotation of A_1 such that one of the basic vectors becomes a normal to the hyperplane B. This time we note that the transformation matrix $(t_{ij}^{(1)})$ is of M - 1 dimensions with the suffix conveniently begining with 2. Corresponding to (4. 4), we have

$$t_{2j}^{(1)} = \frac{\int H_1 s_j^{(1)}(x)dx/V}{[\sum_{k\geq 2} \{\int_X H_1 s_k^{(1)}(x)dx/V\}^2]^{1/2}} , \quad j \geq 2 \qquad (4.\ 9)$$

on account of (4. 1). The distance between B and the origin of A_1 is given as

$$b_{2o}^{(2)} = \frac{e - n\int H_1 c_1(x)dx/V}{n[\sum_{j\geq 2}\{\int_X H_1 s_j^{(1)}(x)dx/V\}^2]^{1/2}} . \qquad (4.\ 10)$$

As a result, a function in B is expressed as

$$z(x) = \sum_{j\geq 3} b_j^{(2)} s_j^{(2)}(x) + c_2(x) + c_1(x) \qquad (4.\ 11)$$

where

$$s_j^{(2)}(x) = \sum_{k\geq 2} t_{jk}^{(1)} s_k^{(1)}(x) , \qquad (4.\ 12)$$

$$c_2(x) = b_{2o}^{(2)} s_2^{(2)}(x) . \qquad (4.\ 13)$$

Hence we know an orthonormal function set in B is given by (4. 12) i.e.

$$s_j^{(2)}(x) = \sum_{k\geq 2} t_{jk}^{(1)} \sum_{l\geq 2} t_{kl} s_l(x) , \ j \geq 3 \qquad (4.\ 14)$$

and $\{b_j^{(2)}\}$ is a set of the Euclidean coordinates based on it; but note that the space R^{M-2} spanned by (4. 14) is not equal by itself but parallel to B, as is seen from (4. 11).

(ii) The explicit form of P

In the frame of R^{M-2} now obtained, z(x) in the master equation (3. 1) should be replaced by

$$z(x) = \bar{z}(x) + c_\perp(x) + c_2(x) ; \qquad (4.\ 15)$$

here and hereafter a function with a bar on top indicates that it belongs to $\bar{B} \equiv R^{M-2}$ (spanned by (4. 14)). Differentiation is invariant to this replacement; $\delta/\delta z(x) = \delta/\delta\bar{z}(x)$. In this frame, let us consider the func-

tional quadratic form with the coefficient kernel function $[\phi;\ z(x)z(x')]$. After the orthogonal transformation in $\bar{B}$ to make it diagonal, it can be written as

$$\int_X \int_X \bar{y}(x)\bar{y}(x')[\phi;\ z(x)z(x')]dxdx' = \sum_{j\geq 3} a_j^{*2} D_j(z) \ , \qquad (4.\ 16)$$

where a_j^* are the Euclidean coordinates of $\bar{y}(x)$; the (real) eigenvalues D_j depend on ϕ and z. Thus, the minimum modification of (4. 16) to make it positive-definite is simply to neglect $D_j(z)$ when $D_j(z) < 0$. This leads to the formula:

$$\int_X \int_X \bar{y}(x)\bar{y}(x')P[\phi;\ z(x)z(x')]dxdx' = \sum_{j\geq 3} a_j^{*2} \tilde{D}_j(z) \qquad (4.\ 17)$$

where

$$\tilde{D}_j(z) = D_j(z) \ , \quad D_j > 0 \ ;$$

$$= 0 \quad , \quad D_j \leq 0 \ . \qquad (4.\ 18)$$

Although this means just "completely prohibiting the anti-irreversible process to happen", as already described, an interesting relation with the coarse-graining idea will be explained in the final subsection.

(iii) General solution for $\tilde{\rho}$

A general solution for $\tilde{\rho}$ can formally be constructed in the form of a repeated multiple integral by the propagation kernel method.[1,16] That is,

$$\tilde{\rho}(z,\ t) = \lim_{\Delta t \to o} \int_{\bar{B}} \cdots \int_{\bar{B}} P_{\Delta t}(z^L/z^{L-1}) \cdots P_{\Delta t}(z^2/z^1)\tilde{\rho}(z^1,\ 0) \prod_{k=1}^{L-1} \delta\bar{z}^k \ , \quad (4.\ 19)$$

where $z = z^L$, $\Delta t = t/L$, and the superscripts indicate the order of the

time-subintervals. The infinitesimal kernel $P_{\Delta t}$ is explicitly obtained from (3. 1) as

$$P_{\Delta t}(z^{k+1}/z^k) = \int_{\bar{B}} \exp[i\int_X \bar{y}^k(x)\{\bar{z}^k(x) - \bar{z}^{k+1}(x) + \Delta t Qz^k(x)\}dx$$

$$- \frac{\Delta t}{2}\int_X\int_X \bar{y}^k(x)\bar{y}^k(x')P[\phi;\ z^k(x)z^k(x')]dxdx']\delta\bar{y}^k \ , \qquad (4.\ 20)$$

and $\tilde{\rho}(z^1,\ 0)$ is the initial condition on $\tilde{\rho}$. It should be noted that the arguments in $\tilde{\rho}$ and $P_{\Delta t}$ are actually $\bar{z}^k$ rather than z^k through (4. 15) in the present frame of $\bar{B}$. The present notation of arguments is entirely for convenience.

The expression (4. 20) may be rewritten in terms of the Euclidean coordinates for $\bar{y}^k(x)$;

$$\bar{y}^k(x) = \sum a_j^{k*} s_j^{k*}(x) \ , \qquad (4.\ 21)$$

where $\{s_j^{k*}(x);\ j \geq 3\}$ is the orthonormal function set in $\bar{B}$ which is related with (4. 14) by the orthogonal transformation described in the preceding subsection. By noting (4. 17), we have

$$P_{\Delta t}(z^{k+1}/z^k) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp[i\sum_{j\geq 3} a_j^{k*}\{\beta_j^{k*} - b_j^{k+1*} + \Delta t\int_X s_j^{k*}(x)Qz^k(x)dx\}$$

$$- \frac{\Delta t}{2}\sum_{j\geq 3}(a_j^{k*})^2\,\tilde{D}_j(z^k)]\prod_{j\geq 3}\{da_j^{k*}/(2\pi)^{1/2}\} \ , \qquad (4.\ 22)$$

where

$$\beta_j^{k*} = \int_X s_j^{k*}(x)\bar{z}^k(x)dx \qquad (4.\ 23)$$

and

$$b_j^{k+1*} = \int_X s_j^{k*}(x)\bar{z}^{k+1}(x)dx \ , \qquad (4.\ 24)$$

which is further calculated as

$$P_{\Delta t}(z^{k+1}/z^k) = \prod_j \frac{1}{\{\Delta t \tilde{D}_j(z^k)\}^{1/2}} \exp\left[-\frac{\{\beta_j^{k*} + \Delta t \int_X s_j^{k*}(x) Q z^k(x) dx - b_j^{k+1*}\}^2}{2\Delta t \tilde{D}_j(z^k)}\right] . \tag{4. 25}$$

Here we note that the j-th factor with $\tilde{D}_j = 0$, if any, reduces to the delta function $\delta(\beta_j^{k*} + \Delta t \int_X s_j^{k*}(x) Q z^k(x) dx - b_j^{k+1*})$.

$P_{\Delta t}$ in (4. 25) is a generalized Gaussian measure factor with respect to $\{b_j^{k+1*}\}$, so that it may be interpreted as the probability density for the stochastic quantity $\{b_j^{k+1*}\}$. Since this probability depends on z^k and since $\{b_j^{k+1*}\}$ represents z^{k+1} in the manner of (4. 24), it may be understood as the transition probability that a random-walker in the space B (or $\bar{B}$) moves from the point z^k (or $\{b_j^{k*}\}$) to the point z^{k+1} (or $\{b_j^{k+1*}\}$) in a small time Δt. A great difference in our random walk from the simple Brownian motion is seen in the complicated dependence of $P_{\Delta t}$ on z^k, i.e. the starting point at each instant. As a consequence, the measure $\tilde{\rho}\delta\bar{z}$ established by (4. 19) together with (4. 25) is far more complicated in shape than the Wiener measure. However, it is worth noting that the present master equation approach has the great mathematical advantage over the original state functional approach[1] in that the existence of the integral $\tilde{\Psi} = \int_{\bar{B}} \exp(i\int yzdx)\, \tilde{\rho}\delta\bar{z}$ is guaranteed by establishment of the measure $\tilde{\rho}\delta\bar{z}$ even in the limit $M \to \infty$[17]. Thus, it is concluded that all $\tilde{F}$s converge as $M \to \infty$.

(iv) The Monte Carlo quadrature

It is now obvious that if (3. 6) is adopted for $\tilde{\rho}(z_1, 0)$, (4. 19) expresses the probability of finding the random walker, who started from $F_o(x)$ in B, at $z(x)$ after a continuous chain of random-walk during the time t. The whole integration in (4. 19), however, is analytically impossible. It is rather fortunate that the first integral with respect to z^1 can be calculated as

$$\int_{\bar{B}} P_{\Delta t}(z^2/z^1)\tilde{\rho}(z^1, 0)\delta\bar{z}^1 = \int_{\bar{B}} P_{\Delta t}(z^2/z^1)\delta[\bar{z}^1(x) + c_1(x) + c_2(x) - F_o(x)]\delta\bar{z}^1$$

$$= P_{\Delta t}(z^2/F_o) \ . \qquad (4.\ 26)$$

But the next successive integrals with respect to $\bar{z}^2$, $\bar{z}^3$.., i.e. in the Euclidean coordinates $\{b_j^{2*}\}$, $\{b_j^{3*}\}$, ...are involved enough to recommend the Monte Carlo quadrature with the use of a high-speed computer; although then we should be satisfied with an approximate value to the true integral.

It is nice for an importance sampling to be applied that the integrand itself constitutes a product of conditional probability densities. Then, the first task to estimate the second integral with respect to $\{b_j^{2*}\}$ is just to sample values for $\{b_j^{2*}\}$ out of the ensemble with the probability distribution $P_{\Delta t}(z^2/F_o)$ and to insert them through $z^2(x)$ into $P_{\Delta t}(z^3/z^2)$. ($\{s_j^{1*}(x)\}$ is known as a set of eigenvectors with the eigenvalues $\{\tilde{D}_j(F_o)\}$. Hence $\bar{z}^2(x)$ is solved for by (4. 24). Together with $\{\tilde{D}_j(z^2)\}$, a new set of eigenvectors $\{s_j^{2*}(x)\}$ is found and hence $\{\beta_j^{2*}\}$ is solved for.) Thus, the probability for $\{b_j^{3*}\}$ is decided and so the same sampling process can be done for $\{b_j^{3*}\}$, and further for $\{b_j^{4*}\}$,... until we arrive at $\{b_j^{L-1*}\}$, when one round of the importance sampling for the whole integral (4. 19) finishes. The next task is, of course, the average over many rounds of sampling.

If we wish to estimate $\tilde{F}_s$ by the formula (3. 7), another sampling is necessary for the integration with respect to $\{b_j^{L*}\}$. In this case we only have as the estimator a function $z(x_1)$ .. $z(x_s)$ made of the sampled values for $\{b_j^{L*}\}$, so that the average over many such sample functions may give $\tilde{F}_s(x_1, .., x_s, t)$. This is the principle of the Monte Carlo quadrature

for calculating $\tilde{F}_s$. Since (4. 25) is a Gaussian probability distribution for $\{b_j^{k+1*}\}$, we can sample the values for $\{b_j^{k+1*}\}$ out of normal random numbers with proper variances and averages. It is interesting to note that each round of the importance sampling simulates nothing but each chain of random-walk during the time t in a segmented way. In the limit when $\Delta t \to 0$ or $L \to \infty$ the simulation becomes perfect. Also, it is expected that the other approximations included in the present procedure are improved with the values of M and V increasing independently.

(v) The relation with the coarse-graining idea

We may point out a slight relation of our master equation approach with the coarse-graining idea. The prescription of (4. 17) - (4. 18) may also be understood to limit the space for $\bar{y}(x)$ into a smaller subspace than R^{M-2} by neglecting all the j-th eigenvectors of the space when $D_j \leq 0$. This means that $\bar{y}(x)$ has been coarse-grained by losing many orders of orthonormal functions which are not desirable for the irreversible description of the system. However, this coarse-graining procedure is not so fixed an operation as the conventionally understood one[15], but is very flexible because it depends on z. If we proceed so thoroughly with the physically motivated coarse-graining idea that we artificially change the domain of integration in (4. 22) from R^{M-2} to the subspace described above, the transition probability in (4. 25) will be the product of only the j-th factors with $D_j(z^k) > 0$. Then, b_j^{k+1} with the same j as that of the neglected eigenvector in $\bar{y}^k(x)$ does not appear in $P_{\Delta t}$, so that $\bar{z}^{k+1}(x)$ and hence $z^{k+1}(x)$ would be coarse-grained in the same way (depending on z^k) as $\bar{y}^k(x)$. Hence we can coarse-grain the distribution function $\tilde{F}_s$ (in a flexible sense) through the relation (3. 7). The above discussion based on the artificial change of the domain of integration

is interesting in suggesting the physical meaning of our master equation approach to some degree, but obviously such an artifice is strictly inexact. Therefore, we can only see by this discussion a roughly sketched, probable physical picture of our theory. All what we may say is that some very flexible kind of averaging process must have been introduced as a result of the operation P.

5. Conclusion

A minimum modification of the functional formalism of classical non-equilibrium statistical mechanics was performed (on the basis of the cylinder functional approach) such that the basic equation turns into the master equation, which includes the irreversible system evolution. The general theory was applied to the case with a gas or a weakly interacting plasma. The method of solution proposed in Sec. 4 has no great technical difficulty but for the use of a high-speed computer. All calculations with the Monte Carlo quadrature will be rather simple for the machine. It may be said that the possibility suggested in ref. 1 of approaching non-equilibrium statistical mechanics by the Monte Carlo quadrature has been clarified in this paper. It is expected that this method will clarify many unsolved problems in relation with the irreversible process of the many-particle system, even for the case with spatial inhomogeneity. If we are interested in a steady state, it can be studied by examining an asymptotic behavior of the solution as $t \to \infty$ for an arbitrary type of initial condition. Together with the tangential approximation to the Riemannian space, the method of solution can extensively be used for the general strong interaction case with an additional care. In these respects the practical value of the present theory depends to a large extent on future works employing a computer. It is interesting to note that a similar type of functional integral (with the Gaussian measure),

which corresponds to a solution for the characteristic functional for the Burgers model turbulence, was recently calculated by the Monte Carlo quadrature with promising success[18].

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