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Renormalized Kinetic Theory of Nonequilibrium Many-Particle Classical Systems

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The far-from-equilibrium statistical dynamics of classical particle systems is formulated in terms of self-consistently determined phase-space density response, fluctuation, and vertex functions. Collective and single-particle effects are treated on an equal footing. Two approximations are discussed, one of which reduces to the Vlasov equation direct interaction approximation of Orszag and Kraichnan when terms that are explicitly due to particles are removed.

KEY WORDS: Kinetic theory; plasma.

1. INTRODUCTION

Renormalized descriptions of statistical field theories usually depend on the existence of a noninteracting limit in which multipoint correlation functions are simply related to the one- and two-point functions. In quantum field theory this relationship is the Wick expansion, and in classical theories it is the case of Gaussianly distributed random variables. The Gaussian relationships may be viewed as a special case of the cumulant expansion when the nth cumulant C_n is zero for $n > 2$. It is also possible to construct a renormalized description even if the noninteracting limit has $C_n \neq 0$ for $n > 2$. For every $C_n \neq 0$, there will appear an effective n-point "bare" vertex function in addition to the bare vertices which describe the nonlinear couplings in the fundamental dynamic equations.[1–3] If there are many significant C_n, any perturbative expansion which only retains a small number of the effective vertices is bound to fail. Of course, even if the Gaussian limit is attainable, the actual statistical state may be so far from this limit that its perturbative description is difficult.

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A classical gas has the property that its statistics, as described by the phase space density

$$f(rpt) = \sum_{i=1}^{N} \delta(r - r_i(t))\, \delta(p - p_i(t))$$

are very non-Gaussian even for noninteracting particles because of the trivial correlation of a particle with itself. Despite the intrinsic non-Gaussianity of f, Mazenko[4] has been able to obtain a fully renormalized kinetic theory in thermal equilibrium.

In this paper we develop a renormalization procedure which can describe nonequilibrium states. It is based upon the variational methods of Schwinger[5] and the occupation number representation for classical many-particle systems of Doi.[6,8] This representation expresses f as $\psi^\dagger\psi$, where ψ and $\psi^\dagger$ are (classical) particle annihilation and creation operators. In addition to the mean value of f, there are coupled equations for the various correlation functions of ψ and $\psi^\dagger$ up to and including those which have four (phase space, time) arguments. These correlation functions correspond to response and fluctuation functions of f. The necessity of both response and fluctuation functions is due to the lack of a fluctuation dissipation theorem for a general nonequilibrium state. This parallels the situation in the formalism of Martin *et al.*,[9] which is applicable to continuous classical fields. The occurrence of fluctuation and response functions requires the use of two memory functions, one of which represents an effective one-body potential and the other an effective random source of particles.

2. THE ESSENTIAL NON-GAUSSIANITY OF *f*

Let $\langle\cdots\rangle$ denote an ensemble average over random initial conditions at time $t = 0$. It is well known[10] that the singular nature of f leads to singularities in the equal-time correlation functions. For example, with the definitions

$$q = (r, p), \qquad f_1 = f(q_1, t_1), \qquad N_1 = \langle f_1 \rangle$$

it follows that

$$\langle f_1 f_2 \rangle_{t_1 = t_2} = N_1 N_2 + H_{12} + N_1\, \delta(q_1 - q_2) \tag{1}$$

where

$$H_{12} = G_{12} - N_1 N_2$$

and G_{12} is the pair distribution function

$$G_{12} = \sum_{i \neq j} \langle \delta(q_1 - q_i(t_1))\, \delta(q_2 - q_j(t_2)) \rangle$$

The delta function in (1) is due to the correlation of a particle with itself and H represents two-particle correlations. If there are no three-particle correlations besides those due to self-correlations and those implied by H, then

$$\begin{aligned}\langle f_1 f_2 f_3\rangle_{t_1=t_2=t_3} = {} & N_1 N_2 N_3 + N_1[N_2\,\delta(q_2 - q_3) + H_{23}] \\ & + N_2[N_3\,\delta(q_3 - q_1) + H_{31}] + N_3[N_1\,\delta(q_1 - q_2) + H_{12}] \\ & + \delta(q_1 - q_2)H_{23} + \delta(q_2 - q_3)H_{31} + \delta(q_3 - q_1)H_{12} \\ & + \delta(q_1 - q_2)\,\delta(q_1 - q_3)N_1 \end{aligned} \tag{2}$$

The one-, two-, and three-point equal-time cumulants of f are

$$\begin{aligned} C_1 &= N_1, \qquad C_{12} = H_{12} + N_1\,\delta(q_1 - q_2) \\ C_{123} &= \delta(q_1 - q_2)H_{23} + \delta(q_2 - q_3)H_{31} + \delta(q_3 - q_1)H_{12} \\ &\quad + \delta(q_1 - q_2)\,\delta(q_1 - q_3)N_1 \end{aligned} \tag{3}$$

Since the three- and higher point cumulants are not small despite the nonexistence of intrinsic higher particle correlations, a cumulant description of the statistics of f is poor.

The essential nature of C_{123} is demonstrated by considering the short-time limit of the random initial value problem for f. Let $u(\mathbf{r})$ be the interparticle potential, $\mathbf{w}(\mathbf{r})$ its gradient, and assume it to be well enough behaved at small and large values of r so that the coefficients in the Taylor series expansion of $\langle f\rangle$ and $\langle ff\rangle$ are finite. Let

$$\mathbf{F}_1 = -\int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2) f_2\, dq_2$$

be the force on a particle at $\mathbf{r}_1$ due to its interaction with all other particles. f evolves according to the Klimontovich equation

$$\frac{\partial f_1}{\partial t_1} + \frac{\mathbf{p}_1}{m}\cdot\frac{\partial f_1}{\partial \mathbf{r}_1} + \mathbf{F}_1\cdot\frac{\partial f_1}{\partial \mathbf{p}_1} = 0$$

For short times t,

$$\begin{aligned} f(q_1, t) &= f(q_1, 0) + t\dot{f}(q_1, 0) + O(t^2) \\ N(q_1, t) &= \langle f(q_1, t)\rangle = \langle f(q_1, 0)\rangle + t\langle \dot{f}(q_1, 0)\rangle + O(t^2) \\ &= N(q_1, 0) + t\left[-\frac{\mathbf{p}_1}{m}\cdot\frac{\partial N(q_1, 0)}{\partial \mathbf{X}_1} - \left\langle \mathbf{F}(x_1, 0)\cdot\frac{\partial f(q_1, 0)}{\partial \mathbf{p}_1}\right\rangle\right] + O(t^2) \\ &= N(q_1, 0) + t\left[-\frac{\mathbf{p}_1}{m}\cdot\frac{\partial N(q_1, 0)}{\partial \mathbf{r}_1} - \langle \mathbf{F}(r_1, 0)\rangle\cdot\frac{\partial N(q_1, 0)}{\partial \mathbf{p}_1}\right. \\ &\quad \left. + \frac{\partial}{\partial \mathbf{p}_1}\cdot\int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_1')H_1{}'{}_1\, dq_1'\right] + O(t^2) \end{aligned} \tag{4}$$

$N(q_1, t)$ may also be calculated as the coefficient of the delta function in the short-time expansion of C_{12}. While the above expansion for N is independent of the initial value of $\langle fff \rangle$, that of C_{12} is not. If C_{12} is calculated, ignoring the existence of C_{123}, then the coefficient of its delta function would coincide with (4) except for the term proportional to H, which is missing. Therefore, an attempt to describe the statistics of f in an approximation which completely ignores its non-Gaussian initial conditions will violate the identity between the strength of the delta function part of C_{12} at equal times (the so-called particle noise) and $\langle f \rangle$. Since particle noise is essential to the statistical description of collisions, its misrepresentation could well lead to poor approximations. Even if the gas is driven very far from equilibrium, it will "remember" its non-Gaussian initial conditions for all times because the form of the equal-time correlation functions as displayed in (3) is invariant.

3. REVIEW OF THE OCCUPATION NUMBER REPRESENTATION

The following results are taken directly from Doi[6] (see also the work of Katz[7]). Consider the operator algebra generated by the fields $\Psi(q)$ and $\Psi^\dagger(q)$, which are assumed to satisfy the commutation relations

$$[\Psi(q), \Psi^\dagger(q')] = \delta(q - q') \tag{5}$$

A space of states is constructed by applying products of $\Psi^\dagger$'s to a vacuum state $|0\rangle$, which is assumed to have the properties

$$\langle 0|0\rangle = 1 \tag{6}$$

$$\Psi|0\rangle = 0 \tag{7}$$

To a given probability distribution function

$$F(q_1, q_2, \ldots, q_N; t) \equiv F(q^N; t) \equiv F^{(N)}$$

of an N-particle system assign the state

$$|F(t)\rangle = \frac{1}{N!} \int dq^N\, F(q^N; t)|q^N\rangle \tag{8}$$

where

$$|q^N\rangle = \Psi^\dagger(q_1) \cdots \Psi^\dagger(q_N)|0\rangle \tag{9}$$

It follows that

$$F(q^N; t) = \langle q^N|F(t)\rangle \tag{10}$$

More generally, if the number of particles is not fixed, the right-hand side of (8) is summed over N. To a linear operator A which transforms

$$F = \{F^{(0)}, F^{(1)}, \ldots\}$$

into

$$F_A = \{F_A^{(0)}, F_A^{(1)}, \ldots\}$$

where

$$F_A^{(N)} = A^{(N)} F^{(N)}$$

and A has the form

$$A^{(N)}(q^N) = \sum_{i=1}^{N} A_1(q_i) + \tfrac{1}{2} \sum_{i \neq j} A_2(q_i, q_j) + \cdots \tag{11}$$

assign the operator $\tilde{A}$,

$$\tilde{A} = \tilde{A}_1 + \tilde{A}_2 + \cdots$$

$$\tilde{A}_1 = \int dq\, \Psi^\dagger(q) A_1(q) \Psi(q)$$

$$\tilde{A}_2 = \tfrac{1}{2} \int dq\, dq'\, \Psi^\dagger(q) \Psi^\dagger(q') A_2(q, q') \Psi(q) \Psi(q') \tag{12}$$

Finally, define the state

$$|\text{sum}\rangle = \exp\left[\int dq\, \Psi^\dagger(q)\right] |0\rangle \tag{13}$$

It can then be shown that

$$\Psi |\text{sum}\rangle = |\text{sum}\rangle, \qquad \langle \text{sum}| \Psi^\dagger = \langle \text{sum}| \tag{14}$$

and

$$\bar{A}(t) \equiv \sum_{N=0}^{\infty} \frac{1}{N!} \int dq^N A^{(N)}(q^N) F^{(N)}(q^N; t) = \langle \text{sum}| \tilde{A} | F(t) \rangle \tag{15}$$

In particular, the normalization of F is expressed by

$$\langle \text{sum} | F(t) \rangle = 1 \tag{16}$$

There are three operators $\tilde{A}$ of prime interest: (1)

$$\tilde{n}(q) \equiv \Psi^\dagger(q) \Psi(q) \tag{17}$$

which for an N-particle system corresponds to $f(q)$; (2)

$$\tilde{n}(q, q') \equiv \Psi^\dagger(q) \Psi^\dagger(q') \Psi(q) \Psi(q') \tag{18}$$

which corresponds to

$$\sum_{1 \leqslant i \neq j \leqslant N} \delta(q - q_i)\, \delta(q' - q_j)$$

and (3) the Liouville operator

$$\tilde{\mathscr{L}} \equiv \int dq_1\, \Psi^\dagger(q_1)\, \frac{\mathbf{p}_1}{m}\cdot\frac{\partial\Psi(q_1)}{\partial\mathbf{r}_1} - \int dq_1\, dq_2\, \Psi^\dagger(q_1)\Psi^\dagger(q_2)\mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)\cdot\frac{\partial\Psi(q_1)}{\partial\mathbf{p}_1}\,\Psi(q_2) \tag{19}$$

which corresponds to

$$\mathscr{L} = \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial\mathbf{r}_i} - \sum_{1\leqslant i\neq j\leqslant N} \mathbf{w}(\mathbf{r}_i - \mathbf{r}_j)\cdot\frac{\partial}{\partial\mathbf{p}_i} \tag{20}$$

$\tilde{\mathscr{L}}$ is the time evolution operator,

$$(\partial/\partial t)|F(t)\rangle = -\tilde{\mathscr{L}}|F(t)\rangle \tag{21}$$

$\tilde{n}(q)$ is the phase-space density operator,

$$\langle\text{sum}|\tilde{n}(q)|F(t)\rangle = N_{qt} \tag{22}$$

and $\tilde{n}(q, q')$ is the (equal time) pair distribution operator,

$$\langle\text{sum}|\tilde{n}(q, q')|F(t)\rangle = G_{qt,q't} \tag{23}$$

It follows from (14) that in (22), $\tilde{n}(q)$ can be replaced by $\Psi(q)$, and in (23), $\tilde{n}(q, q')$ can be replaced by $\Psi(q)\Psi(q')$. The normalization of F as expressed in (16) is preserved in time because

$$\langle\text{sum}|\tilde{\mathscr{L}} = 0 \tag{24}$$

This is a consequence of (14) and the presence of the derivatives $\partial/\partial\mathbf{r}_1$ and $\partial/\partial\mathbf{p}_1$ in (19).

As in quantum field theory, the time evolution can be shifted from $|F\rangle$ to Ψ and $\Psi^\dagger$ by going into the equivalent of the Heisenberg representation. Since the Liouville operator of (20) is time independent,

$$|F(t)\rangle = [\exp(-\tilde{\mathscr{L}}t)]|F(0)\rangle \tag{25}$$

and

$$\bar{A}(t) = \langle\text{sum}|\tilde{A}\exp(-\tilde{\mathscr{L}}t)|F(0)\rangle = \langle\text{sum}|\exp(\tilde{\mathscr{L}}t)\,\tilde{A}\exp(-\tilde{\mathscr{L}}t)|F(0)\rangle \tag{26}$$

where (24) is used to replace $\langle\text{sum}|$ by $\langle\text{sum}|\exp(\tilde{\mathscr{L}}t)$. If $\tilde{A}$ is expressed as in (12), then $\tilde{A}(t) \equiv \exp(\tilde{\mathscr{L}}t)\,\tilde{A}\exp(-\tilde{\mathscr{L}}t)$ is expressed as a sum of products of $\Psi(t)$ and $\Psi^\dagger(t)$, where

$$\Psi(t) \equiv \exp(\tilde{\mathscr{L}}t)\,\Psi\exp(-\tilde{\mathscr{L}}t), \qquad \Psi^\dagger(t) \equiv \exp(\tilde{\mathscr{L}}t)\,\Psi^\dagger\exp(-\tilde{\mathscr{L}}t) \tag{27}$$

4. TIME-DEPENDENT PERTURBATION FORMALISM

Schwinger's equations are obtained by adding time-dependent sources and sinks of particles to $\tilde{\mathscr{L}}$, and then calculating the variation in the correlation function equation of motion. This variation leads to the appearance of objects like

$$\langle \text{sum}|\Psi(t_1)\Psi(t_2)\cdots|F(0)\rangle$$

where t_1 is not necessarily equal to t_2. We will now show how some of the unequal-time correlation functions can be related to response functions.

Allow $\tilde{\mathscr{L}}$ to be time dependent. Equations (25) and (26) are replaced by

$$|F(t)\rangle = U(t)|F(t=0)\rangle \tag{28}$$

$$\bar{A}(t) = \langle \text{sum}|\tilde{A}(t)|F(0)\rangle \tag{29}$$

where

$$\tilde{A}(t) \equiv U^{-1}(t)\tilde{A}U(t) \tag{30}$$

and

$$U(t) \equiv T\exp - \int_0^t \tilde{\mathscr{L}}(t')\,dt' \tag{31}$$

$$U^{-1}(t) \equiv T^*\exp \int_0^t \tilde{\mathscr{L}}(t')\,dt' \tag{32}$$

T is the chronological ordering operator, T^* is the anti-chronological ordering operator, and the time displacement operators U and U^{-1} satisfy

$$U^{-1}(t)U(t) = U(t)U^{-1}(t) = 1$$

$$\partial U(t)/\partial t = -\tilde{\mathscr{L}}(t)U(t), \qquad U(0) = 1 \tag{33}$$

$$\partial U^{-1}(t)/\partial t = U^{-1}(t)\tilde{\mathscr{L}}(t), \qquad U^{-1}(0) = 1 \tag{34}$$

Note that $\tilde{\mathscr{L}}(t)$ does not depend upon $\Psi(t)$ or $\Psi^\dagger(t)$, where

$$\Psi(t) \equiv U^{-1}(t)\Psi U(t), \qquad \Psi^\dagger(t) \equiv U^{-1}(t)\Psi^\dagger U(t) \tag{35}$$

Its time dependence arises through that of external particle sources and external forces. It is convenient to define

$$\tilde{\mathscr{L}}_H(t) = U^{-1}(t)\tilde{\mathscr{L}}(t)U(t) \tag{36}$$

Since $\tilde{\mathscr{L}}(t)$ is a product of Ψ's and $\Psi^\dagger$'s, $\tilde{\mathscr{L}}_H(t)$ has the same form as $\tilde{\mathscr{L}}(t)$ with the replacements $\Psi \to \Psi(t)$, $\Psi^\dagger \to \Psi^\dagger(t)$. In terms of $\tilde{\mathscr{L}}_H$ the equations of motion for U, Ψ, and $\Psi^\dagger$ are

$$\partial U(t)/\partial t = -U(t)\tilde{\mathscr{L}}_H(t)$$

$$\partial\Psi(t)/\partial t = [\Psi(t), -\tilde{\mathscr{L}}_H(t)], \qquad \partial\Psi^\dagger(t)/\partial t = [\Psi^\dagger(t), -\tilde{\mathscr{L}}_H(t)] \tag{37}$$

Note that

$$[\Psi(q,t), \Psi^\dagger(q',t)] = \delta(q-q')$$

The analogy with quantum field theory may now be completed by obtaining formal expressions for the response to time-dependent perturbations. Let

$$\tilde{\mathscr{L}} = \tilde{\mathscr{L}}_0 + \delta\tilde{\mathscr{L}}$$

where $\tilde{\mathscr{L}}_0$ is an "unperturbed" evolution operator. Denote the time displacement operator and the time-dependent representations of Ψ and $\Psi^\dagger$ that correspond to $\tilde{\mathscr{L}}_0$ by $U_0(t)$, $\Psi_0(t)$, and $\Psi_0{}^\dagger(t)$, respectively. Define

$$\tilde{\mathscr{L}}_{0H_0} = U_0{}^{-1}\tilde{\mathscr{L}}_0 U_0, \qquad \tilde{\mathscr{L}}_{0H} = U^{-1}\tilde{\mathscr{L}}_0 U,$$
$$\delta\tilde{\mathscr{L}}_{H_0} = U_0{}^{-1}\,\delta\tilde{\mathscr{L}}\,U_0, \qquad \delta\tilde{\mathscr{L}}_H = U^{-1}\,\delta\tilde{\mathscr{L}}\,U$$

where the time indices have been suppressed. Let

$$U = U_0\cdot\delta U$$

and equate the following two expressions for $\partial U/\partial t$:

$$\partial U/\partial t = -U(\tilde{\mathscr{L}}_{0H} + \delta\tilde{\mathscr{L}}_H)$$
$$\partial U/\partial t = -U_0\tilde{\mathscr{L}}_{0H_0}\,\delta U + U_0\,\partial\delta U/\partial t$$

to obtain

$$\partial\delta U/\partial t = \tilde{\mathscr{L}}_{0H_0}\,\delta U - \delta U(\tilde{\mathscr{L}}_{0H} + \delta\tilde{\mathscr{L}}_H)$$

Since

$$\tilde{\mathscr{L}}_{0H} = \delta U^{-1}U_0^{-1}\tilde{\mathscr{L}}_0 U_0\,\delta U = \delta U^{-1}\tilde{\mathscr{L}}_{0H_0}\,\delta U$$

and

$$\delta\tilde{\mathscr{L}}_H = \delta U^{-1}\,\delta\tilde{\mathscr{L}}_{H_0}\,\delta U$$

it follows that

$$\partial\delta U/\partial t = -\delta\tilde{\mathscr{L}}_{H_0}\,\delta U$$

or

$$\delta U(t) = T\exp - \int_0^t \delta\tilde{\mathscr{L}}_{H_0}(t')\,dt' \tag{38}$$

Similarly

$$U^{-1}(t) = \delta U^{-1}(t)U_0^{-1}(t)$$

with

$$\delta U^{-1}(t) = T^*\exp\int_0^t \delta\tilde{\mathscr{L}}_{H_0}(t')\,dt' \tag{39}$$

Note that $\delta\tilde{\mathscr{L}}_{H_0}(t)$ is a functional of

$$\Psi_0(t) \equiv U_0^{-1}(t)\Psi U_0(t) \qquad \text{and} \qquad \Psi_0{}^\dagger(t) \equiv U_0^{-1}(t)\Psi^\dagger U_0(t)$$

If we further define $A_0(t) = U_0^{-1}(t)AU_0(t)$, then

$$\bar{A}(t) = \langle \text{sum}|\delta U^{-1}(t)A_0(t)\,\delta U(t)|F(t=0)\rangle \tag{40}$$

As in (26), $\delta U^{-1}(t)$ may be replaced by unity.

If $\delta\tilde{\mathscr{L}}$ is "small," the exponential in (38) can be expanded in powers of $\delta\tilde{\mathscr{L}}$ to obtain the linear response of $\bar{A}$, the quadratic response of $\bar{A}$,.... For example, to linear order, the change in $\bar{A}$ due to the perturbation $\delta\tilde{\mathscr{L}}$ is

$$\delta\overline{A(t)} = -\int_0^t dt'\,\langle \text{sum}|A_0(t)\,\delta\tilde{\mathscr{L}}_{H_0}(t')|F(0)\rangle \tag{41}$$

The meaning of $\langle \text{sum}|\Psi(t)\Psi^\dagger(t')|F(0)\rangle$ can be found by considering the linear response of N to a source of particles. Let

$$\delta\tilde{\mathscr{L}}(t) = [1 - \Psi^\dagger(q')]\,\delta(t-t')$$

Since $\langle \text{sum}|\delta\tilde{\mathscr{L}} = 0$, the normalization of $|F\rangle$ is preserved. To calculate δN, set $A = \Psi$: $\delta N(q,t) = \langle \text{sum}|(\Psi(q,t)\Psi^\dagger(q't') - \Psi(qt))|F(0)\rangle$. The equal-time commutation relation between Ψ and $\Psi^\dagger$ implies that

$$\lim_{t\to t'} \delta N(q,t) = \delta(q-q')$$

Therefore,

$$\begin{aligned} R_{12} &\equiv \langle \text{sum}|T\Psi_1\Psi_2{}^\dagger|F(0)\rangle - \langle \text{sum}|\Psi_1|F(0)\rangle \\ &= \langle \text{sum}|T\Psi_1\Psi_2{}^\dagger|F(0)\rangle - \langle \text{sum}|\Psi_1|F(0)\rangle\cdot\langle \text{sum}|\Psi_2{}^\dagger|F(0)\rangle \end{aligned} \tag{42}$$

gives the retarded linear response in the mean particle density at 1 $[=(q_1, t_1)]$ to the injection of a single particle at 2.

Let us also examine the pair distribution response $\delta G_{q_1t,q_2t}$ to the injection of a pair of particles at (q_1', t') and (q_2', t'). For this perturbation

$$\delta\tilde{\mathscr{L}}(t) = [2 - \Psi^\dagger(q_1') - \Psi^\dagger(q_2')]\,\delta(t-t')$$

The exponential in (38) must be expanded to second order in $\delta\tilde{\mathscr{L}}$ to see the interaction of the two injected particles with each other. Suppressing the contribution from all but the lowest order pair interaction term, we have

$$\delta G_{q_1t,q_2t} = \langle \text{sum}|\Psi(q_1t)\Psi(q_2t)\Psi^\dagger(q_1't')\Psi^\dagger(q_2't')|F(0)\rangle \tag{43}$$

Besides the response to the injection of particles, there is the more traditional response to an external force. If the Hamiltonian is changed by

$$\delta H(t) = \sum_i V(r_i, p_i, t)$$

then

$$\delta\mathscr{L}(t) = \sum_i \frac{\partial V}{\partial \mathbf{p}_i}\cdot\frac{\partial}{\partial \mathbf{r}_i} - \frac{\partial V}{\partial \mathbf{r}_i}\cdot\frac{\partial}{\partial \mathbf{p}_i}$$

$$\delta\tilde{\mathscr{L}}(t) = \int dq\, V(q,t)\left[\frac{\partial \Psi^\dagger}{\partial \mathbf{r}}\cdot\frac{\partial \Psi}{\partial \mathbf{p}} - \frac{\partial \Psi^\dagger}{\partial \mathbf{p}}\cdot\frac{\partial \Psi}{\partial \mathbf{r}}\right]$$

$$\frac{\delta N(q,t)}{\delta V(q',t')} = \langle \mathrm{sum}|\Psi(q,t)\left[\frac{\partial \Psi^\dagger(q',t')}{\partial \mathbf{p}'}\cdot\frac{\partial \Psi(q',t')}{\partial \mathbf{r}'} - \frac{\partial \Psi^\dagger(q',t')}{\partial \mathbf{r}'}\cdot\frac{\partial \Psi(q',t')}{\partial \mathbf{p}'}\right]|F(0)\rangle \tag{44}$$

The interpretation of $\langle \mathrm{sum}|\Psi(qt)\Psi(q't')|F(0)\rangle$ for $t \neq t'$ is deferred until Section 6.

5. THE SCHWINGER VARIATIONAL EQUATIONS

Introduce the two-component matrix

$$\Phi(1) \equiv \Phi(q_1, \alpha_1, t_1), \qquad \alpha_1 = \pm$$

where

$$\Phi(q_1, +, t) \equiv \Psi(q,t) \qquad \text{and} \qquad \Phi(q, -, t) \equiv \Psi^\dagger(q,t)$$

All the correlation functions of interest can be generated from the functional

$$W(\eta) \equiv \ln\langle \mathrm{sum}|T \exp \Phi(1)\eta(1)|F(0)\rangle \tag{45}$$

by differentiation with respect to the numerical valued matrix η. In (45) a summation convention is used where repeated continuous (discrete) indices are integrated (summed). The functions

$$G^\eta(1,\ldots,k) \equiv \delta^k W/\delta\eta(1)\cdots\delta\eta(k)$$

reduce to the cumulants of Φ when $\eta = 0$. For example,

$$\lim_{\eta\to 0} G^\eta(1) = \begin{pmatrix} N_1 \\ 1 \end{pmatrix}, \qquad \lim_{\eta\to 0} G^\eta(1,2) = \begin{bmatrix} C_{12} & R_{12} \\ R_{21} & 0 \end{bmatrix}$$

where

$$C_{12} \equiv \langle \mathrm{sum}|\Psi(1)\Psi(2)|F(0)\rangle - N_1 N_2$$

Note that $G(q_1 + t, \ldots, q_N + t)$ is the N-particle Ursell function, and that

$$\lim_{\eta\to 0} G^\eta(-,-) = 0$$

because

$$\langle \mathrm{sum}|\Psi^\dagger\Psi^\dagger|F(0)\rangle = 1 = \langle \mathrm{sum}|\Psi^\dagger|F(0)\rangle$$

In terms of Φ, the Liouville operator in (19) can be written as

$$-\tilde{\mathscr{L}}(t_1) = \hat{\gamma}_2(12)\Phi(1)\Phi(2) + \hat{\gamma}_4(1234)\Phi(1)\Phi(2)\Phi(3)\Phi(4)$$

(no integration over t_1), with

$$\hat{\gamma}_2(q_1\alpha_1t_1, q_2\alpha_2t_2) \equiv -\delta_{\alpha_1 -}\delta_{\alpha_2 +}\frac{\mathbf{p}_1}{m}\cdot\frac{\partial}{\partial \mathbf{r}_1}\,\delta(q_1 - q_2)\,\delta(t_1 - t_2) \tag{46}$$

$$\hat{\gamma}_4(q_1\alpha_1t_1, q_2\alpha_2t_2, q_3\alpha_3t_3, q_4\alpha_4t_4)$$
$$\equiv \delta_{\alpha_1 -}\delta_{\alpha_2 -}\delta_{\alpha_3 +}\delta_{\alpha_4 +}\mathbf{w}_{12}\cdot\frac{\partial}{\partial \mathbf{p}_1}\,\delta(q_1 - q_3)\,\delta(q_2 - q_4)\,\delta(t_1 - t_3)\,\delta(t_2 - t_4) \tag{47}$$

and

$$\mathbf{w}_{12} \equiv \delta(t_1 - t_2)\mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)$$

Since

$$[\Psi^\dagger, \Psi\Psi^\dagger] = [\Psi^\dagger, \Psi^\dagger\Psi]$$

and

$$[\Psi, \Psi\Psi^\dagger] = [\Psi, \Psi^\dagger\Psi] \qquad \text{(at equal times)}$$

$\hat{\gamma}_2$ can be replaced by $\frac{1}{2}\gamma_2$, where

$$\gamma_2(12) \equiv \hat{\gamma}_2(12) + \hat{\gamma}_2(21) \tag{48}$$

In the $\hat{\gamma}_4$ term of $\tilde{\mathscr{L}}$, any rearrangement of the Φ's can be compensated for by modifying γ_2, and hence $\hat{\gamma}_4$ may be replaced by $(1/4!)\gamma_4$, where

$$\gamma_4(1234) \equiv \text{sum of } \hat{\gamma}_4 \text{ over all 4! permutations of its indices} \tag{49}$$

$\tilde{\mathscr{L}}$ can now be expressed in the symmetric form

$$-\tilde{\mathscr{L}}(t_1) = \tfrac{1}{2}\gamma_2(12)\Phi(1)\Phi(2) + (1/4!)\gamma_4(1234)\Phi(1)\Phi(2)\Phi(3)\Phi(4) \tag{50}$$

If the interparticle potential is an even function, $\mathbf{w}$ is an odd function and the γ_2 in (50) is the same as in (48).

The commutators of Φ satisfy

$$[\Phi(q_1\alpha_1t), \Phi(q_2\alpha_2t)] = \tau_{\alpha_1\alpha_2}\,\delta(q_1 - q_2)$$

where

$$\tau \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Therefore

$$\dot{\Phi}(1) = [\Phi(1), -\tilde{\mathscr{L}}] = \tau\gamma_2(12)\Phi(2) + (1/3!)\tau\gamma_4(1234)\Phi(2)\Phi(3)\Phi(4)$$

or

$$G_0^{-1}(12)\Phi(2) = (1/3!)\gamma_4(1234)\Phi(2)\Phi(3)\Phi(4)$$

where

$$\begin{aligned} G_0^{-1}(12) &\equiv -\tau \frac{\partial}{\partial t_1} \delta(q_1 - q_2)\, \delta(t_1 - t_2) - \gamma_2(12) \\ &= -\tau\left(\frac{\partial}{\partial t_1} + \frac{\mathbf{p}_1}{m}\cdot\frac{\partial}{\partial \mathbf{r}_1}\right) \delta(q_1 - q_2)\, \delta(t_1 - t_2) \end{aligned} \tag{51}$$

The occupation number operator algebra is now in a form which exactly parallels that of quantum field theory. The reader is referred to DeDominicis and Martin[11] for the details of the renormalization procedure. The key results are summarized below. $G^\eta(1)$ satisfies

$$\begin{aligned} G_0^{-1}(12)G^\eta(2) = \eta(1) + (1/3!)\gamma_4(1234)[&G^\eta(234) + 3G^\eta(2)G(34) \\ &+ G^\eta(2)G^\eta(3)G^\eta(4)] \end{aligned} \tag{52}$$

It is convenient to work with the inverse of $G(12)$,

$$G^{-1}(12)G(23) = G(12)G^{-1}(23) = \delta(q_1 - q_3)\, \delta(t_1 - t_3)\delta_{\alpha_1\alpha_3}$$

which is determined by a memory function Σ,

$$G^{-1}(12) \equiv G_0^{-1}(12) - \Sigma(12) \tag{53}$$

Σ in turn can be expressed in terms of $G(12)$ and the renormalized three- and four-point vertex functions defined by

$$\Gamma_3(123) \equiv \delta^3[W - \eta(4)G(4)]/\delta G(1)\delta G(2)\delta G(3) \tag{54}$$

$$\Gamma_4(1234) = \delta\Gamma_3(123)/\delta G(4) \tag{55}$$

It can be shown that

$$\Gamma_3(123) = G(\bar{1}\bar{2}\bar{3})G^{-1}(\bar{1}1)G^{-1}(\bar{2}2)G^{-1}(\bar{3}3) \tag{56}$$

$$\begin{aligned} \Gamma_4(1234) = {} & G(\bar{1}\bar{2}\bar{3}\bar{4})G^{-1}(\bar{1}1)G^{-1}(\bar{2}2)G^{-1}(\bar{3}3)G^{-1}(\bar{4}4) \\ & - \Gamma_3(523)G(56)\Gamma_3(164) - \Gamma_3(153)G(56)\Gamma_3(264) \\ & - \Gamma_3(125)G(56)\Gamma_3(364) \end{aligned} \tag{57}$$

$$\begin{aligned} \Sigma(11') = {} & (1/3!)\gamma_4(1234)[3\delta(21')G(3)G(4) \\ & + 3\delta(21')G(34) + 3G(4)\Gamma_3(\bar{2}\bar{3}1')G(\bar{2}2)G(\bar{3}3) \\ & + \Gamma_4(\bar{2}\bar{3}\bar{4}1')G(\bar{2}2)G(\bar{3}3)G(\bar{4}4) \\ & + 3\Gamma_3(5\bar{3}\bar{4})G(56)\Gamma_3(61'\bar{2})G(\bar{2}2)G(\bar{3}3)G(\bar{4}4)] \end{aligned} \tag{58}$$

$$\Gamma_3(123) = \frac{\delta\Sigma(12)}{\delta G(3)} + \frac{\delta\Sigma(12)}{\delta G(45)} G(46)\Gamma_3(376)G(75) \tag{59}$$

$$\begin{aligned}\Gamma_4(1234) = D(12;34) &- \Gamma_3(135)G(56)\Gamma_3(624)\\ &- \Gamma_3(164)G(56)\Gamma_3(523)\end{aligned} \tag{60}$$

$$\tfrac{1}{2}D(12;34) = \frac{\delta\Sigma(12)}{\delta G(34)} + \frac{1}{2}\frac{\delta\Sigma(12)}{\delta G(78)} G(7\bar{7})G(8\bar{8})D(\bar{7}\bar{8};34) \tag{61}$$

Equations (52), (53), and (58)–(61) are a closed set of equations. Though not apparent from the functional manipulations[11] which led to them, this set is exact if and only if the initial conditions satisfy a Wick-type theorem. This means that $G_N(+, +, \ldots, +) = 0$ for $N > 2$, which corresponds to the initial absence of three- and higher particle correlations (see Appendix A).

If η is set equal to zero, the above set deals with physically realizable fluctuation and response functions. If $\eta(+) = 0$, but $\eta(-) \neq 0$, the set refers to the usual classical gas supplemented with a source of particles $\eta(-)$. In either of these two cases, we can make the following general statements. Since $G(-) = 1$, one of the two equations contained in (52) is trivial. The other is the exact equation of motion for N in terms of itself and the equal-time pair distribution function. Replacing the latter by $C + NN$, we obtain the usual

$$\frac{\partial N_1}{\partial t_1} + \frac{\mathbf{p}_1}{m}\cdot\frac{\partial N_1}{\partial \mathbf{r}_1} + \langle \mathbf{F}_1\rangle\cdot\frac{\partial N_1}{\partial \mathbf{p}_1} = \frac{\partial}{\partial \mathbf{p}_1}\cdot\int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2) C_{q_1t_1q_2t_1}\, dq_2 \tag{62}$$

The vanishing of $G(-, -, \ldots, -)$ implies that $\Sigma(+, +)$, $\Gamma_3(+, +, +)$, and $\Gamma_4(+, +, +, +)$ vanish. The retarded nature of R implies that $\Sigma_{-+}(t_1, t_2)$ also vanishes unless $t_1 \geqslant t_2$. Equations (53) and (51) and the above properties of Σ yield

$$\begin{aligned}\left(\frac{\partial}{\partial t_1} + \frac{1}{m}\mathbf{p}_1\cdot\frac{\partial}{\partial \mathbf{r}_1}\right) R_{q_1t_1,q_3t_3} - \int_{t_3}^{t_1} \Sigma(q_1, -, t_1; q_2, +, t_2) R_{q_2t_2,q_3t_3}\, dt_2\, dq_2\\ = \delta(q_1 - q_3)\,\delta(t_1 - t_3)\end{aligned} \tag{63}$$

$$\begin{aligned}\left(\frac{\partial}{\partial t_1} + \frac{1}{m}\mathbf{p}_1\cdot\frac{\partial}{\partial \mathbf{r}_1}\right) C_{q_1t_1,q_3t_3} - \int_0^{t_1} \Sigma(q_1, -, t_1; q_2, +, t_2) C_{q_2t_2,q_3t_3}\, dt_2\, dt_3\\ = \int_0^{t_3} \Sigma(q_1, -, t_1; q_2, -, t_2) R_{q_3t_3,q_2t_2}\, dt_2\, dq_2\end{aligned} \tag{64}$$

If the system is spatially homogeneous, C, R, and Σ may be represented by their Fourier transforms $\tilde{C}(k)$, $\tilde{R}(k)$, and $\tilde{\Sigma}(k)$. Suppressing the dependence upon momentum indices, and denoting the operation of time history integrals by an asterisk, we have schematically

$$\frac{\partial}{\partial t}\tilde{C}(k) - \tilde{\Sigma}_{-+}(k)^*\hat{C}(k) = \tilde{\Sigma}_{--}(k)^*\tilde{R}(-k)$$

Given a certain level of fluctuations at k, Σ_{-+} can cause them to grow or decay, and when viewed as a matrix in its velocity indices, transfer fluctuations from one component of C to another. Since R is the linear response δN of the mean phase-space density to a source of particles η,

$$[\partial/\partial t - \tilde{\Sigma}_{-+}(k)^*]\, \delta\hat{N}(k) = \tilde{\eta}(k) \tag{65}$$

or

$$\delta\tilde{N}(k) = \tilde{R}(k)^* \tilde{\eta}(k) \tag{66}$$

Let $k \to -k$ in (66), and multiply (65) and (66) together,

$$[\partial/\partial t - \tilde{\Sigma}_{-+}(k)^*]\, \delta\tilde{N}(k)\cdot\delta\tilde{N}(-k) = \tilde{\eta}(k)\tilde{\eta}(-k)^*\tilde{R}(-k)$$

If η is random with zero mean, and if $\langle|\eta(k)|^2\rangle$ is its covariance, then

$$[\partial/\partial t - \tilde{\Sigma}_{-+}(k)^*]\langle|\delta\tilde{N}(k)|^2\rangle = \langle|\eta(k)|^2\rangle^*\tilde{R}(-k)$$

Comparing this with (64), we may interpret $\Sigma(-,-)$ as an effective random source of particles. Since, as we will later show, $\Sigma(-,-)$ includes terms which are quadratic in C, it can transfer fluctuations from one wave number to another.

6. THE REPRESENTATION OF MULTI-TIME FLUCTUATION FUNCTIONS

To make contact with other methods of calculation, we must identify the correlation function C, and more generally all unequal-time correlation functions which are not response functions. If $\tilde{A}$ and $\tilde{B}$ are operators of the kind described in (11) and if $t_1 \geqslant t_2$, then

$$\overline{A(t_1)B(t_2)} = \langle \mathrm{sum}|\tilde{A}(t_1)\tilde{B}(t_2)|F(0)\rangle \tag{67}$$

This follows from the arbitrariness in the choice of time origin.[12] If instead of "0," t_2 is chosen as the origin, then $\tilde{B}|F(t_2)\rangle$ takes the place of $\tilde{B}(t_2)|F(0)\rangle$. Since $\tilde{B}|F(t_2)\rangle$ may be regarded as a new phase space function, (67) follows from (29).

Another derivation of (67) is presented because it is easily generalized to the product of any number of operators and because it may aid in the proof of the realizability (see Section 8) of certain approximations. The states $|q^N\rangle$ are a complete set, and we may symbolically write

$$1 = \sum_{N=0}^{\infty} \int \frac{dq^N}{N!}\, |q^N\rangle\langle q^N|$$

which for convenience will also be written in the form

$$1 = |q^N\rangle\langle q^N| \tag{68}$$

It then follows from (30) that

$$\langle \text{sum}|\tilde{A}(t_1)\tilde{B}(t_2)|F(0)\rangle = \langle \text{sum}|\tilde{A}U(t_1)U^{-1}(t_2)|q^N\rangle\langle q^N|\tilde{B}U(t_2)|F(0)\rangle \tag{69}$$

$\langle q^N|U(t_2)|F(0)\rangle$ is the probability that the state $F(0)$ has evolved into the state q^N at time t_2, and $\langle q^N|\tilde{B}U(t_2)|F(0)\rangle/\langle q^N|U(t_2)|F(0)\rangle$ is the mean value of B in that state. Given that the system is in state $|q^N\rangle$ at time t_2, $\langle \text{sum}|\tilde{A}U(t_1)U^{-1}(t_2)|q^N\rangle$ is the mean value of A at the time t_1, since $U(t_1)U^{-1}(t_2)$ is the time displacement operator between times t_2 and t_1. Therefore, (69) is a representation of $\overline{A(t_1)B(t_2)}$ as a summation over the mean values conditioned upon being in a particular state q^N at the intermediate time t_2. This is easily generalized to prove that

$$\overline{A(t_1)B(t_2)\cdots C(t_n)} = \langle \text{sum}|\tilde{A}(t_1)\tilde{B}(t_2)\cdots \tilde{C}(t_n)|F(0)\rangle \tag{70}$$

Now $C_{qt,q't'}$ can be related to the phase-space density–density fluctuation function. Recalling (17) and the notation used in (1), and taking $t_1 \geqslant t_2$,

$$\begin{aligned}\overline{f_1 f_2} &= \langle \text{sum}|\Psi^\dagger(q_1t_1)\Psi(q_1t_1)\Psi^\dagger(q_2t_2)\Psi(q_2t_2)|F(0)\rangle\\ &= \langle \text{sum}|T\Psi(q_1t_1)\Psi^\dagger(q_2t_2{}^+)\Psi(q_2t_2)|F(0)\rangle\end{aligned}$$

where

$$\begin{aligned}t_2{}^+ &= t_2 + \text{a positive infinitesimal}\\ \overline{f_1 f_2} &= G(q_1, +, t_1; q_2, -, t_2{}^+; q_2, +, t_2) + G(q_1, +, t_1; q_2, -, t_2)N_2\\ &\quad + G(q_1, +, t_1; q_2, +, t_2) + G(q_2, -, t_2{}^+; q_2, +, t_2)N_1 + N_1N_2\end{aligned}$$

Since $G(q_2, -, t_2{}^+; q_2, +, t_2) = 0$, we obtain

$$\begin{aligned}(\overline{f_1 f_2})_{t_1\geq t_2} &= G(q_1, +, t_1; q_2, -, t_2{}^+; q_2, +, t_2)\\ &\quad + N_2R_{q_1t_1,q_2t_2} + C_{q_1t_1,q_2t_2} + N_1N_2\end{aligned} \tag{71}$$

and a similar result if $t_2 > t_1$. The three-point cumulant in (71) is expressible in terms of R, C, and Γ_3, which to the lowest order in perturbation theory (see Section 7) is essentially γ_4 integrated over one of its arguments. Together, Eqs. (44) and (71) constitute a generalization of the well-known relationship between the density–density fluctuation function and the density response to an external field which couples to the density.

7. CORRESPONDENCE WITH OTHER METHODS

The renormalized kinetic theory of Mazenko (see the review by Mazenko and Yip[4]) is a natural candidate for comparison because it too deals with a renormalized description of classical many-particle systems. Unfortunately, the steps necessary to reduce the general formalism presented in this paper to the special case of thermal equilibrium are not apparent. In the application of the Martin *et al.*[9] formalism to continuous systems which satisfy a detailed balance condition, a reduction from two propagators (R and C) to one is made possible through the use of a fluctuation dissipation theorem.[13] This theorem gives a linear relationship between $\dot{C}$ and R. However, for a gas in thermal equilibrium, the fluctuation dissipation theorems do not address themselves to the response to the injection of particles. While there are relationships between this kind of response function and the more usual ones, as outlined in the previous section, it is not clear whether or not there exists a simple closed form relationship between C and R. An attempt to follow the manipulations used in the quantum field theory of thermal equilibrium, whereby $\langle \Psi\Psi^\dagger \rangle$ is related to $\langle \Psi^\dagger\Psi \rangle$, breaks down because there does not seem to be any correspondence with the cyclic invariance of the trace operation.

Let us now examine some simple perturbative approximations to the exact system of equations presented in Section 5. The perturbative method will be one in which the interparticle potential is regarded as weak. This is unsuitable in the case of hard-core interactions, for which a generalized T-matrix approximation is introduced in Section 9.

If γ_4 is weak, then Γ_3 and Γ_4 may be expanded as a power series in γ_4 whose leading terms are essentially γ_4. The first-order contribution to Σ, $\Sigma^{(1)}$, is therefore found directly from (57):

$$\Sigma^{(1)}(12) = \tfrac{1}{2}\gamma_4(1234)[G(3)G(4) + G(34)]$$

$$\begin{aligned}\Sigma^{(1)}&(q_1, -, t_1; q_2, +, t_2)\\ &= \delta(t_1 - t_2)\left[\mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)\cdot\frac{\partial N_1}{\partial \mathbf{p}_1} - \frac{\partial\delta(q_1 - q_2)}{\partial \mathbf{p}_1}\cdot\langle \mathbf{F}_1\rangle\right]\end{aligned}$$

$$\Sigma^{(1)}(q_1, -, t_1; q_2, -, t_2) = \delta(t_1 - t_2)\mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)\cdot\left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2}\right)(N_1N_2 + C_{12})$$

Equations (64) and (72) yield

$$\begin{aligned}&\left(\frac{\partial}{\partial t_1} + \frac{1}{m}\mathbf{p}_1\cdot\frac{\partial}{\partial \mathbf{r}_1} + \langle \mathbf{F}_1\rangle\cdot\frac{\partial}{\partial \mathbf{p}_1}\right)C_{13}\\ &\quad - \frac{\partial N_1}{\partial \mathbf{p}_1}\cdot\int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)C_{q_2t_1,q_3t_3}\,dq_2\\ &\quad = \int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)\cdot\left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2}\right)(N_{q_1t_1}N_{q_2t_1} + C_{q_1t_1,q_2t_1})R_{q_3t_3,q_2t_1}\,dq_2 \qquad (73)\end{aligned}$$

while the equation for R coincides with that obtained from the linearized Vlasov equation.

If $t_3 = t_1{}^+$, then $R_{q_3t_3,q_2t_1} = \delta(q_3 - q_2)$, and in the corresponding equation for $\partial C_{13}/\partial t_3$, the right-hand side of (73) is replaced by zero:

$$\left(\frac{\partial}{\partial t_3} + \frac{1}{m}\mathbf{p}_3\cdot\frac{\partial}{\partial \mathbf{r}_3} + \langle \mathbf{F}_3\rangle\cdot\frac{\partial}{\partial \mathbf{p}_3}\right)C_{q_3t_3,q_1t_1}$$
$$- \frac{\partial N_3}{\partial \mathbf{p}_3}\cdot\int \mathbf{w}(\mathbf{r}_3 - \mathbf{r}_2)C_{q_2t_3,q_1t_1}\,dq_2 = 0$$

If the system is spatially homogeneous, $\langle \mathbf{F}\rangle = 0$, $\partial/\partial\mathbf{r}_3 = -\partial/\partial\mathbf{r}_1$, and it follows that

$$\left[\frac{\partial}{\partial t_1} + \frac{1}{m}(\mathbf{p}_1 - \mathbf{p}_3)\cdot\frac{\partial}{\partial \mathbf{r}_1}\right]C_{q_1t_1,q_3t_1}$$
$$- \int\left[\frac{\partial N_1}{\partial \mathbf{p}_1}\cdot\mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)C_{q_2t_1,q_3t_1} + \frac{\partial N_3}{\partial \mathbf{p}_3}\cdot\mathbf{w}(\mathbf{r}_3 - \mathbf{r}_2)C_{q_2t_1,q_1t_1}\right]dq_2$$
$$= \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_3)\cdot\left(\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_3}\right)(N_{q_1t_1}N_{q_3t_1} + C_{q_1t_1,q_3t_1}) \tag{74}$$

This is precisely the equation used by Book and Frieman[15] in their close collision improvement upon the Balescu–Lenard equation. They obtained it from the BBGKY hierarchy by setting the three-body correlation function equal to zero.

The second-order approximation for Σ requires a first-order approximation for Γ_3 and Γ_4. From (59) and (60) we obtain to this order

$$\Gamma_3(123) = \delta\Sigma(12)/\delta G(3) = \gamma_4(1234)G(4),\ \Gamma_4(1234) = \gamma_4(1234) \tag{75}$$

The $\gamma_4\Gamma_4$ term in (58) makes no contribution because with $\Gamma_4 = \gamma_4$, there will either appear a factor $G(-, -) = 0$, or the factors $R_{t_1,t_2}R_{t_2,t_1} = 0$. The second-order contribution to Σ, $\Sigma^{(2)}$, can therefore be written as

$$\Sigma^{(2)}(12) = \tfrac{1}{2}\Gamma_3(134)G(35)G(46)\Gamma_3(562) \tag{76}$$

Superficially, this has the form of the direct interaction approximation (DIA) for quadratically nonlinear equations of motion, such as the Vlasov equation and the Navier–Stokes equation.[16–18] However, there are essential differences due to the presence of explicit particle noise terms. To first order in the interparticle potential, this is the $(NN + C)$ term in (72), and to second order in the potential it arises from the existence of two components to Γ_3:

$$\Gamma_3(++-) \sim \gamma_4(++--), \qquad \Gamma_3(+--) \sim \gamma_4(+--+)N \tag{77}$$

If only the $(++-)$ component is used in (76), and if $\Sigma^{(1)}(-, -)$ is ignored, the equations for C and R precisely correspond to the Vlasov plasma DIA.[16] Including the particle noise terms, (76) yields

$$
\begin{aligned}
&\Sigma^{(2)}(q_1, -, t_1; q_2, +, t_2) \\
&\quad = \frac{\partial C_{12'}}{\partial \mathbf{p}_1}\cdot \mathbf{w}_{2'2}\mathbf{w}_{11'}\cdot \frac{\partial R_{1'2}}{\partial \mathbf{p}_2} + \mathbf{w}_{1'1}\cdot \frac{\partial^2 R_{12}}{\partial \mathbf{p}_1\,\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} C_{1'2'} \\
&\qquad + \mathbf{w}_{22'}\cdot \frac{\partial^2 C_{12'}}{\partial \mathbf{p}_{2'}\,\partial \mathbf{p}_1}\cdot \mathbf{w}_{1'1} R_{1'2'} + \frac{\partial R_{12'}}{\partial \mathbf{p}_1}\cdot \mathbf{w}_{11'}\frac{\partial C_{1'2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} \\
&\qquad + \mathbf{w}_{1'1}\cdot \frac{\partial^2 R_{12}}{\partial \mathbf{p}_1\,\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} R_{1'2'} N_{2'} + \frac{\partial R_{12}}{\partial \mathbf{p}_1}\cdot \mathbf{w}_{11'} R_{1'2'}\frac{\partial N_{2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} \\
&\qquad + \mathbf{w}_{1'1}\cdot \frac{\partial R_{12'}}{\partial \mathbf{p}_1} N_{2'}\frac{\partial R_{1'2}}{\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} + \frac{\partial R_{12'}}{\partial \mathbf{p}_1}\cdot \mathbf{w}_{11'} R_{1'2}\frac{\partial N_{2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2}
\end{aligned}
\tag{78}
$$

$$
\begin{aligned}
&\Sigma^{(2)}(q_1, -, t_1; q_2, -, t_2) \\
&\quad = \left\{\frac{1}{2}\mathbf{w}_{11'}\cdot \frac{\partial^2 C_{12}}{\partial \mathbf{p}_1\,\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} C_{1'2'} + \frac{1}{2}\frac{\partial C_{12'}}{\partial \mathbf{p}_1}\cdot \mathbf{w}_{11'}\frac{\partial C_{21'}}{\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'}\right. \\
&\qquad + \mathbf{w}_{11'}\cdot \frac{\partial R_{12'}}{\partial \mathbf{p}_1} C_{1'2}\frac{\partial N_{2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} + \mathbf{w}_{11'}\cdot \frac{\partial R_{12'}}{\partial \mathbf{p}_1} N_{2'}\frac{\partial C_{1'2}}{\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} \\
&\qquad + \mathbf{w}_{11'}\cdot \frac{\partial C_{12}}{\partial \mathbf{p}_1} R_{1'2'}\frac{\partial N_{2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} + \mathbf{w}_{11'}\cdot \frac{\partial^2 C_{12}}{\partial \mathbf{p}_1\,\partial \mathbf{p}_2}\cdot \mathbf{w}_{22'} R_{1'2'} N_{2'} \\
&\qquad + \mathbf{w}_{11'}\cdot \frac{\partial R_{12'}}{\partial \mathbf{p}_1} C_{1'2'}\mathbf{w}_{22'}\cdot \frac{\partial N_2}{\partial \mathbf{p}_2} + \mathbf{w}_{11'}\cdot \frac{\partial R_{12'}}{\partial \mathbf{p}_1}\frac{\partial C_{1'2'}}{\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} N_2 \\
&\qquad \left. + \mathbf{w}_{11'}\frac{\partial C_{12'}}{\partial \mathbf{p}_1} R_{1'2'}\mathbf{w}_{2'2}\cdot \frac{\partial N_2}{\partial \mathbf{p}_2} + \mathbf{w}_{11'}\cdot \frac{\partial^2 C_{12'}}{\partial \mathbf{p}_1\,\partial \mathbf{p}_{2'}}\cdot \mathbf{w}_{2'2} N_2 R_{1'2'}\right\} \\
&\qquad + \{1 \leftrightarrow 2\}
\end{aligned}
\tag{79}
$$

In the above equations there is an implicit integration over $dq_{1'}\,dq_{2'}$ and over $dt_{1'}\,dt_{2'}$. Since $\mathbf{w}$ has a delta-function dependence on its time difference variable, all the correlation functions are evaluated at the time t_1 and t_2. We shall call the equations for N, C, and R obtained from the expansion of Σ to second order in the interparticle potential the "particle direct interaction approximation" (PDIA).

To better understand the significance of the non-Vlasov DIA terms in Σ, we refer the reader to a recent paper by DuBois and Espedal.[17] They describe a plasma in the Vlasov approximation and also construct an approximate statistical theory for the Klimontovich equation in the limit of large plasma parameter by regarding the phase-space density field f as the limit of a continuous field which has its equal-time covariance constrained by (1).

We have shown that the preservation of (1) is dependent on the proper treatment of the non-Gaussian initial conditions; DuBois and Espedal do not consider the initial value problem, but rather impose (1) at equal times. This procedure can be shown to be valid only to lowest order in the inverse plasma parameter. The Vlasov DIA is used and the covariance of f is decomposed into two parts, $\hat{H} + C^s$, where $\hat{H}$ at equal times is the H of (1) and C^s at equal times is the singular part of (1). For unequal times, C^s is "renormalized particle noise," and it roughly corresponds to the RN term in (71), while $\hat{H}$ roughly corresponds to our C. The Vlasov DIA equation for $C^v \equiv \langle \delta f \cdot \delta f \rangle$ is of the form

$$(\partial/\partial t - \Sigma_{-+})C^v = \Sigma_{--}R \tag{80}$$

If one writes

$$C^v = \hat{H} + C^s \tag{81}$$

and then attempts to separate (80) into equations for $\hat{H}$ and C^s, it is possible to make a correspondence with some of the explicit particle noise terms in the PDIA. If (81) is substituted into (80) and if C^s is replaced by RN, then

$$(\partial/\partial t - \Sigma_{-+})\hat{H} = (\Sigma_{-+}N + \Sigma_{--})R - \partial C^s/\partial t$$

The Vlasov DIA expression for Σ_{--} is supplemented by some of the terms in $\Sigma_{-+}N$ (some, because those that go into $\partial C^s/\partial t$ remain to be specified). In particular, one of the first-order terms in Σ_{-+} is of the form $\mathbf{w} \cdot \partial N/\partial \mathbf{p}$, and it contributes to Σ_{--} a term which corresponds to one of the first-order terms in the PDIA. In addition to the terms generated by $\Sigma_{-+}N$, if each C^v in the Vlasov DIA expressions for Σ is replaced by (81), then some other particle noise terms in the PDIA are reproduced.

Independent of questions concerning particle noise, DuBois and Espedal have made an important connection between R and the more traditional dielectric response function d defined by

$$d_{12} = -[\delta U(\mathbf{r}_1, t_1)/\delta \rho^{\text{ext}}(\mathbf{r}_2 t_2)]_\eta$$

where U is the total electrostatic potential, and ρ^{ext} is an external charge density. ρ^{ext} determines an external potential

$$U^{\text{ext}}(\mathbf{r}_1, t_1) = \int \frac{\rho^{\text{ext}}(\mathbf{r}_2, t_1)\, d\mathbf{r}_2}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}$$

whose gradient pushes particles but does not create or destroy them. U is the sum of U^{ext} and the induced potential U^{ind},

$$U^{\text{ind}}(\mathbf{r}_1, t_1) = -e \int \frac{N(q_2, t_1)\, dq_2}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|}$$

R and d are related through the phase-space density response function

$$G(q_1t_1, q_2t_2) \equiv [\delta N_1/\delta\eta(q_2, -, t_2)]_U \tag{82}$$

The essential difference between R and G is that the former gives δN at constant U^{ext}. DuBois and Espedal find the exact relation

$$-\int \frac{R(q_3t_1, q_2t_2)}{4\pi|\mathbf{r}_1 - \mathbf{r}_3|}\, dq_3 = d_{13}G_{32} \tag{83}$$

To the extent that some turbulent plasmas are described by N, d, and the charge density covariance, there is redundant information in R and C which can be eliminated through the use of G and d.

Since (83) involves the integral of R over its first momentum variable, another relation is required if R is to be replaced by G. DuBois and Espedal have found such a relation [Eq. (89)] between R^{-1} and G^{-1}. It is derived perturbatively, with the level of potential fluctuations as the small parameter. Section 8–10 of this paper are independent of the immediately following paragraphs, which are devoted to a formally exact generalization of Eq. (89).

First, an alternative proof of (83) is presented. Let

$$\rho^{\text{ind}} = -\Delta U^{\text{ind}}$$

or

$$\rho^{\text{ind}}(\mathbf{r}_1, t_1) = -e\int N(q_1, t_1)\, d\mathbf{p}_1$$

The definition of G implies that

$$-e\int G(q_1t_1, q_2t_2)\, d\mathbf{p}_1 = [\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)/\delta\eta_2]_U$$

By use of the chain rule

$$\begin{aligned}\left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\eta_2}\right)_U \\ = \left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\eta_2}\right)_{U_{\text{ext}}} + \left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}\right)_\eta \left(\frac{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}{\delta\eta_2}\right)_U\end{aligned} \tag{84}$$

and

$$\begin{aligned}\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} &= -\Delta_3\delta(\mathbf{r}_3 - r_4)\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\rho^{\text{ext}}(\mathbf{r}_4, t_3)} \\ &= \Delta_1\Delta_3\delta(\mathbf{r}_3 - \mathbf{r}_4)\frac{\delta U^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\rho^{\text{ext}}(\mathbf{r}_4, t_3)} \\ &= \Delta_3[-\Delta_1 d_{13} + \delta(\mathbf{r}_1 - \mathbf{r}_3)\,\delta(t_1 - t_3)]\end{aligned}$$

Also,

$$\left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\eta_2}\right)_{U_{\text{ext}}} = -e\int R(q_1t_1, q_2t_2)\, d\mathbf{p}_1$$

and

$$\left(\frac{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}{\delta\eta_2}\right)_U = -\left(\frac{\delta U^{\text{ind}}(\mathbf{r}_3, t_3)}{\delta\eta_2}\right)_U = \Delta_{34}^{-1}\left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_4, t_3)}{\delta\eta_2}\right)_U$$

$$= -e\int \Delta_{34}^{-1}G(q_4t_3, q_2t_2)\, dq_4$$

Make the above three substitutions in (84) to obtain

$$\left(\frac{\delta\rho^{\text{ind}}(\mathbf{r}_1, t_1)}{\delta\rho_2}\right)_U = -e\int [R(q_1t_1, q_2t_2) + G(q_1t_1, q_2t_2)]\, d\mathbf{p}_1$$

$$+ e\Delta_1\int d_{13}G(q_3t_3, q_2t_2)\, dq_3\, dt_3$$

Therefore

$$\int R(q_1t_1, q_2t_2)\, d\mathbf{p}_1 = \Delta_1 d_{13}G_{32}$$

from which (83) follows directly.

Now consider the inverse of (82):

$$G_{12}^{-1} = \left(\frac{\delta\eta(q_1, -, t_1)}{\delta N_2}\right)_U$$

$$= \left(\frac{\delta\eta(q_1, -, t_1)}{\delta\eta_2}\right)_{U_{\text{ext}}} + \left(\frac{\delta\eta(q_1, -, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}\right)_N\left(\frac{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}{\delta N_2}\right)_U$$

$$= R_{12}^{-1} - \left(\frac{\delta\eta(q_1, -, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}\right)_N\left(\frac{\delta U^{\text{ind}}(\mathbf{r}_3, t_3)}{\delta N_2}\right)_U$$

$$= R_{12}^{-1} + e\int \left(\frac{\delta\eta(q_1, -, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)}\right)_N \frac{\delta(t_3 - t_2)}{4\pi|\mathbf{r}_3 - \mathbf{r}_2|}\, d\mathbf{r}_3\, dt_3$$

The equation of motion for N in the presence of an external potential and a source of particles $\eta(-)$ is

$$\frac{\partial N_1}{\partial t_1} + \frac{1}{m}\mathbf{p}_1\cdot\frac{\partial N_1}{\partial \mathbf{r}_1} + e\left[\frac{\partial U^{\text{ext}}(\mathbf{r}_1, t_1)}{\partial \mathbf{r}_1} + \frac{\partial U^{\text{ind}}(\mathbf{r}_1, t_1)}{\partial \mathbf{r}_1}\right]\cdot\frac{\partial N_1}{\partial \mathbf{p}_1}$$

$$= \eta(q_1, -, t_1) + \frac{\partial}{\partial \mathbf{p}_1}\cdot\int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2)C_{q_1t_1,q_2t_1}\, dq_2 \tag{85}$$

Therefore

$$e \frac{\partial N_1}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{r}_1} \delta(\mathbf{r}_1 - \mathbf{r}_3)\, \delta(t_1 - t_3)$$

$$= \left(\frac{\delta \eta(q_1, -, t_1)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N + \frac{\partial}{\partial \mathbf{p}_1} \cdot \int \mathbf{w}(\mathbf{r}_1 - \mathbf{r}_2) \left(\frac{\delta C_{q_1 t_1, q_2 t_1}}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N dq_2 \tag{86}$$

By use of the chain rule

$$\left(\frac{\delta C_{12}}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N$$

$$= \left(\frac{\delta C_{12}}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_{\eta(-)} + \left(\frac{\delta C_{12}}{\delta \eta(q_4, -, t_4)} \right)_{U_{\text{ext}}} \left(\frac{\delta \eta(q_4, -, t_4)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N$$

$$= \left(\frac{\delta C_{12}}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_{\eta(-)}$$

$$+ G(q_1, +, t_1; q_2, +, t_2; q_4, -, t_4) \left(\frac{\delta \eta(q_4, -, t_4)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N$$

Substitute the above into (86) to obtain

$$\left[\delta(q_1 - q_4)\, \delta(t_1 - t_4) + \frac{\partial}{\partial \mathbf{p}_1} \cdot \mathbf{w}_{12} G(q_1, +, t_1; q_2, +, t_2; q_4, -, t_4) \right]$$

$$\times \left(\frac{\delta \eta(q_4, -, t_4)}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_N$$

$$= e \frac{\partial N_1}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{r}_1} \delta(\mathbf{r}_1 - \mathbf{r}_3)\, \delta(t_1 - t_3) - \mathbf{w}_{12} \cdot \frac{\partial}{\partial \mathbf{p}_1} \left(\frac{\delta C_{12}}{\delta U^{\text{ext}}(\mathbf{r}_3, t_3)} \right)_{\eta(-)} \tag{87}$$

To calculate $\delta C / \delta U^{\text{ext}}$, use the response function formalism of Section 4. The effect of δU^{ext} is described by a change in the Liouville operator $\delta \tilde{\mathscr{L}}$:

$$\delta \tilde{\mathscr{L}}(t_5) = e \int U^{\text{ext}}(r_5, t_5) \frac{\partial}{\delta \mathbf{r}_5} \cdot \left[\frac{\partial \Psi^{\dagger}(q_5 t_5)}{\partial \mathbf{p}_5} \Psi(q_5 t_5) \right] dq_5$$

$$\left(\frac{\delta C_{12}}{\delta U^{\text{ext}}(\mathbf{r}_3 t_3)} \right)_{\eta(-)}$$

$$= -e \int \delta(\mathbf{r}_3 - \mathbf{r}_5)\, \delta(t_3 - t_5) \frac{\partial}{\partial \mathbf{r}_5} \cdot \frac{\delta^2}{\delta \eta(q_1, +, t_1)\, \delta \eta(q_2, +, t_2)}$$

$$\times \langle \text{sum} | \frac{\partial \Psi^{\dagger}(q_5 t_5)}{\partial \mathbf{p}_5} \Psi(q_5, t_5) | F(0) \rangle\, dq_5\, dt_5$$

$$= -e \int \delta(\mathbf{r}_3 - \mathbf{r}_5)\, \delta(t_3 - t_5) \lim_{4 \to 5^+} \frac{\partial^2}{\partial \mathbf{r}_5 \cdot \partial \mathbf{p}_4}$$

$$\times [G(q_1, +, t_1; q_2, +, t_2; q_5, +, t_5; q_4, -, t_4)$$

$$+ N_5 G(q_1, +, t_1; q_2, +, t_2; q_4, -, t_4) + C_{15} R_{24} + C_{25} R_{14}]\, dq_5\, dt_5 \tag{88}$$

When (88) is substituted into (87), which is solved for $(\delta\eta/\delta U^{\text{ext}})_N$ and then substituted into (85), the desired relation between R^{-1} and G^{-1} is obtained.

To $O(\gamma_4)$,

$$\left(\frac{\delta\eta(q_4, -, t_4)}{\delta U^{\text{ext}}(r_3 t_3)}\right)_N = e\frac{\partial N_1}{\partial \mathbf{p}_1}\cdot\frac{\partial}{\partial r_1}\,\delta(\mathbf{r}_1 - \mathbf{r}_3)\,\delta(t_1 - t_3)$$

$$+ e\left(\mathbf{w}_{12}\cdot\frac{\partial}{\partial \mathbf{p}_1}\right)\frac{\partial}{\partial \mathbf{r}_3}\cdot\int \delta(\mathbf{r}_3 - \mathbf{r}_5)\,\delta(t_3 - t_5)$$

$$\times\left[C_{15}\frac{\partial R_{25}}{\partial \mathbf{p}_5} + C_{25}\frac{\partial R_{15}}{\partial \mathbf{p}_5}\right] dq_5\, dt_5$$

Therefore, to $O(\gamma_4)^2$,

$$G_{12}^{-1} = R_{12}^{-1} + \frac{\partial N_1}{\partial \mathbf{p}_1}\cdot\mathbf{w}_{12} - \int dq_4\, dt_4 \int dq_3\, dt_3\left(\mathbf{w}_{14}\cdot\frac{\partial}{\partial \mathbf{p}_1}\right)$$

$$\times\left(C_{13}\frac{\partial R_{43}}{\partial \mathbf{p}_3} + C_{43}\frac{\partial R_{13}}{\partial \mathbf{p}_3}\right)\cdot\mathbf{w}_{32} \tag{89}$$

This is the second relation reported by DuBois and Espedal.

8. CONSERVATION LAWS AND REALIZABILITY

What properties of the exact correlation function equations are shared by the PDIA? When there are no initial three- or higher particle correlations, the fundamental equations (52), (53), and (58)–(61) are exact, and it is easily shown that the short-time Taylor series expansion of C and R (if it exists) coincides with that of the PDIA to $O(t^2)$. In particular, this means that all the conservation laws and realizability conditions are satisfied for short times. By realizability [18,19] we mean those relations which follow from the representation of the correlation functions as expectation values.

The conservation of particle number, momentum, and energy is easily satisfied for all times. Particle and momentum conservation follow directly from the equation for N whose form is independent of our approximation procedures. The evolution of the fluctuating electrostatic potential energy is determined by the evolution of $\int C(r_1 p_1 t, r_2 p_2 t)\, dp_1\, dp_2$. Since $\Sigma(q_1, -, t_1; q_2, +, t_2)$ and $\Sigma(q_1, -, t_1; q_2, -, t_2)$ always have a leading factor of $\partial/\partial p_1$, the approximate equation for the fluctuating potential energy obtained from (64) is in fact independent of the approximation used for Σ. The cancellation between the time rates of change of kinetic and total potential energy then follows in essentially the same way as it does for the Klimontovich equation.

Is the PDIA realizable for all times? A strong affirmative answer would consist in demonstrating the existence of a model particle system whose *exact*

N, R, and C satisfy the PDIA. This would not necessarily imply that it is a "good" approximation. The model system, for example, might have unphysical instabilities. For continuous fields, Kraichnan[18] has constructed a stochastic model which proves that the DIA is realizable; however, for the Vlasov DIA, this realizability does not include those constraints which follow from the positivity of f. If the PDIA is realizable in terms of a model *particle system*, then by definition it follows that $N_q = \langle \sum_i \delta(q - q_i) \rangle \geqslant 0$.

A weaker affirmative answer to the above question would consist in first establishing certain properties of the true N, R, and C functions, and then showing that these properties are also true for the corresponding PDIA functions. We have already mentioned that N should be nonnegative. For the Vlasov DIA, the function which corresponds to C is a covariance and it must be a positive-definite matrix. The C function in the PDIA *is not a covariance*. Indeed, in thermal equilibrium, the fact that like charges repel each other implies that $C(q_1 t, q_2 t) < 0$ for a one-species plasma. Since the potential energy of two approaching similar charges goes to positive infinity in spatial dimensions $d \geqslant 2$,

$$\lim_{r_1 \to r_2} C(r_1 p_1 t; r_2 p_2 t) + N(r_1 p_1 t) N(r_2 p_2 t) = 0$$

This is true regardless of the statistical state.

Kraichnan[20] has also constructed stochastic models for many-particle quantum systems to prove the realizability of some well-known approximate statistical theories.[18] It is conceivable that the realizability of approximations in the context of the classical occupation number formalism may be demonstrated in a similar manner. This will not be entirely straightforward, because the quantum mechanical models are generated by model Hamiltonians which are constrained to be Hermitian, whereas we require a model Liouville operator which must be constrained to maintain the positivity of the N-particle probability distribution functions.

9. THE *T*-APPROXIMATION

While individual collisions, for hard-core interactions, are singular, the mean collision frequency is regular since it is determined by the dynamics between collisions. By solving (60) for γ_4 in terms of Γ_4 and inserting this solution into the expression for Σ, attention is shifted to this mean rate. This procedure yields the so-called vertex-renormalized approximations.

Assume that Γ_3 and Γ_4 are "small." More properly, the two dimensionless variables schematically denoted by $(GGG)^{1/2}\Gamma_3$ and $(GGGG)^{1/2}\Gamma_4$, where G is the two-point matrix cumulant, are assumed to be small.[11] To obtain γ_4 as a functional power series in Γ_3 and Γ_4, it is simplest to revert the ex-

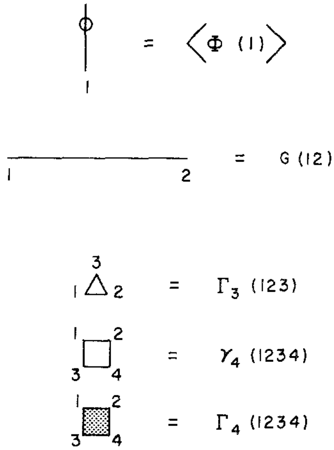

Fig. 1

pansions of Γ_3 and Γ_4 in powers of γ_4. These are represented in Fig. 2. The fundamental graphical elements are defined in Fig. 1.

The reversions of the equations in Fig. 2 are shown in Fig. 3. The equations in Fig. 3 imply that

$$\Gamma_3(123) = \Gamma_4(1234)\langle\Phi(4)\rangle + O(\Gamma_4)^3 \tag{90}$$

To obtain an $O(\Gamma)^2$ approximation to Σ, we first illustrate the exact equation (58), omitting the $\gamma_4(\Gamma_3)^2$ term, in Fig. 4. In Appendix B we demonstrate that the $\gamma_4\Gamma_4$ term in Σ, with Γ_4 determined by Fig. 3, vanishes.

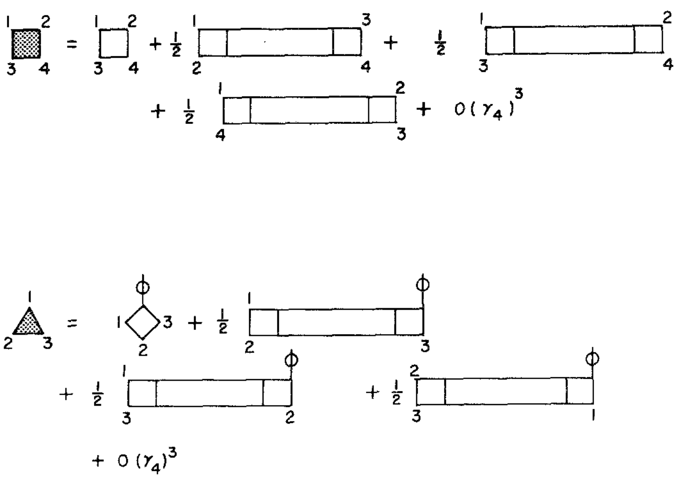

Fig. 2

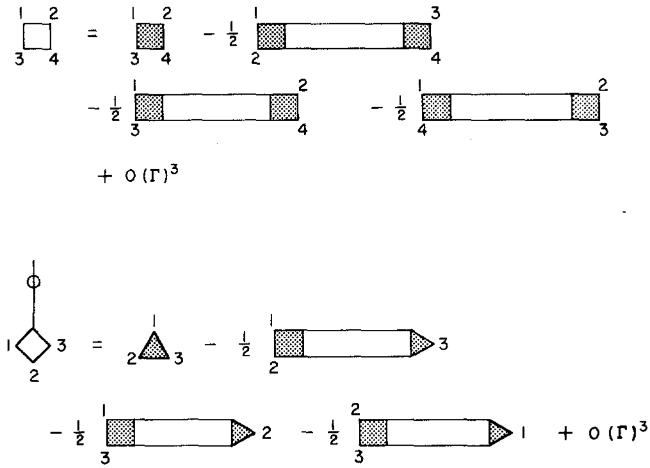

Fig. 3

Ignore this term, substitute for γ_4 as given in Fig. 3 and for Γ_3 as given in (90) to obtain Fig. 5. Figures 3 and 5, and the equation obtained from (62) by expressing $\mathbf{w}$ in terms of Γ_4, constitute a generalized T approximation.

It differs from the corresponding quantum mechanical approximation[1] in three respects. The latter has an equation for Γ_4 whose homogeneous terms are linear in Γ_4. We could obtain a simpler approximation with this feature by replacing each of the $\Gamma_4\Gamma_4$ terms in Fig. 3 by $\frac{1}{2}(\Gamma_4\gamma_4 + \gamma_4\Gamma_4)$. Though easier to deal with analytically, we have no fundamental reason for preferring it over the original. Another difference is the retention of the $O(\Gamma)^2$ terms in Σ. Presumably there are situations in which their deletion would not lead to any qualitative changes. We have retained them so that in the special case where γ_4 itself is weak, the PDIA is recovered, in which the $(\gamma_4)^2$ terms describe fluctuation–fluctuation interactions. Third and most important, the iterative solution for Γ_4 generated by Fig. 3 contains more than the usual ladder diagrams. For example, to third order in γ_4, there

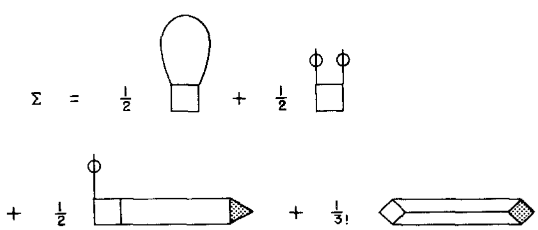

Fig. 4

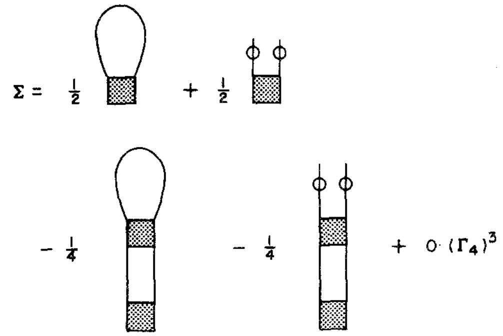

Fig. 5

appear the diagrams in Fig. 6. The non-ladder (second) diagram in Fig. 6 occurs because there are two propagators, R and C; which in turn implies that Γ_4 may have components $\Gamma(-, +, +, +)$, $\Gamma(-, -, -, +)$, and $\Gamma(-, -, -, -)$ in addition to the component $\Gamma(-, -, +, +)$. It is shown in Appendix B that $\Gamma(-, +, +, +)$ vanishes and that only the ladder diagrams contribute to $\Gamma(-, -, +, +)$. There are diagrams, including both of those in Fig. 6, which do contribute to $\Gamma(-, -, -, +)$ and $\Gamma(-, -, -, -)$. It is easily shown that the Γ_4 of Fig. 3 has the property that $\Gamma(-, -, +, +)$ has no factors of C, $\Gamma(-, -, -, +)$ has a single factor, and $\Gamma(-, -, -, -)$ has two factors. To first order in Γ_4, we have from Fig. 5

$$\Sigma(-, +) \sim \Gamma(-, -, +, +)N + \Gamma(-, -, -, +)$$

Very roughly, let us write

$$\Gamma(-, -, -, +) \sim (C/R)\Gamma(-, -, +, +)$$

and then

$$\Sigma(-, +) \sim [\Gamma(-, -, +, +)/R](RN + C)$$

Similarly,

$$\Gamma(-, -, -, -) \sim (C/R)(C/R)\Gamma(-, -, +, +)$$

and

$$\Sigma(-, -) \sim [\Gamma(-, -, +, +)/R^2][(RN)^2 + RN\cdot C + C^2]$$

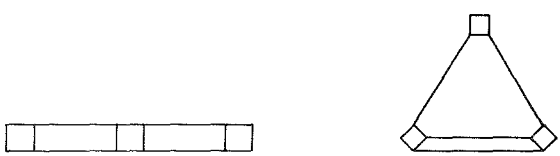

Fig. 6

In a crude way, this shows that the contributions of the non-ladder diagrams compare with those of the ladder diagrams as C compares with RN. We recall from (71) that C is a measure of the correlation between two distinct particles, and RN is the correlation of a particle with itself at (possibly) two different times. In plasma physics, RN would be called particle noise. There are clearly many situations, including a low-density system for which $C \sim N^2$, in which the non-ladder diagrams are unimportant, and our T-approximation then has a close formal similarity to the usual one.

Generally speaking, the above analysis illustrates the tendency for a given approximation scheme to contain more information in the case of a classical gas than in the case of a quantum mechanical gas. Two other illustrations are of particular importance for a plasma. The first-order (in γ_4) approximation (72) contains the linearized Vlasov equation and hence a reasonable description of screening, whereas in quantum mechanics screening is not obtained so simply. Even more striking is the ability of (72) to correctly describe (at least) the short-distance behavior of the thermal equilibrium pair distribution function for a single-species plasma, while an adequate quantum mechanical treatment is considerably more involved. One essential reason for the above is that the equal-time density–density correlation function can be described by the two-point function C, while in quantum mechanics this requires a four-point function.

In addition to the case of hard-core interactions, the PDIA is unsuitable for attractive interactions which can lead to (classical) bound states. The T-approximation may be adequate for a description of, for example, the formation and dissolution of Kepler orbits in a many-body gravitational system. We will have more to say about this in a future publication.

10. SUMMARY AND DISCUSSION

A renormalized kinetic theory has been presented which can describe the evolution of a classical N-body system from an arbitrary initial state. It is based upon a recently introduced occupation number formalism of Doi. Though there are formal similarities to the quantum mechanical second-quantized representation, there are many major differences, of which we list a few:

a. The operator Φ has position *and momentum* as independent variables.

b. Probability amplitudes are real and are obtained as a matrix element, $\langle N| \cdots |F(0)\rangle$, not the absolute value squared of a matrix element.

c. The matrix elements of Φ alone are generally nonzero.

d. The evolution of Φ is determined by a Liouville operator which is distinct from the Hamiltonian operator.

A second-order mass renormalized approximation, called the PDIA, has been introduced and related to the Vlasov plasma turbulence DIA of Orszag and Kraichnan, and to the recent plasma turbulence approximation of DuBois and Espedal.

The PDIA is not suitable for hard-core interactions or for interactions which lead to classical bound states, but the formal development of T-matrix-like approximations which should be appropriate in these cases is straightforward. Though the classical description of bound states in a plasma may not be of interest, because if they are ever significant a quantum mechanical description is called for, they are of great interest in the gravitational N-body problem. We believe that the formalism outlined in this paper would be suitable for a systematic analysis of gravitational turbulence.

Of course, the task of extracting useful information from a formal approximation such as the PDIA is formidable. The technical difficulties will be much greater than they are in thermal equilibrium, where equal-time correlation functions are known, where there are fluctuation dissipation theorems, and where there is translational invariance in time. We will soon attempt to numerically integrate the PDIA for a one-species plasma in one spatial dimension.

Perhaps the most distinctive new element presented in this paper is the unified treatment of the correlations between a particle and itself and the correlations between two distinct particles. This is of special significance in plasma turbulence, where the effects of the former (particle noise) are usually added to the latter (usually derived from a theory of Vlasov plasma turbulence) in an ad hoc fashion. Even when particle noise may be treated as a small perturbation, and its effects adequately described by the methods of DuBois and Espedal, there remain the spuriously large particle noise effects found in computer simulations which use a relatively small number of particles. In practice, these effects are reduced by the use of various smoothing techniques, which could be improved through a better understanding of strong particle noise.

APPENDIX A. CORRELATION FUNCTION EQUATIONS FOR ARBITRARY INITIAL CONDITIONS

The generalization of the Schwinger variational equations for initial states with $G_N(+, +, \ldots, +) \neq 0$ for $N > 2$ can be obtained in a manner similar to that used in the case of classical random processes with non-Gaussian initial conditions. We shall not provide a complete proof of the former; instead, a brief outline of its essential features is given and the reader is referred to Deker's [21] analysis for more details.

The mean field equation of motion in the presence of the external source η is incomplete in the sense that its initial condition has an unknown η dependence. However, if the initial state is the vacuum, then $G^{\eta}(q, +, t = 0) = 0$. The actual initial state can be developed from the vacuum by applying an impulsive, random particle source. Consider

$$\tilde{\mathscr{L}}(t) = \tilde{\mathscr{L}}_0(t) + \int dq\, \beta(q)\, \delta(t)[1 - \Psi^{\dagger}(q)] \tag{A1}$$

where $\tilde{\mathscr{L}}_0$ is the original Liouville operator, and β is a random function specified below. Immediately after the source has acted, the state of the system is

$$|F(0^+)\rangle = \exp \int dq\, \beta(q)[\Psi^{\dagger}(q) - 1]|0\rangle$$

and the particle statistics can be obtained from the generating function S

$$S(b) = \ln\langle\langle\text{sum}|\exp\int dq\,\{b(q)\Psi(q) + \beta(q)[\Psi^{\dagger}(q) - 1]\}|0\rangle\rangle \tag{A2}$$

The outer brackets $\langle\cdots\rangle$ refer to an average over β. Denote the argument $b\Psi$ by A and the argument $\beta[\Psi^{\dagger} - 1]$ by B. Since the commutator of A and B is a c-number, and since

$$e^A|0\rangle = |0\rangle, \qquad \langle\text{sum}|e^B = \langle\text{sum}|$$

we may use the well-known operator identity

$$e^A e^B = e^B e^A e^{[A,B]}$$

to obtain

$$S(b) = \ln<\exp\int dq\, b(q)\beta(q)> \tag{A3}$$

The cumulants of β are therefore chosen to be in a one to one correspondence with the initial value Ursell functions, $U_N(q^N; 0)$.

Before deriving an expression for the full generating function W defined in Eq. (45), it is useful to make the transformation

$$\theta = \Psi, \qquad \theta^{\dagger} = \Psi^{\dagger} - 1 \tag{A4}$$

Let $\theta_0(q, t)$ and $\theta_0^{\dagger}(q, t)$ denote the operators which evolve according to $\tilde{\mathscr{L}}_0$. Instead of W, calculate Z, defined by

$$e^Z = \langle\langle\text{sum}|T\exp\int_0^{\infty} dq\, dt\,[\eta(q, +, t)\theta(q, t) + \eta(q, -, t)\theta^{\dagger}(q, t)]|0\rangle\rangle \tag{A5}$$

Use the time-dependent perturbation formalism of Section 4 to obtain in the usual way

$$e^Z = \langle\langle \mathrm{sum}|T\exp\int_0^\infty dq\, dt\, [\eta(q, +, t)\theta_0(q, t)$$

$$+ \eta(q, -, t)\theta_0^\dagger(q, t) + \beta(q)\, \delta(t)\theta_0^\dagger(q, t)]|0\rangle\rangle$$

$$= \langle \mathrm{sum}|T\exp\int_0^\infty dt \left\{\int dq\, [\eta(q, +, t)\theta_0(q, t) + \eta(q, -, t)\theta_0^\dagger(q, t)]\right.$$

$$\left. + \delta(t) \sum_{N=1}^{\infty} \frac{1}{N!} \int dq^N\, U_N(q^N; 0)\theta_0^\dagger(q_1, t) \cdots \theta_0^\dagger(q_N, t)\right\}|0\rangle \tag{A6}$$

Equation (A6) is the interaction representation of Z for a system with the effective Liouville operator $\tilde{\mathscr{L}}_{\mathrm{eff}}$,

$$\tilde{\mathscr{L}}_{\mathrm{eff}}^{(t)} = \tilde{\mathscr{L}}_0(t) + \delta(t) \sum_{N=1}^{\infty} \frac{1}{N!}\, \theta^\dagger(q_1) \cdots \theta^\dagger(q_N) U_N(q^N; 0) \tag{A7}$$

We have thus transformed a system whose initial state is described by the collection of Ursell functions $\{U_N\}$ and whose evolution is determined by $\tilde{\mathscr{L}}_0$ into another system which has the vacuum as its initial state and whose evolution is determined by $\tilde{\mathscr{L}}_{\mathrm{eff}}$. As shown by Deker,[21] the standard manipulations[11] can now be applied to the latter to obtain the renormalized correlation function equations.

APPENDIX B. PROPERTIES OF Γ_4 IN THE T-APPROXIMATION

Since all the cumulants of $\Psi^\dagger$ vanish, so must $\Gamma_4(+, +, +, +)$. The integral equation in Fig. 3 for Γ_4 therefore has four components, one for each of $\Gamma_4(-, +, +, +)$, $\Gamma_4(-, -, +, +)$, $\Gamma_4(-, -, -, +)$, and $\Gamma_4(-, -, -, -)$, and in this appendix our attention is focused only on some of the properties of the first two.

The bare vertex function γ_4 is the source of Γ_4. The $\gamma_4(-, -, +, +)$ is the sole component of the former that is nonzero, and hence it is only the corresponding component of the latter that effectively has a source. Consider now the equation for $\Gamma_4(-, +, +, +)$. Since $G(-, -) = 0$, each of its terms contains at least one factor of $\Gamma_4(-, +, +, +)$. It follows that the iterative solution of the T-approximation, which takes $\Gamma_4 = \gamma_4$ as the zeroth iteration, yields $\Gamma_4(-, +, +, +) = 0$. Since $G(-, -) = \Gamma_4(-, +, +, +) = 0$, the equation for $\Gamma_4(-, -, +, +)$ has the form

$$\begin{aligned}\Gamma_4(t_1, -; t_2, -; t_3, +; t_4, +) \\ &= \gamma_4(t_1, -; t_2, -; t_3, +; t_4, +) \\ &\quad + \Gamma_4(t_1, -; t_2, -; t_5, +; t_6, +)R(t_5, t_7)R(t_6, t_8) \\ &\quad \times \Gamma_4(t_7, -; t_8, -; t_3, +; t_4, +) \\ &\quad + \Gamma_4(t_1, -; t_3, +; t_5, +; t_7, -)R(t_5, t_6)R(t_8, t_7) \\ &\quad \times \Gamma_4(t_6, -; t_8, +; t_2, -; t_4, +) \end{aligned} \tag{B1}$$

In Eq. (B1), the second term on the right-hand side by itself would generate the ladder diagrams. It is easy to show that

$$\Gamma_4(t_1, -; t_2, -; t_3, +; t_4, +) \sim \delta(t_1 - t_2)\,\delta(t_3 - t_4)$$

Since R is a retarded response function, it then follows that

$$\Gamma_4(t_1, -; t_2, -; t_3, +; t_4, +) = 0 \qquad \text{if} \quad t_1 < t_3 \tag{B2}$$

Equations (B1) and (B2) imply that the third term on the right-hand side of (B1) vanishes. For future reference, we also note that

$$\Gamma_4(t_1, -; t_2, -; t_3, -; t_4, +) = 0 \tag{B3}$$

if any of t_1, t_2, or t_3 is less than t_4.

In order to show that the self-energy Σ receives no contribution from the $\gamma_4\Gamma_4$ term (within the framework of the T-approximation), consider $\Sigma(-, -)$,

$$\begin{aligned}\Sigma(t_1, -; t_2, -) = \cdots &+ \gamma_4(-, -, +, +)R(t_4, t_1)R(t_1, t_5)C(t_1, t_3) \\ &\times \Gamma_4(t_4, +; t_5, -; t_3, +; t_2, -) \\ &+ \gamma_4(-, -, +, +)R(t_4, t_1)R(t_1, t_5)R(t_1, t_3) \\ &\times \Gamma_4(t_4, +; t_5, -; t_3, -; t_2, -)\end{aligned}$$

where only the terms of interest have been schematically displayed. Equations (B2) and (B3) imply that the above expression vanishes. Similarly, it can be shown that the corresponding expression for $\Sigma(-, +)$ vanishes.

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