Field Theoretic Formulation of Kinetic theory:

I. Basic Development

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Abstract

We show how kinetic theory, the statistics of classical particles obeying Newtonian dynamics, can be formulated as a field theory. The field theory can be organized to produce a self-consistent perturbation theory expansion in an effective interaction potential. The need for a self-consistent approach is suggested by our interest in investigating ergodic-nonergodic transitions in dense fluids. The formal structure we develop has been implemented in detail for the simpler case of Smoluchowski dynamics. One aspect of the approach is the identification of a core problem spanned by the variables $\rho$ the number density and $B$ a response density. In this paper we set up the perturbation theory expansion with explicit development at zeroth and first order. We also determine all of the cumulants in the noninteracting limit among the core variables $\rho$ and $B$. 
I. INTRODUCTION

There exists a well defined approach to the problem of classical many-particle dynamics. Kinetic theory governs the kinetics of particles obeying Newtonian dynamics. It is one of the oldest disciplines in all of science. From the early work of Bernoulli[1] to the seminal work of Boltzmann[2] and Maxwell[3], kinetic theory has been applied to dilute systems out of equilibrium. More systematic modern methods have been developed for systems fluctuating in equilibrium. Based on work by Koopman[4] and von Neumann[5], one can express the time evolution in terms of Koopman’s operator $e^{iLt}$ where $L$ is the Liouville operator. For example one can develop in a rather straightforward way density expansions for transport coefficients[6,7] and memory functions[8]. Similarly one can develop expansions in terms of the interaction potential[9,10]. However these approaches have their limitations. It is not known how to systematically rearrange the respective density or potential expansions in a self-consistent manner. By self-consistent we mean here the interaction kernels of the associated kinetic equations can be expressed in terms of the full unknown correlation functions. Thus one obtains a nonlinear kinetic equation that must be solved self-consistently. While there are many formal reasons why this self-consistency is desirable, our motivation for pursuing such a theory in the present case is more practical. We want to understand the role of ergodic-nonergodic (ENE) transitions[11]. Self-consistency is essential if one is to investigate whether one does or does not have an ENE transition in dense fluids.

The liquid cooled to low temperature or compressed to high densities reach a stage in which it behaves like a frozen solid without any long range order. Understanding the formation of the amorphous solid state of the liquid coming from the ergodic liquid state has remained an unresolved problem of physics. A theory of the formation of the amorphous solid like state with self generated disorder will require developing techniques for testing the possibilities of ENE transitions in the dense liquid. There is compelling evidence that as one approaches the glass transition one comes close to an ENE transition. Even if we finally rule out the existence of a physical ENE transition, we need a formal structure which potentially can show such a transition. We present the outline of such a self-consistent theory here for the case of Newtonian dynamics (ND). Elsewhere one of us has developed[12,13] such a self-consistent theory for a classical set of particles which obey the simpler Smoulochowski dynamics[14](SD). In that case a program of investigating the existence of ENE transitions
is well along and one has a well defined approach to the problem. A key attribute of this theory is that well-defined approximations are available with well-defined corrections. In this paper we show at the formal level that Newtonian dynamics can be organized in the same self-consistent fashion. Our main goal is to investigate the status of ergodic-nonergodic transitions in dense liquids. How does one approach the liquid-glass transition? In Ref. [13] the question of an ENE transition in a system obeying SD by working at one-loop order was addressed. With the simplest interaction vertices it was demonstrated that a system of hard spheres does not undergo an ENE transition until a packing fraction of $\eta^* = 0.76$. This is the result of the simplest calculation. There are a variety of perturbations and extensions one can work out to test the robustness of this result. A better description for the static structure and/or improvements of the vertex functions to include interaction effects can also be used in the calculation. Going to higher loop order is also another way of improving the predictions of the theory. We anticipate that all of these calculations will eventually be carried out for SD.

There are differences between Newtonian and Smolukowksi dynamics. First, Newtonian dynamics are reversible and Smoluchowski dynamics have a noise component. Related is the fact that ND has additional conservation laws (energy and momentum) compared to SD. Finally there is the technically very important fact that the phase-space in the ND case contains the particle momenta while one has only the positions in the SD case. In the SD case the kinetic equations lack the momentum index labeling labeling ND kinetic equations. This is a large technical advantage of working with the SD. In the present work we take the point of view, which can be checked, that as one approaches the glass transition the slow kinetics are associated with structural rearrangements of the density, and couplings to energy and momentum currents are less important. This is one of the assumptions of simplest version of the mode-coupling theory [15]. A related working assumption is that the glassy kinetics of SD and ND are very similar. We know that they share the same static correlation functions-static structure factors. We will eventually be able to show this similarity.

An important formal point is that within the theory there exists a core problem involving $\rho$, the particle density, and $B$, a response density. One must address this core problem in both SD and ND before including other variables like momentum variables in ND. More specifically a discussion of the rich hydrodynamical structure of this system is addressed as
one introduces additional variables. For example the shear viscosity is associated with the inclusion of transverse currents in the development.

In the next section we show how kinetic theory can be reexpressed in terms of path integrals. The path integral formulation is similar to that found in the SD case with the initial condition playing a role similar to that for the noise in the SD case. In the SD case the path integral approach involved the same core fields: $\rho$ and $B$. The ND case can also be organized most simply in terms the same two variables. With respect to their respective interaction structures, the formulations are same for ND and SD dynamics. We find that the noninteracting cumulants for the set of variables $\rho$ and $B$ are qualitatively similar for the two cases. Thus we follow here the development in Ref. and construct a self-consistent approach to the dynamics.

It has turned out in the SD case that we can replace the bare potential with an effective potential expressed in terms of the physical structure factor. Thus the theory can be applied to systems with hard-sphere interactions. Here we develop a perturbation expansion for the two-point cumulant in terms of the pseudo interaction potential. The glue which ties together the terms in perturbation theory are the three-point vertices which are constructed from the noninteracting three-point cumulants among the variables $\rho$ and $B$. We show that all of these cumulants can be evaluated in the time and wave number regime. We focus here on the two-point cumulants and their determination to first order in the interaction including the renormalization of the bare potential.

At the formal level we show that the collective contribution to the self-energies for $\rho$ and $B$ have the same form in the ND case as for the SD case to second order in the expansion. The main calculation carried out in this paper is the determination of all the cumulants between $\rho$ and $B$ for the noninteracting system. In the next paper in this sequence we address the development of the theory at second-order in the interaction. The first important development there is to show, more simply than in the SD case, that one has a fluctuation dissipation symmetry relating the response functions to the correlation functions. In this case one can establish a set of nonperturbative identities satisfied by the three-point cumulants and irreducible vertices. Additional identities are clearly available for higher order quantities. In turn one shows that the set of matrix Dyson’s equations, satisfied by the two-point cumulants, reduce to a single kinetic equation for the correlation function as assumed in mode-coupling theory. It is from this kinetic equation that one can develop the
machinery associated with the ENE transition and the slow dynamics one can observe even if one can not access a sharp ENE transition.

In this paper we lay the groundwork for the analogous calculations for Newtonian dynamics. These calculations are in some ways harder in the ND case. For example, the three-point vertex functions are more complicated. However, in other ways the evaluations are easier. The treatment of the FD symmetry is simpler in ND case. The expansion parameter in this problem is a pseudo-interaction potential just as in Ref. [13] mentioned above. Indeed we expect to find the same interaction pseudo-potential in the two cases.

At second order we have an expression for the static structure factor $S(q)$ in terms of the potential. We assume we can pick the best result for $S(q)$ and solve for the associated pseudo-potential. Plots of $\tilde{V}(q)$ for various packing fractions (e.g., see eqn. (218) and Fig. 2 in Ref. [13]) shows that the pseudo-potential is a rather smooth quantity even for rigid hard spheres potentials.

A key difference between SD and ND is the noise in the SD case driving the system toward equilibrium. At low orders in the ND system it needs to be told it is in equilibrium. In conventional kinetic theory the initial state is chosen to be in equilibrium. Once in equilibrium the system typically stays there. Thus one option is to fix an initial condition at $t = t_0$. We show how this works in the zeroth and first-order cases for the dynamic structure factor. In the first-order case one has two effects on the theoretical structure. First one has (see Eq. (27) below) that the interaction matrix has a piece which imposes an initial condition and, second, the time integrations are restricted to the time regime $t_0 < t$. We show that the fluctuation-dissipation theorem [17] (FDT) is crucial in seeing that these breaks in time-translational invariance (TTI) cancel out and one obtains correlation functions compatible with TTI. In our treatment of FDT we find that the system is invariant over a set of symmetry operations which depends on an undetermined parameter. We propose to fix the system at temperature $T$ by choosing that all cumulants and vertices satisfy the FDS associated with equilibrium.

II. NEWTONIAN DYNAMICS

Consider a system of $N$ particles with mass $m$ with configurations specified by the phase-space coordinates $\Psi_i = (R_i, P_i)$ which satisfy the equations of motion:
\[ \dot{R}_i = \frac{P_i}{m} \]  
\[ \dot{P}_i = f_i \]  
(1)  
(2)

where the particles experience force

\[ f_i = -\frac{\partial}{\partial R_i} U(R) \]  
(3)

with total potential energy

\[ U(R) = \frac{1}{2} \sum_{i \neq j} V(R_i - R_j) \]  
(4)

and we have suppressed vector labels to unclutter the equations. If we form the vectors

\[ \Psi_i = (R_i, P_i) \]

then the equations of motion (1) and (2) can be put into the form

\[ \dot{\Psi}_i = K_i \]  
(5)

where \( K_i \) is a function of the \( \Psi \). We treat the phase-space coordinates as our fields in a MSR structure \[18\] and the physical observables are treated as conjugate to external fields which label the generators of the physical observables. The \( N \)-particle partition function is given by

\[ Z_N[H, h, \hat{h}] = \mathcal{N} \int \prod_{i=1}^{N} \mathcal{D} (\Psi_i) \mathcal{D} (\dot{\Psi}_i) d\Psi_i^{(0)} P_0(\Psi_0) e^{-A} \]
\[ \times \exp (H \cdot \phi) \exp (h \cdot \Psi + i \hat{h} \cdot \hat{\Psi}) \]  
(6)

where \( \mathcal{N} \) is a normalization constant, and we have an initial probability distribution \( P_0(\Psi_0) \). We assume the system is in equilibrium initially and the initial distribution is canonical:

\[ P_0 = e^{-\beta \mathcal{H}(\Psi_0) / Z_0} \]  
(7)

where \( \mathcal{H} \) is the hamiltonian, which is the sum of the kinetic and potential energies. The MSR action for the problem is given by

\[ A_\Psi = \int_{t_0}^{\infty} dt \left[ i \dot{\Psi}_i(t) \cdot \left( \dot{\Psi}_i(t) + K_i(t) \right) \right] \]  
(8)
Finally we have the contribution in Eq.(8) due to external fields that couple to $\Phi$ the collective core variables of interest:

$$H \cdot \Phi = \sum_\alpha \int d1H_\alpha(1)\Phi_\alpha(1).$$

As explained in Ref. [12], the minimal set for $\Phi$ includes the particle density and the response field $B$. For convenience we have also included the fundamental source fields $h_i$. It is useful to show that this development can be mapped onto the traditional representation. Set $H = 0$ in Eq.(8). No information is lost as long as we keep the full set of external fields $h$:

$$Z_N[h] = N \int \mathcal{D}(\Psi)\mathcal{D}(\hat{\Psi})d\Psi(0)P_0(\Psi_0)e^{[i\hat{\Psi} \cdot (\hat{\Psi} + K)]} \exp(h \cdot \Psi)$$

where in each of the arguments of the exponentials on the RHS there is a summation over particle label, an index labeling position and momentum, and an integral over time. Now we do the functional integral over $\hat{\Psi}$ to obtain a functional $\delta$-function:

$$Z_N[h] = N \int \mathcal{D}(\Psi)d\Psi(0)P_0(\Psi_0)\delta(\hat{\Psi} + K) \exp(h \cdot \Psi)$$

The next step is to recognize that in a deterministic system the probability of finding the system in configuration $\Psi(t)$ after starting at time $t_0$ in configuration $\Psi_0$ is proportional to

$$\delta(\Psi(t) - \Psi(t_0))$$

where $\Psi(t; t_0)$ is the unique configuration at time $t$ evolving from $\Psi(t_0)$. In the operator formulation

$$\Psi(t; t_0) = e^{i\mathcal{L}(t-t_0)}\Psi(t_0)$$

where $\mathcal{L}$ is the Liouville operator. As discussed in some detail by Penco and Mauro[19], one can use the following argument to connect our development here to the standard formulation. If a function $f(\phi)$ has a zero at $\phi = \phi_0$ then

$$\delta(\phi - \phi_0) = \delta[f(\phi)]|f'(\phi_0)|$$

In our case we choose $f$ to be $\hat{\Psi} + K$, we have the identity
\[
\delta (\Psi(t) - \Psi(t; t_0)) = \delta (\dot{\Psi}(t) + K(t)) \mathcal{N}
\] (15)

and the factor \(\mathcal{N}\) in Eqs. (11) and (15) is the functional determinant

\[
\mathcal{N} = \text{det} \frac{\delta (\dot{\Psi}(t) + K(t))}{\delta \Psi(t')}
\] (16)

This quantity is essentially the Jacobian discussed in Ref. [12] which opens up the discussion again to ghost fermions, supersymmetry, unification [20]. Importantly, for our purposes here, \(\mathcal{N}\) is a constant [21] independent of \(\Psi\). Using Eq. (15) in Eq. (11) leads to the partition function as

\[
Z_N[h] = \int D(\Psi)d\Psi(0)P_0(\Psi_0)\prod_t \delta (\Psi(t) - \Psi(t; t_0)) \exp(h \cdot \Psi)
\] (17)

We can immediately do the functional integral over \(\Psi(t)\) to obtain

\[
Z_N[h] = \int d\Psi(0)P_0(\Psi_0)\exp\left(\int_{t_0}^{\infty} dt \sum_{i=1}^{N} h_i(t) \cdot \dot{\Psi}_i(t; t_0)\right)
\] (18)

Clearly by taking functional derivatives we can generate the average of any set of phase-space observables:

\[
\langle A(t_1)B(t_2) \ldots D(t_n) \rangle = \int d\Psi(0)P_0(\Psi_0)A(\Psi(t_1; t_0))B(\Psi(t_2; t_0)) \ldots D(\Psi(t_n; t_0))
\] (19)

and we see that our representation is equivalent to the standard theory.

The appropriate generating functional for the problems discussed here, working in the grand canonical ensemble, is given by

\[
W[H, h, \hat{h}] = lnZ_T[H, h, \hat{h}]
\] (20)

where

\[
Z_T[H, h, \hat{h}] = \sum_{N=0}^{\infty} \frac{p_0^N}{N!}Z_N[H, h, \hat{h}]
\] (21)

and \(Z_N[H, h, \hat{h}]\) is given by Eq. (18).

For the method to be effective we have a minimum of two collective fields dictated by the structure of the interactions. One essential field is the particle density
\[ \rho(1) = \sum_{i=1}^{N} \delta(x_i - R_i(t_1)) \]  

(22)

and it is crucial to include the response field

\[ B(1) = \sum_{i=1}^{N} \left[ (\hat{P}_i(t_1))_i \nabla_1 \right] \delta(x_1 - R_i(t_1)) . \]  

(23)

Notice that \( B \) depends on the MSR hatted field \( \hat{P}_i(t) \). Unlike the SD case the \textit{Jacobian} does not contribute to the definition of \( B(1) \) here.

We can then write the canonical partition function given by Eq.(10) in the form

\[ Z_N[H, h, \hat{h}] = \int \prod_{i=1}^{N} D(\Psi_i) D(\hat{\Psi}_i) D(\Psi_i^{(0)}) e^{-A_0 - A_I + H \cdot \phi + h \cdot \psi + \hat{h} \cdot \hat{\psi}} \]  

(24)

where \( A_0 \) is the quadratic part of the action including the quadratic contribution to the initial probability distribution

\[ A_0 = \int_{t_0}^{\infty} dt_1 \left[ \sum_{i=1}^{N} i\hat{\Psi}_i \cdot \left( \dot{\Psi}_i + K_i^{(0)} \right) \right] + \beta K_0 . \]  

(25)

\( K_0 \) is the initial kinetic energy. Notice that we have constructed things such that the phase-space variables are constrained to their initial values at \( t = t_0 \). We then average over these values. Here we are explicitly treating the case where the system is in equilibrium at \( t = t_0 \), but more general situations are clearly compatible with the development. The interaction part of the action is given in the compact form

\[ A_I = \frac{1}{2} \sum_{\alpha, \beta} \int d1d2\Phi_{(1)}(1)\sigma_{\alpha\nu}(12)\Phi_{(2)}(12) \]  

(26)

where the Greek labels range over \( \rho \) and \( B \) and the interaction matrix is defined just as in SD, by

\[ \sigma_{\alpha\beta}(12) = V(12) \left[ \delta_{\alpha \rho} \delta_{\beta \rho} \delta(t_1 - t_0) + \delta_{\alpha B} \delta_{\beta \rho} + \delta_{\alpha \rho} \delta_{\beta B} \right] \]  

(27)

where the first contribution is from the potential energy contribution to the initial condition and

\[ V(12) = V(x_1 - x_2) \delta(t_1 - t_2) . \]  

(28)
Notice that the response field $B$ is chosen such that the interaction part of the action has the form given by Eq. (26). The canonical partition function (24) can be written in the convenient form

$$Z_N = \tilde{\text{Tr}} e^{-A_I + H \Phi} \quad (29)$$

where we have introduced the average

$$\tilde{\text{Tr}} = \int \prod_{i=1}^N \mathcal{D}(\Psi_i) \mathcal{D}(\hat{\Psi}_i) d\Psi^{(0)}_i e^{-A_0}. \quad (30)$$

We have thus shown that ND can be written in a path-integral form as given in Eqns. (B15)-(B17). These expressions look like the formulation for SD with an important exception. The action $A_\psi$, given by Eq. (8), does not have a contribution from noise. A noise component, as in Fokker-Planck dynamics, adds a term to the action

$$A_{\text{noise}} = \int_{t_0}^{\infty} dt_1 \int_{t_0}^{\infty} dt_2 \sum_{i=1}^N \dot{\psi}_i(t_1) D(t_1, t_2) \dot{\psi}_i(t_2) \quad (31)$$

which contributes to the noninteracting part of the action Eq. (2.20). The noise has the property of continuously telling the system to equilibrate at temperature $T$. How in the case of Newtonian reversible dynamics does the system know it is in equilibrium? One mechanism is to satisfy an initial condition. In the conventional formulation an equilibrium correlation function is given by

$$C_{AB}(t) = Tr P_0 B e^{\mathcal{L}t} A \quad (32)$$

where $\mathcal{L}$ is the Liouville operator and $P_0$ the equilibrium probability distribution and at $t = 0$ one has explicitly an equilibrium probability distribution. The use of initial conditions is one important way of treating nonequilibrium kinetics as discussed in Ref. [12]. The use of initial conditions in the case where the system is in equilibrium for all times, including the $t = t_0$, is inconvenient since formally it looks like one has broken time-translational invariance (TTI). As shown below for an ideal gas and to first order in the interaction, one can tell the gas its in equilibrium with an initial condition in equilibrium and maintaining TTI. However there is a cleaner way of maintaining equilibrium and TTI. This is to require that the fluctuation-dissipation symmetry hold at all times.
A. Fluctuation-Dissipation relations

The correlation functions, via its definition as the average of the product of commuting (classical) fields satisfies the time reversal symmetry

$$G_{ij}(t - t') = G_{ji}(t' - t) \tag{33}$$

The physical fields are real so $G_{ij}^*(t - t') = \langle \psi_i(t)\psi_j(t') \rangle^* = G_{ij}(t - t')$. In a stationary state we have time translational invariance. The full MSR action as outlined above is obtained in the following form for the Newtonian Dynamics

$$A = \sum_i \int \left[ i\dot{R}_i(t) \left\{ \dot{R}_i(t) - \frac{P_i(t)}{m} \right\} + i\dot{P}_i(t) \left\{ \dot{P}_i(t) - F_i(t) \right\} \right] dt \tag{34}$$

Under complex conjugation the MSR action transforms as

$$A^*(\psi, \hat{\psi}) = A(\psi, -\hat{\psi}) \tag{35}$$

We introduce the following transformation:

$$\tau R_i(t) = R_i(-t)$$
$$\tau \dot{R}_i(t) = -\dot{R}_i(-t) + i\beta F_i(-t)$$
$$\tau P_i(t) = P_i(-t)$$
$$\tau \dot{P}_i(t) = -\dot{P}_i(-t) - \frac{i\beta}{m} P_i(-t) \tag{36}$$

where $F_i(t) = (\partial U/\partial R_i(t))$ is the force on the particle $i$. We now consider how the action $A$ changes under this transformation

$$A' = \tau A$$
$$= \sum_i \int dt \left[ -i\dot{R}_i(-t) \left\{ \frac{\partial R_i(-t)}{\partial(-t)} - \frac{P_i(-t)}{m} \right\} - i\dot{P}_i(-t) \left\{ \frac{\partial P_i(-t)}{\partial(-t)} - F_i(-t) \right\} \right]$$
$$+ \beta \int_{-\infty}^{+\infty} \frac{\partial H(-t)}{\partial(-t)} d(t)$$
Looking at individual terms, and letting \( t \to -t \) in the integrals, we obtain \( A' = \tau A = A - \beta H(-\infty) + \beta H(\infty) \). We take the two limits of time integration \( t_2 \to \infty \) and \( t_1 \to -\infty \) here. Treating the last part as a constant (=0 in a conserved case) we conclude that the MSR action remains invariant under this transformation.

**B. FDT involving the \( \rho \) and \( B \) fields**

Let us consider the transformation rule for the field \( B(x, t) \) under time reversal \( \tau \)

\[
B(x, t) = -\sum_{i=1}^{N} \vec{P}_i \cdot \frac{\partial}{\partial \vec{R}_i} \delta(x - R_i(t))
\]

In the present formulation we are working so far with the density variable \( \rho(x, t) \) as the only collective variable and \( B(x, t) \) is the hatted counterpart. Under \( \tau \) the field \( B(x, t) \) changes as

\[
\tau B(x, t) = -B(x, -t) - \frac{i}{m} \beta \left[ \frac{\partial \rho(x, t)}{\partial t} \right]
\]

Using this relation we obtain for any function \( f[\rho] \) the following FDT relation linking to the \( B(x, t) \)

\[
G_{fB}(t - t') = \frac{i}{m} \theta(t - t') \beta \frac{\partial}{\partial t} G_{f\rho}(t - t')
\]

**III. SELF-CONSISTENT DEVELOPMENT**

The self consistent theory for the liquid state dynamics is developed in terms of correlation functions of collective variables \( \Phi_\alpha \)'s introduced in the previous section. We use the notation for the variable \( \Phi_\alpha \) as

\[
\Phi_\alpha = \sum_i \phi^{(i)}_\alpha
\]

with the index \( \alpha \) denoting the space of collective variables and \( i \) is the particle label. We work here with the density variable \( \rho \) and conjugate variable \( B(x, t) \) which are respectively denoted as:
\[ \phi^{(i)}_\rho(1) = \delta(x_1 - R_i(t_1)) \quad (40) \]

and

\[ \phi^{(i)}_B(1) = i\tilde{P}_i(t_1)\nabla_{x_1}\delta(x_1 - R_i(t_1)) \quad (41) \]

Working in the grand canonical ensemble, the grand partition function \( Z_T \) for the interacting problem is given by Eq. (21). The cumulants of the fields \( \Phi_i \) are generated by taking functional derivatives of the generating functional

\[ W[H] = \ln Z_T \quad . \quad (42) \]

with respect the fields \( H \) introduced in eqn. (9) above. The one-point average in a field is given by

\[ G_i = \frac{\delta}{\delta H_i}W \quad (43) \]

In the above equation we have used a compact notation where the index \( i \) labels space, time and fields \( \rho \) or \( B \). We maintain the notation from here on. In Ref. [12] we derived the fundamental identity

\[ G_i = Tr\phi_i e^{H\phi + \Delta W} \quad (44) \]

where

\[ \Delta W = W[H + F] - W[H] \quad (45) \]

with \( H \) denoting the external field and \( F_i \) being given by

\[ F_i = \sum_j \sigma_{ij} \phi_j \quad . \quad (46) \]

with the interaction kernel \( \sigma_{ij} \) obtained in Eq. (27). The important result Eq. (44) was established in FTSPD. It is more useful to derive here this result in a completely different fashion. This is presented in Appendix A in which we derive Eq.(44) without using functional techniques.
IV. FORMAL DEVELOPMENT OF PERTURBATION THEORY

The dependence of the theory on the pair potential is controlled by the quantity

$$\Delta W = W[H + F] - W[H]$$  \hspace{1cm} (47)

in eqn.(44) where $F$ is proportional to the interaction potential. We can expose the dependence on the potential by constructing the functional Taylor-series expansion

$$\Delta W = \sum_i F_i \frac{\delta}{\delta H_i} W[H] + \sum_{ij} \frac{1}{2} F_i F_j \frac{\delta^2}{\delta H_i \delta H_j} W[H] + \cdots$$  \hspace{1cm} (48)

and we can introduce the full cumulants:

$$G_{ij...k} = \frac{\delta}{\delta H_i} \frac{\delta}{\delta H_j} \cdots \frac{\delta}{\delta H_k} W[H]$$  \hspace{1cm} (49)

to obtain

$$\Delta W = \sum_i F_i G_i + \sum_{ij} \frac{1}{2} F_i F_j G_{ij} + \sum_{ijk} \frac{1}{3!} F_i F_j F_k G_{ijk} + \cdots$$  \hspace{1cm} (50)

Clearly in this form we can take $\Delta W$ to be a functional of $G_i$. One can then use functional differentiation to express higher order cumulants in terms of $G_i$ and $G_{ij}$. One has for example the manipulation expressing the three-point cumulant in terms of $G_{ij}$

$$G_{ijk} = \frac{\delta}{\delta H_k} G_{ij} = \sum_{mnp} -G_{im} G_{jn} G_{kp} \Gamma_{mnp}$$  \hspace{1cm} (51)

and the irreducible three-point vertex. $\Gamma_{ijk}$ in turn is given as a functional derivative of the two-point irreducible vertex,

$$\Gamma_{ijk} = \frac{\delta}{\delta G_k} \Gamma_{ij}$$  \hspace{1cm} (52)

with respect to $G_k$. $\Gamma_{ij}$ is precisely the matrix inverse of the two-point cumulant $G_{kj}$:

$$\sum_k \Gamma_{ik} G_{kj} = \delta_{ij}$$  \hspace{1cm} (53)

where we refer to this as Dyson’s equation.
As in the SD case \cite{13}, we can establish a dynamic generalization of the static Ornstein-Zernike relation \cite{22}. Starting with the functional equation for the two-point cumulant, we use the chain-rule for functional differentiation to obtain:

\[
G_{ij} = \frac{\delta}{\delta H_j} G_i \\
= Tr\phi_{i} \phi_{j} e^{H + \phi + \Delta W} + \sum_{k} Tr\left(\delta_{i} \frac{\delta}{\delta G_k} e^{H + \phi + \Delta W} \right) \frac{\delta}{\delta H_j} G_k \\
= G_{ij} + \sum_{k} c_{ik} G_{kj}
\]  

(54)

where

\[
G_{ij} = Tr\phi_{i} \phi_{j} e^{H + \phi + \Delta W}
\]

(55)

is roughly speaking a one-body object, and \(c_{ij}\) is defined as

\[
c_{ij} = Tr\phi_{i} e^{H + \phi + \Delta W} \frac{\delta}{\delta G_k} \Delta W
\]

(56)

Since \(\Delta W\) can be treated as a functional of \(G_{i}\) we see at this stage that we have available a self-consistent theory. To formulate this we define the matrix-inverse of the one body quantity \(G_{ij}\) as \(\gamma_{ij}\),

\[
\sum_{k} \gamma_{ik} G_{kj} = \delta_{ij}
\]

(57)

Now multiplying the correlation matrix \(G\) defined in eqn. (54) with the matrix \(\gamma\), and using definitions (53) and (57), we obtain the two-point vertex function (without any approximation):

\[
\Gamma_{ij} = \gamma_{ij} + K_{ij}
\]

(58)

where the collective part or the dynamic self-energy is given by

\[
K_{ij} = - \sum_{k} \gamma_{ik} c_{kj}
\]

(59)
A. Collective Self-Energy at First and Second Order

At the formal level we can work out the collective part of the self-energy in perturbation theory. Using Eq. (56) we have at first order

\[
C^{(1)}_{ij} = \text{Tr}\phi_i e^{H + \Delta W} \frac{\delta}{\delta G_j} \Delta W^{(1)}. \tag{60}
\]

where

\[
\Delta W^{(1)} = \sum_i F_i G_i. \tag{61}
\]

Clearly

\[
\frac{\delta}{\delta G_j} \Delta W^{(1)} = F_j \tag{62}
\]

and

\[
C^{(1)}_{ij} = \text{Tr}\phi_i e^{H + \Delta W} F_j = \text{Tr}\phi_i e^{H + \Delta W} \sum_k \phi_k \sigma_{kj} = G_{ik} \sigma_{kj}. \tag{63}
\]

The collective contribution to the self-energy at first-order is

\[
K^{(1)}_{ij} = -\gamma_{it} G_{tk} \sigma_{kj} = -\sigma_{ij}. \tag{64}
\]

Next, we consider the second-order contribution

\[
C^{(2)}_{ij} = \text{Tr}\phi_i e^{H + \Delta W} \frac{\delta}{\delta G_j} \Delta W^{(2)}. \tag{65}
\]

where

\[
\Delta W^{(2)} = \frac{1}{2} \sum_{ij} F_i F_j G_{ij}. \tag{66}
\]

It is shown in Ref. [13] that the second order contribution to the dynamic self energy is obtained in the symmetric form in terms of the screened matrix correlation function \(\tilde{G}\) as
\[
K^{(2)}_{ij} = -\frac{1}{2} \gamma^{(0)}_{iuv} G_{uw} G_{vq} \gamma^{(0)}_{jrq}
\]

where \(\gamma^{(0)}_{ijk}\) denotes the three point vertex function \(\Gamma_{ijk}\) defined in eqn. (52) at the lowest order i.e., for a noninteracting system. This is referred to as the collective one-loop contribution.

The \(G\) matrix elements are obtained as

\[
\tilde{G}_{ij}(1) = \frac{1}{2} \sum_{kl} \left[ G_{ik}^{(0)} \sigma_{kl} G_{lj}^{(0)} + G_{ik}^{(0)} \sigma_{kl} G_{lj}^{(0)} \right]
\]

and plays the role of an effective propagator. The above result obtained for the SD case in Ref. [13] also holds for the ND case. The relations (68) and (67) form a closed set of self-consistent equations for the correlation matrix \(G_{ij}\). This gives rise to a feedback mechanism which becomes strong enough at high density to drive the system to a possible ENE transition. Evaluating the strength of the feedback mechanism even at the lowest order will involve evaluating the three-point vertex functions \(\gamma^{(0)}_{ijk}\) for the noninteracting system. Later we describe the basic calculation for obtaining the correlations in the ideal gas. Analysis of the feedback process with evaluation of the vertex functions and the possibility of the ENE transition will be taken up in a companion paper.

**B. First-Order Theory**

To obtain the correlation functions at the first order we need as an input the correlation functions for the noninteracting system. We present computation of the two point correlation functions \(G^{(0)}_{\alpha\beta}\) at the zeroth order in the next section. We list the zeroth-order results here as a starting point of the first-order calculation:

\[
G^{(0)}_{\rho\rho}(k, t_1, t_2) = \rho_0 e^{-\frac{k^2}{2m} (t_2 - t_1)^2}
\]

\[
G^{(0)}_{\rho B}(k, t_1, t_2) = -\frac{k^2}{m} (t_1 - t_2) e^{-\frac{k^2}{2m} (t_2 - t_1)^2} \theta(t_1 - t_2) \rho_0
\]

\[
G^{(0)}_{B\rho}(k, t_1, t_2) = -\frac{k^2}{m} (t_2 - t_1) e^{-\frac{k^2}{2m} (t_2 - t_1)^2} \theta(t_2 - t_1) \rho_0
\]

\[
G^{(0)}_{BB}(k, t_1, t_2) = 0
\]

where we have the same structure as in the SD case. \(G_{\rho\rho}\) is real, \(G_{\rho B}\) is retarded, \(G_{B\rho}\) is advanced, and \(G_{BB}\) is zero. For the time translational invariance we obtain the frequency
transformed quantities as

\[ G_{\rho \rho}^{(0)}(k, \omega) = \sqrt{2 \pi} \frac{\rho_0}{k v_0} e^{-\frac{\omega^2}{2 k v_0}} \]

\[ G_{\rho B}^{(0)}(k, \omega) = -\rho_0 \beta S\left(\frac{\omega}{\sqrt{2 k v_0}}\right) \]

where \( m v_0^2 = k_B T \) and where the integral \( S(x) \) is defined as

\[ S(x) = 1 - 2x^2 \int_0^x du e^{u^2} + i \sqrt{\pi} x e^{-x^2} \]

Let us look at the first-order theory for the one point function or the equation of state. Starting from the basic relation (44) we obtain for the one point function

\[ G_i = G_i^{(0)} + Tr \phi_i \Delta W^{(1)} \]

\[ = G_i^{(0)} + G_{ik}^{(0)} \sigma_{kl} G_l \]

For \( i = \rho \) using the corresponding \( \sigma_{B\rho} \) element and using the result \( G_\rho^{(0)}(1) = 2\pi \delta(\omega) G_\rho^{(0)}(k) \)

we obtain

\[ G_\rho(k) = \frac{G_\rho^{(0)}(k)}{1 - V(k) G_{\rho B}^{(0)}(k, 0)} \]

Since \( G_\rho^{(0)}(0) \equiv \rho_0 \) we obtain the equation of state to first order in \( V \) as

\[ \bar{\rho} = \frac{\rho_0}{1 + \beta \rho_0 V} \]

where we have used the result from eqn. (74) that \( G_\rho^{(0)}(0, 0) = -\beta \rho_0 \) to zeroth order in the interaction. Notice that we self-consistently determine the static properties as we solve the dynamic problem.

It turns out to be more useful to write eqn. (78) in the form:

\[ \rho_0 = \frac{\bar{\rho}}{1 - \beta \bar{\rho} V(0)} \]

\[ = \bar{\rho} e^{\exp(\tilde{V}(0))} \]
We now relate this to the conventional equation of state. First, since we are working in the grand canonical ensemble, \( \rho_0 \) is the fugacity

\[
\rho_0 = \frac{e^{\beta \mu}}{\ell^d}
\]  

(81)

where \( \ell \) is a microscopic length independent of density and \( \mu \) is the chemical potential. There is the Gibbs-Duhem relation

\[
\frac{\partial \rho}{\partial \rho} = \frac{\partial \mu}{\partial \rho}
\]

or

\[
\frac{\partial \beta \rho}{\partial \rho} = \frac{\partial \beta \mu}{\partial \rho}
\]

(82)

\[
\frac{\partial \beta \rho}{\partial \rho} = \frac{\rho_0}{\bar{\rho}} \frac{\partial \rho_0}{\partial \rho}
\]

(83)

(84)

Working at first order in the potential it is easy to show

\[
\frac{\partial \rho_0}{\partial \rho} = e^{\tilde{\nu}[0]} (1 + \tilde{V}[0])
\]

(85)

Then

\[
\frac{\partial \beta \rho}{\partial \rho} = (1 + \tilde{V}[0])
\]

(86)

\[
\beta \rho = \rho + \frac{1}{2} \beta \rho^2 V[0]
\]

(87)

The first term is the ideal gas law. The complete expression with \( V \) an effective potential is sensible over a broad range of densities.

Let us look at the first-order theory for the two-point correlation functions. To obtain the correlation functions at this order we begin with the eqn. (54) and use the corresponding order expression for the self energy \( c_{ij}^{(1)} \) and \( \Delta W^{(1)} \) obtained respectively in eqns. (63) and (61) to write the matrix kinetic equation [12]:

\[
G_{ij} = G_{ij}^{(0)} + \sum_{l,k} G_{ijl}^{(0)} \sigma_{lk} G_k + \sum_{l,k} G_{il}^{(0)} \sigma_{lk} G_{kj}
\]

(88)

The role of the second term on the RHS of the above equation gives rise to a factor [12] of \( \rho_0 / \rho_0 \) with the first term. In time space we write,
\[ G_{ij}(k, t_1, t_2) = \frac{\bar{\rho}}{\rho_0} G_{ij}^{(0)}(k, t_1, t_2) + \int_{t_0}^{\infty} d\bar{t} \sum_{k,l} G_{ik}^{(0)}(k, t_1, \bar{t}) \sigma_{kl}(k) G_{lj}(k, \bar{t}, t_2) . \] 

(89)

The average density \( \bar{\rho} \) is defined in the equation of state given by eqn. (78) in the time translational invariant form. Now from eqn.(89) we obtain setting \( i = j = B \) and \( t_2 = t_0 \) (the initial time)

\[ G_{BB}(k, t_1, t_2) = \frac{\bar{\rho}}{\rho_0} G_{BB}^{(0)}(k, t_1, t_2) + G_{B\rho}^{(0)}(k, t_1, t_0)(-\beta V(k))G_{\rho B}(k, t_0, t_2) \quad . \] 

(90)

Since \( G_{BB}^{(0)}(k, t_1, t_2), G_{B\rho}^{(0)}(k, t_1, t_0) \) and \( G_{\rho B}^{(0)}(k, t_0, t_2) \) are zero, we find \( G_{BB}(k, t_1, t_2) = 0. \)

Consider the response functions \( G_{\rho B}(k, t_1, t_2) \) and \( G_{B\rho}(k, t_1, t_2) \) by taking the \( \rho - B \) and \( B - \rho \) matrix elements of Eq.(89) results in the equations

\[ G_{\rho B}(k, t_1, t_2) = \frac{\bar{\rho}}{\rho_0} G_{\rho B}^{(0)}(k, t_1, t_2) + \int_{t_0}^{\infty} d\bar{t}G_{\rho B}^{(0)}(k, t_1, \bar{t})V(k)G_{\rho B}(k, \bar{t}, t_2) \] \[ G_{B\rho}(k, t_1, t_2) = \frac{\bar{\rho}}{\rho_0} G_{B\rho}^{(0)}(k, t_1, t_2) + \int_{t_0}^{\infty} d\bar{t}G_{B\rho}^{(0)}(k, t_1, \bar{t})V(k)G_{B\rho}(k, \bar{t}, t_2) \] 

(91)

It is easy to see that \( G_{\rho B}(k, t_0, t_2) \) and \( G_{B\rho}(k, t_1, t_0) \) are both equal to zero. Since \( G_{\rho B}(k, \bar{t}, t_2) \) is retarded and \( G_{B\rho}^{(0)}(k, t_1, \bar{t}) \) is advanced, eqn.(91) are solved by Fourier transformation:

\[ G_{\rho B}^{(1)}(k, \omega) = \frac{(\bar{\rho}/\rho_0)G_{\rho B}^{(0)}(k, \omega)}{1 - V(k)G_{\rho B}^{(0)}(k, \omega)} \] \[ G_{B\rho}^{(1)}(k, \omega) = \frac{(\bar{\rho}/\rho_0)G_{B\rho}^{(0)}(k, \omega)}{1 - V(k)G_{B\rho}^{(0)}(k, \omega)} \] 

(92)

Using the results from eqn. (74) that \( G_{\rho B}^{(0)}(0, k) = -\beta \rho_0 \), to zeroth order in the interaction, we obtain the zero-frequency \( G_{\rho B} \) at the first order as,

\[ G_{\rho B}^{(1)}(k, 0) = -\frac{\beta \bar{\rho}}{1 + \beta \rho_0 V(k)} \] \[ G_{B\rho}^{(1)}(k, 0) = -\frac{\beta \bar{\rho}}{1 + \beta \rho_0 V(k)} \] 

(93)
Now we consider the $\rho - \rho$ matrix element of Eq.(89)

\[ G_{\rho\rho}(k, t_1, t_2) = \bar{\rho}\rho_0 G^{(0)}(k, t_1, t_2) + G^{(0)}_{\rho \rho}(k, t_1, t_0)(-\beta V(k))G_{\rho \rho}(k, t_0, t_2) + \int_{t^o}^{\infty} d\bar{t}G^{(0)}_{\rho \rho}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) + \int_{t^o}^{\infty} d\bar{t}G^{(0)}_{\rho B}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) \] (94)

We rewrite this equation in the following form

\[ G_{\rho\rho}(k, t_1, t_2) = \bar{\rho}\rho_0 G^{(0)}(k, t_1, t_2) + \int_{-\infty}^{\infty} d\bar{t}G^{(0)}_{\rho \rho}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) + \int_{-\infty}^{\infty} d\bar{t}G^{(0)}_{\rho B}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) + K(k, t_1, t_2) \] (95)

where all of the terms dependent on $t_0$ are included in

\[ K(k, t_1, t_2) = G^{(0)}_{\rho \rho}(k, t_1, t_0)(-\beta V(k))G_{\rho \rho}(k, t_0, t_2) - \int_{-\infty}^{t_0} d\bar{t}G^{(0)}_{\rho \rho}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) - \int_{-\infty}^{t_0} d\bar{t}G^{(0)}_{\rho B}(k, t_1, \bar{t})V(k)G_{\rho \rho}(k, \bar{t}, t_2) \]. (96)

All of the elements contributing to the breaking TTI are collected into $K$. By direct calculation one can show that $K = 0$ and TTI holds. This analysis is rather involved. Instead we consider the case where the FDT holds

\[ G_{\rho B}(t - s) = \theta(t - s)\beta \frac{\partial}{\partial t} G_{\rho \rho}(t - s) \] . (97)

Now in $K$ eliminate the response functions in terms of the density-density correlation function. Notice that the two terms involving an integration can be combined into a single term where inside the integral one has an exact derivative. Doing the integration the contribution from $\bar{t} = t_0$ cancels the term from the initial condition and one has $K = 0$. Eqn.(95) with $K = 0$ can be solved by Fourier transformation and one has

\[ G_{\rho \rho} = \frac{(\bar{\rho}/\rho_0)G^{(0)}_{\rho \rho}}{1 - V(k)G^{(0)}_{\rho B}} \left[ 1 + \frac{V(k)G^{(0)}_{\rho B}}{1 - V(k)G^{(0)}_{\rho B}} \right] \] (98)

20
and we have used the previously determined result for the response functions. After a little rearrangement we have the real result

$$G_{ρρ} = \frac{(\bar{ρ}/ρ_0)G_{ρρ}^{(0)}}{[1 - V(k)G_{ρB}^{(0)}][1 - V(k)G_{Bρ}^{(0)}]} \tag{99}$$

where

$$G_{ρB}^{(0)} = [G_{Bρ}^{(0)}]^* \tag{100}$$

This is the solution to our first order problem.

There are other ways of looking at the information contained in the solution. If the FDT holds we have in Fourier space

$$\frac{2}{βω}ImG_{ρB} = G_{ρρ} \tag{101}$$

which also holds for the noninteracting limit

$$\frac{2}{βω}ImG_{ρB}^{(0)} = G_{ρρ}^{(0)} \tag{102}$$

These lead to an integral form for the FDT. We start with the identity for the Laplace transform of $G_{ρB}$

$$G_{ρB}(z) = \int_{-∞}^{∞} \frac{dω}{π} \frac{ImG_{ρB}}{z - ω}$$

$$= \int_{-∞}^{∞} \frac{dω}{2πβω} G_{ρρ} \tag{103}$$

where the Laplace transform of the density-density correlation function is defined as

$$G_{ρρ}(k, z) = \int_{-∞}^{∞} \frac{dω}{2π} G_{ρρ}(k, ω) \frac{z - ω}{z - ω} \tag{104}$$

We have used above the result
$$G_{\rho B}(z = 0) = -\beta \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\rho\rho}(\omega)$$
$$= -\beta \bar{\rho} S(k) \ ,$$

(105)

where $S(k)$ is the static structure factor. Using eqn. (93) we obtain our first order approximation for the structure factor

$$S(k) = \frac{1}{1 + \rho_0 \beta V(k)}$$

(106)

which is equivalent to taking the two point Ornstein-Zernike direct correlation function as

$$c(k) = -\beta V(k) \ .$$

(107)

We then equate the two expressions for $G_{\rho B}(k, z)$ obtained in eqns. (92) and (103)

$$G_{\rho B}(z) = -\beta \bar{\rho} \rho S(k) + z \beta G_{\rho\rho}(k, z)$$
$$= \frac{(\bar{\rho}/\rho_0) G_{\rho B}^{(0)}(k, z)}{1 - V(k)G_{\rho B}^{(0)}(k, z)} \ .$$

(108)

Solving for $G_{\rho\rho}$ we find

$$G_{\rho\rho}(k, z) = \frac{\bar{\rho}}{z} \left[ S(k) + \frac{G_{\rho B}^{(0)}(k, z)}{1 - V(k)G_{\rho B}^{(0)}(k, z)} \right]$$

(109)

In the noninteracting limit, we define $\psi(z)$ as the density autocorrelation function normalized with respect to its equal time value

$$\psi(z) = G_{\rho\rho}^{(0)}(k, z)/\rho_0 \ .$$

(110)

Laplace transforming the FDT relation (102) for the noninteracting system we obtain

$$G_{\rho B}^{(0)}(z) = -\beta \rho_0 (1 - z \psi(z))$$

(111)

Using this we obtain from eqn. (109) the result

$$G_{\rho\rho}(k, z) = \frac{\bar{\rho}}{z} \left[ \frac{1}{1 + \beta \rho_0 V(k)} + \frac{(1 - z \psi(z))}{1 + \beta \rho_0 V(k)(1 - z \psi(z))} \right] \ .$$

(112)
After some algebra we have for the density correlation function,

\[ G_{\rho\rho}(k, z) = \bar{\rho}S(k) \left[ \frac{\psi(z)}{1 + \beta \rho_0 V(k)\{1 - z\psi(z)\}} \right] \]  (113)

where

\[ \psi(z) = -i \int_0^\infty dt e^{izt} e^{-\frac{1}{2}(kv_0 t)^2} \]  (114)

Let us look at this in the small k limit. We easily find

\[ \psi(z) = \frac{1}{z} \left[ 1 + \frac{(kv_0)^2}{z^2} \right] \]  (115)

plus terms of order \( k^4 \). Putting this into Eq. (113) and rearranging we find

\[ G_{\rho\rho}(k, z) = \frac{\bar{\rho}S(0)}{2} \left[ \frac{1}{z - ck} + \frac{1}{z + ck} \right] \]  (116)

The two poles represent the two propagating sound modes respectively with speed \( c(k) \) is obtained as,

\[ c(k) = v_0\{1 + \beta \rho_0 V(k)\}^{1/2} = \frac{1}{\sqrt{\beta mS(k)}}. \]  (117)

V. MOMENTUM VARIABLES, CURRENTS, AND THE HIERARCHICAL STRUCTURE OF THEORY

A. Additional Degrees of Freedom

So far the theory has been set up to deal with what we will call the core problem. This is the determination of the observables involving the core variables \( \Phi_0 = (\rho, B) \). In the case of SD this covers essentially all of the degrees of freedom of interest. For ND this is not the case. We have a number of additional degrees of freedom. This is because we have a larger phase-space due to the momentum degrees of freedom. Choices of variables to be included from the simplest to the most involved are:
1. Couple to the two transverse currents \( g_{\perp,1}, g_{\perp,2} \)
2. Couple to the whole current \( g \) and/or the kinetic energy density \( g_K \).
3. Couple to the phase-space density

\[ f(x, p, t) = \sum_{i=1}^{N} \delta(p - P_i(t))\delta(x - R_i(t)) \quad . \] (118)

Choice 1 is the simplest since there is no direct coupling between the longitudinal and transverse degrees of freedom. This is also the simplest way of determining the shear viscosity. If one goes to choice 2 things are more complicated since we have all the correlation functions among \( \rho, B \) and \( g \). One needs \( g_K \) to determine the thermal conductivity.

If one wants to investigate the Boltzmann equation and momentum distributions one needs to include the phase-space density \( f(x, p, t) \) as one of the variables. This will be discussed elsewhere.

**B. Generic Inclusion Of Additional Variables**

Suppose that we have a single-particle additive variable \( g_\alpha \) we want to include in our set \( \Phi = (\rho, B, g) \). This inclusion simply involves an additional term in the basic action

\[ A - H \cdot \Phi_0 \rightarrow A - H \cdot \Phi_0 - J \cdot g \quad (119) \]

which introduces a new external coupling \( J_\alpha \) into the problem. The fundamental generating functional is now given by

\[ W[H, J] = \ln Z_T[H, J] \quad (120) \]

where

\[ Z_T[H, J] = \sum_{i=1}^{N} \rho_0^N \frac{N!}{N!} Z_N[H, J] \quad (121) \]

and

\[ Z_N[H, J] = Tr N e^{A - H \cdot \Phi_0 - J \cdot g} \quad (122) \]

Functional derivatives with respect to \( J \) generates a factor of \( g \) in an average

\[ \langle g_\alpha \rangle = \frac{\delta}{\delta J_\alpha} W[H, J] \quad (123) \]

**C. Perturbation Theory and Hierarchial Structure of Theory**

It is trivial to see that the fundamental identity of the theory takes the form
\[ G_\alpha = Tr_0^0 \phi_\alpha e^{H\phi_0 + J\cdot g} e^{\Delta W[H;J]} \] (124)

where

\[ \Delta W[H;J] = W[H + F;J] - W[H;J] \] (125)

in the extended space.

We can again construct a dynamical OZ equation of the form

\[ G_{\alpha\beta} = G_{\alpha\beta} + c_{\alpha\mu} G_{\mu\beta} \] (126)

where the single-particle contribution is given by

\[ G_{\alpha\beta} = Tr_0^0 \phi_\alpha \phi_\beta e^{H\phi_0 + J\cdot g} e^{\Delta W[H;J]} \] (127)

and the dynamic direct correlation function

\[ c_{\alpha\mu} = Tr_0^0 \phi_\alpha e^{H\phi_0 + J\cdot g} e^{\Delta W[H;J]} \delta_{\delta G_{\mu}} \Delta W[H;J] \] (128)

The key point is that to first order in perturbation theory

\[ \Delta W[H;J]^{(1)} = \sum_{u_0} F_{u_0} G_{u_0} \] (129)

where the sum over \( u_0 \) is only over the core variables \( \phi_0 = \{\rho, B\} \). This happens because the Hamiltonian and hence the corresponding MSR action involves only these core variables. The first order dynamical direct correlation function \( c_{\alpha\mu}^{(1)} \) vanishes if \( \mu = g \). This means at first order we have the kinetic equation

\[ G_{\alpha\beta} = G_{\alpha\beta} + G_{\alpha\rho} V G_{\rho\beta} + G_{\alpha B} V G_{B\beta} \cdot \] (130)

The structure of this equation is very interesting. If we restrict \( \alpha \) and \( \beta \) to the core variables then Eq. (130) reduces to the first- order core problem we solved earlier. The correlation functions for the extended variables \( \Phi \) can be expressed in terms of (roughly) noninteracting correlation functions between all the variables and solutions to the core problem associated with \( \Phi_0 \).
This suggests that one can not get around the core problem. This problem is self-contained and must be treated first. These self-consistent solutions then enter into the extended space $\Phi$ as determined sub-matrices in the matrix kinetic equation. The second order order corrections to the dynamic direct correlation functions $c_{ij}^{(2)}$ and hence the self energy matrix $K_{ij}^{(2)}$ will involve the extended set of collective variables.

VI. NON-INTERACTING SYSTEM

A. Generating functional

In this section we present the calculation of the zeroth- order cumulants for the Newtonian dynamics case. We first work out the generating functional for a rather general single-particle gaussian model in the Appendix B. This model includes SD, ND and Fokker-Planck dynamics as special cases. For a quadratic action of fields $\psi_i$ and response fields $\hat{\psi}_i$ we have

$$A_0[\psi, \hat{\psi}] = \sum_{ij} \int_{t_0}^{\infty} dt \dot{\psi}_i(t) \bar{D}_{ij} \dot{\psi}_j(t) + \sum_{i} \int_{t_0}^{\infty} dt \left[ i \dot{\psi}_i(t) (\psi_i(t) + \sum_{j} K_{ij} \dot{\psi}_j(t)) \right]$$

$$- \sum_{i} \int_{t_0}^{\infty} dt \left[ h_i(t) \dot{\psi}_i(t) + \hat{h}_i(t) \dot{\psi}_i(t) \right]$$

(131)

where $\bar{D}_{ij}$ is the damping matrix, $K_{ij}$ is a force matrix, and $h_i$ and $\hat{h}_i$ are the detailed external fields that couple to $\psi_i(t)$ and $\hat{\psi}_i(t)$. In Appendix B we find that the associated generating functional is given by

$$\ln Z_0(h, \hat{h}; \psi^{(0)}) = \sum_{ij} \int dt \int dt' \left[ \frac{1}{2} h_i(t) c_{ij}(t - t') h_j(t') + h_i(t) g_{ij}(t - t') \hat{h}_j(t') \right]$$

$$+ \sum_{i j} \int dt h_i(t) i g_{ij}(t - t_0) \psi_j^{(0)}$$

(132)

where $\psi_i^{(0)}$ is the initial value of the fields, the normalization is such that $Z_0[0,0] = 1$,

$$c_{ij}(t, t') = -2 \sum_{k,\ell} \int_{-\infty}^{\infty} d\bar{t} g_{ik}(t, \bar{t}) \bar{D}_{k\ell} g_{\ell j}^T(\bar{t}, t')$$
\[ = -\sum_{k,\ell} \int_{-\infty}^{\infty} d\bar{r} g_{ij}(t, \bar{r}) 2 \bar{D}_{k\ell} g_{\bar{k}\bar{l}}(\bar{r}, t') = c_{ij}(t', t) \]

(133)

and the function \( g_{ij} \) is now obtained from the solution of the Green’s function equation

\[ \partial \frac{\partial}{\partial t} g_{ij}(t, t') + \sum_{k} K_{ik} g_{kj}(t, t') = -i\delta(t - t')\delta_{ij} . \]

(134)

These equations govern SD, ND and FPD. Notice that all information about the equilibrium state of the system is carried by the damping matrix \( \bar{D} \approx k_B T \). If we restrict ourselves to simple fluids, then the damping term with \( c_{ij} \) is zero and the state of the system enters via the initial condition. We have

\[ Z_0(h, \dot{h}, \psi(0)) = \exp(\int_{t_0}^{\infty} dt \int_{t_0}^{\infty} dt' \sum_{ij} h_i(t) g_{ij}(t - t') [\dot{h}_j(t) + i\delta(t' - t_0) \psi_j(0)] \]

(135)

with an average over initial conditions remaining. If the initial conditions are gaussian

\[ P_0(\psi(0)) = \mathcal{N} e^{-\frac{1}{2} \psi_i(0) M_{ij} \psi_j(0)} \]

(136)

one can carry out the average over \( \psi_i(0) \) and obtain

\[ \ln Z_0(h, \dot{h}) = \frac{1}{2} \int_{t_0}^{\infty} dt \int_{t_0}^{\infty} dt' \sum_{ij} h_i(t) c_{ij}^T(t - t') h_j(t') + h_i(t) g_{ij}(t - t') \dot{h}_j \]

(137)

and

\[ c_{ij}^T(t, t') = c_{ij}(t, t') + c_{ij}^I(t, t') \]
\[ c_{ij}^I(t, t') = \sum_{k,\ell} g_{ik}(t, t_0) (M^{-1})_{k\ell} g_{\ell j}^T(t_0, t') . \]

(138)

B. Newtonian Dynamics

For Newtonian dynamics there are two phase-space coordinates, \( R \) and \( P \), with an elementary force matrix \( K_{ij} = \delta_{iR} \delta_{jP} \frac{1}{m} \) for the noninteracting system. We first have to solve the matrix equation following from Eq. (134) in the Newtonian case for which indices \( i \) and \( j \) run over the set \( \{ R, P \} \).
\[
\frac{\partial}{\partial t} g_{RR} - \frac{g_{PR}}{m} = -i\delta(t) \quad (139)
\]
\[
\frac{\partial}{\partial t} g_{RP} - \frac{g_{PP}}{m} = 0
\]
\[
\frac{\partial}{\partial t} g_{PR} = 0
\]
\[
\frac{\partial}{\partial t} g_{PP} = -i\delta(t) \quad (140)
\]

The straight forward solution \( g_{ij}(t - t') \) is listed in Table 1.

Since there is no dissipation put into the model, \( \bar{D}_{ij} = 0, \ c^{(0)}_{ij} = 0 \) the generating functional simplifies

\[
\ln Z_0[h, \hat{h}; \psi^{(0)}_i] = \int_{t_0}^{\infty} dt \int_{t_0}^{\infty} dt' \sum_{ij} h_i(t) g_{ij}(t - t') \hat{h}_j(t')
+ \int_{t_0}^{\infty} dt \left[ h_R(t) \theta(t - t_0) R_0 + i \sum_i h_i(t) i g_{iP}(t - t_0) P_0 \right]. \quad (141)
\]

The general result for the solution of the differential equation

\[
\frac{\partial}{\partial t} <\psi_i(t)> + \sum_j K_{ij} <\psi_j(t)> = \psi^{(0)}_i \delta(t - t_0) \quad (142)
\]
is obtained in terms of the Green’s function \( g(t, t') \)
\[ < \psi_i(t; t_0) > = \sum_j i \int dt' g_{ij}(t - t') \psi_j^{(0)}(t' - t_0) = ig_{ij}(t - t_0)\psi_j^{(0)}. \quad (143) \]

For \( c_{ij} = 0 \) and \( \hat{h} = h = 0 \) we obtain the same relation from eqn. (B12). In this particular case, we obtain the following reversible (and deterministic) equations of motion are given for the two coordinates \( \{ R, P \} \).

\[
\begin{align*}
R(t) &= ig_{RR}(t - t_0)R_0 + ig_{RP}(t - t_0)P_0 \\
P(t) &= ig_{PR}(t - t_0)R_0 + ig_{PP}(t - t_0)P_0
\end{align*}
\quad (144)
\]

These equations are also obtained from the relations

\[
\begin{align*}
<R(t)> &= \frac{\delta}{\delta h_R} \ln Z_0 \bigg|_{h, \hat{h} = 0} \\
<P(t)> &= \frac{\delta}{\delta h_P} \ln Z_0 \bigg|_{h, \hat{h} = 0}
\end{align*}
\]

Inserting the \( g' \)'s leads to the standard phase-space trajectories for free streaming particles.

\[
\begin{align*}
R(t) &= \theta(t - t_0) \left[ R_0 + (t - t_0) \frac{P_0}{m} \right] \\
P(t) &= \theta(t - t_0)P_0
\end{align*}
\quad (145)
\]

The generating function for ND is given by

\[
\ln Z_0[h, \hat{h}] = \int_{t_0}^{\infty} dt \int_{t_0}^{\infty} dt' \sum_{ij} h_i(t) g_{ij}(tt') \hat{h}_j(t') \\
+ \int_{t_0}^{\infty} dt(h_R(t)\theta(t - t_0)R_0 + \int_{t_0}^{\infty} dt \sum_i h_i(t)g_{iP}(t - t_0)P_0.
\quad (146)
\]

C. Computation of \( \phi \)-Correlations

It is not the direct correlations of the phase-space coordinates that are of interest but the correlations of the \( \Phi \). It is clear that we need to evaluate all of the \( \rho - B \) cumulants generated by

\[ W_0[H] = Tr e^{H\phi}. \quad (147) \]
We begin by introducing the microscopic sources \( h_i, \hat{h}_i \) and treating
\[
Z_0[H, h, \hat{h}] = Tr e^{H \cdot \phi + h \cdot \psi + \hat{h} \cdot \hat{\psi}}.
\] (148)

Remember that the spatial Fourier transforms of the \( \phi \) are in terms of the phase-space coordinates \( \psi \):
\[
\phi_\rho(1) = e^{-ik_1 R(t_1)}
\]
\[
\phi_B(1) = -k_1 \cdot \hat{P}(t_1) e^{-ik_1 R(t_1)}.
\] (149)

Introducing the operators
\[
\hat{\phi}_\rho(1) = e^{-ik_1 \delta \delta h R(t_1)}
\]
\[
\hat{\phi}_B(1) = \hat{b}(1) \hat{\phi}_\rho(1)
\] (150)

where
\[
\hat{b}(1) = -k_1 \cdot \frac{\delta}{\delta h P(t_1)}.
\] (153)

We can write
\[
Z_0[H, h, \hat{h}] = Tr e^{H \cdot \phi + h \cdot \psi + \hat{h} \cdot \hat{\psi}}
\] (154)
\[
= e^{H \cdot \phi} Tr e^{h \cdot \psi + \hat{h} \cdot \hat{\psi}}
\] (155)
\[
= e^{H \cdot \phi} \rho_0 e^{h \cdot |\hat{h}| \psi_0} \int d\psi_0 P[\psi_0] e^{h \cdot i \psi_0}
\] (156)
\[
= e^{H \cdot \phi} \rho_0 \int d\psi_0 P[\psi_0] e^{h \cdot g \cdot [\hat{h} + i \psi_0]}
\] (157)

One can then express an arbitrary noninteracting cumulant, in the presence of \( h \) and \( \hat{h} \), in the form
\[
G_{BB...B\rho...\rho}(12...\ell \ell + 1...n; h, \hat{h}) = \hat{b}(1) \ldots \hat{b}(\ell) \hat{\phi}(1) \ldots \hat{\phi}(n) Z_0[h, \hat{h}]
\] (158)
\[
= \hat{b}(1) \ldots \hat{b}(\ell) \hat{\phi}(1) \ldots \hat{\phi}(n) \rho_0 \int d\psi_0 P[\psi_0] e^{h \cdot g \cdot [\hat{h} + i \psi_0]}
\] (159)
The analysis is very similar to that for the SD case in Appendix C in Ref. 12. The $\hat{\phi}$ are translation operators:

$$G_{BB...B\rho...\rho}(12...\ell+1...n; h, \hat{h}) = \hat{b}(1) \ldots \hat{b}(\ell) \rho_0 \int d\psi_0 P[\psi_0] e^{[h+L] \cdot g \cdot \hat{h} + i\psi_0}$$

where in more detail

$$h + L \rightarrow h_{\alpha}(t_j) + L_{\alpha}^{(n)}(t_j)$$

with

$$L_{\alpha}^{(n)}(t_j) = -i\delta_{\alpha,R} \sum_{s=1}^{n} k_s \delta(t_j - t_s)$$

Application of the operators $\hat{b}(i)$ is multiplicative

$$G_{BB...B\rho...\rho}(12...\ell+1...n; h, \hat{h}) = b_n(1) \ldots b_n(\ell) \rho_0 \int d\psi_0 P[\psi_0] e^{[h+L] \cdot g \cdot \hat{h} + i\psi_0}$$

and

$$b_n(j) = -k_j \int_{t_0}^{\infty} dt \sum \alpha [h_{\alpha}(\bar{t} + L_{\alpha}^{(n)}(\bar{t})) g_{\alpha P}(\bar{t}, t_j)$$

Thus we have the cumulants for arbitrary $h$ and $\hat{h}$. Setting $h$ and $\hat{h}$ to zero we have

$$G_{BB...B\rho...\rho}(12...\ell+1...n) = b_n(1) \ldots b_n(\ell) \rho_0 \int d\psi_0 P[\psi_0] e^{L \cdot g \cdot \psi_0}$$

where

$$\kappa_\alpha = iL \cdot g = iL_{\mu}^{(n)}(\bar{t}) g_{\mu \alpha}(\bar{t}, t_0)$$

and

$$b_n(j) = -k_j \int_{t_0}^{\infty} d\bar{t} (-i \sum_{s=1}^{n} k_s \delta(\bar{t} - t_s)) \left( -\frac{i}{m} \theta(\bar{t} - t_j)(\bar{t} - t_j) \right)$$

$$= \frac{k_j}{m} \sum_{s=1}^{n} k_s \theta(t_s - t_j)(t_s - t_j)$$
We have after a little work

\[ \kappa_R = -i \sum_{s=1}^{n} k_s \]  

(170)

\[ \kappa_P = -i \sum_{s=1}^{n} k_s (t_s - t_0) \]  

(171)

\[ = -i T \]  

(172)

and

\[ G_{BB...B \rho...\rho} (12 \ldots \ell \ell + 1 \ldots n) = b_n(1) \ldots b_n(\ell) \]  

(173)

\[ \times \rho_0 \int d^d R_0 P[R_0] e^{i \sum_{s=1}^{n} k_s \cdot R_0} \int d^d P_0 P[P_0] e^{-i T \cdot P_0} \]  

(174)

\[ = b_n(1) \ldots b_n(\ell) \rho_0 (2\pi)^d \left( \sum_{s=1}^{n} k_s \right) e^{N_n} \]  

(175)

where

\[ e^{N_n} = \int d^d P_0 P[P_0] e^{-i T \cdot P_0} \].  

(176)

The probability of finding a particle at a given position is uniform and the position average enforces the translational invariance in the system

\[ \int d^d R_0 e^{\kappa_R \cdot R_0} = (2\pi)^d \delta(k_1 + k_2 + \ldots + k_n) \].  

(177)

The momentum is assumed to obey a Maxwell-Boltzmann distribution and the average gives the contribution

\[ e^{N_n} = \int \frac{d^d P}{(2\pi P_0)^{d/2}} e^{-\beta \frac{p^2}{2m}} e^{-i T \cdot P} \]  

(178)

where \( p_0^2 = m\beta^{-1} = m^2 v_0^2 \) is the thermal momentum. This is a complete the square calculation giving

\[ e^{N_n} = e^{-\frac{1}{2} \beta v_0^2 T^2} \]  

(179)

and we identify the effective \( N_n \)

\[ N_n = -\frac{1}{2} p_0^2 T^2 \].  

(180)

The correlation function \( G_{BB...B \rho...\rho} \) with \( \ell \) number of \( B \) fields is obtained as
\[ G_{BB\ldots B\rho\ldots \rho}(12\ldots \ell \ell + 1\ldots n) = b_n(1)\ldots b_n(\ell)\rho_0(2\pi)^d \left( \sum_{s=1}^{n} k_s \right) e^{N_n} . \tag{181} \]

Let us focus on \( N_n \). Writing it out we have

\[ N_n = -\frac{p_0^2}{2m^2} \left[ \sum_{s=1}^{n} k_s(t_s - t_0) \right]^2 . \tag{182} \]

Using the conservation law Eq. (177) we see this expression is independent of \( t_0 \) and is time translationally invariant. The effective \( N_n \) can be written in a form similar to the SD case.

We can rewrite \( N_n \)

\[ N_n = -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} k_i k_j C_{ij} \tag{183} \]

where

\[ C_{ij} = \frac{p_0^2}{m^2} t_i t_j \tag{184} \]

Then define

\[ D_{ij} = C_{ii} + C_{jj} - 2C_{ij} \tag{185} \]

\[ = v_0^2 (t_i - t_j)^2 . \tag{186} \]

We then have

\[ N_n = -\frac{v_0^2}{2} \left[ \sum_{i=1}^{n} k_i^2 C_{ii} + \sum_{i\neq j=1}^{n} k_i k_j \frac{1}{2} [C_{ii} + C_{jj} - D_{ij}] \right] \]

\[ = -\frac{v_0^2}{2} \left[ \sum_{i=1}^{n} k_i^2 C_{ii} + \sum_{i\neq j=1}^{n} k_i k_j \frac{1}{2} [C_{ii} + C_{jj} - D_{ij}] \right] \]

\[ = -\frac{v_0^2}{2} \left[ \sum_{i=1}^{n} k_i^2 C_{ii} + \sum_{i\neq j=1}^{n} k_i k_j \frac{1}{2} [C_{ii} + C_{jj} - D_{ij}] \right] \]

\[ = -\frac{v_0^2}{2} \left[ \sum_{i=1}^{n} k_i^2 C_{ii} + \sum_{i\neq j=1}^{n} k_i k_j \frac{1}{2} (-D_{ij}) \right] \]

\[ = -\frac{v_0^2}{2} \left[ \sum_{i=1}^{n} k_i^2 C_{ii} + \sum_{i\neq j=1}^{n} k_i k_j \frac{1}{2} (-D_{ij}) \right] \]

\[ = \frac{v_0^2}{4} \sum_{i=1}^{n} \sum_{j=1}^{n} K_{ij} (t_i - t_j)^2 . \tag{187} \]
where

\[ K_{ij} = k_i \cdot k_j \]  \quad (188)

The noninteracting correlation and response cumulants are now all in a time-translationally invariant form.

**D. Two-Point Cumulants**

Let us extract the two-point cumulants needed in our first-order discussion. For the density-density correlation function

\[ G^{(0)}_{\rho\rho}(12) = \rho_0(2\pi)^d \delta(k_1 + k_2) e^{-\frac{1}{2} \kappa_1 v_0^2 (t_1 - t_2)^2} \]  \quad (189)

where

\[ \kappa_1 = k_1^2 \]  \quad (190)

For the response function we have

\[ G^{(0)}_{\rho B}(12) = b_2(2)G^{(0)}_{\rho\rho}(12) \]  \quad (191)

where

\[ b_2(2) = -\frac{\kappa_1}{m} \theta(t_1 - t_2)(t_1 - t_2) \]  \quad (192)

and

\[ G^{(0)}_{BB}(12) = b_2(1)b_2(2)G^{(0)}_{\rho\rho}(12) = 0 \]  \quad (193)

Notice the relationship

\[ G^{(0)}_{\rho B}(12) = \theta(t_1 - t_2)\beta \frac{\partial}{\partial t_1} G^{(0)}_{\rho\rho}(12) \]  \quad (194)

holds at the zeroth order. We return to these results in the next paper in this series.

**VII. CONCLUSIONS**

We have developed the fundamental theory for conventional fluids in which the particles follow reversible Newtonian dynamics. The theory is remarkably similar to that developed to treat particles following Smoluchowski dynamics (SD). We have a field theoretic formulation with similar nonlinear interactions in terms of a pair potential. The question of
self-consistency is addressed in a very similar manner. The role of initial conditions and broken time translational symmetry are addressed at zeroth and first order in the theory. At zeroth order the average over initial conditions is shown for cumulants of the collective variables to satisfy TTI. At first order we can impose equilibrium and sustain TTI if we require the system to obey fluctuation dissipation symmetry (FDS).

As for the treatment of SD the second order self-energies require the zeroth order irreducible three-point vertices. These three-point functions turn out to be more complicated in the case of ND. In the present paper we have shown how to compute all cumulants for the non interacting system. The three-point cumulants enter into the determination of the three-point irreducible vertices. These vertices enter into the computation of the second order self-energy. This becomes the necessary input for analysis of a possible ENE transition in such systems at high density. In the next paper in this series we show that there is a FDS and it can rather easily be applied to the cumulants and irreducible vertices of the fully interactive fluid ND system. We derive identities obeyed by the three-point objects in a manner similar to the application of nonperturbative FDS to the two-point cumulants and vertices. We then focus on the use of this machinery to explore whether we have ENE transitions in ND systems.

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Appendix A: Fundamental Identities

We have the definition of the grand partition function

\[ Z_T[H; x] = \sum_{N=0}^{\infty} \frac{x^N}{N!} T_T^N e^{H \Phi_N + \frac{1}{2} \Phi_N \sigma \Phi_N} \quad (A1) \]

where \( \Phi_N = \sum_{i=1}^{N} \phi^{(i)} \) and we have the important result that self-energies (the interaction of the \( i \)-th particle with itself does not contribute, \( i.e., \)

\[ \phi^{(i)} \sigma \phi^{(i)} = 0 \quad (A2) \]

for all \( i \). We need the following identity

\[ \Phi_{N+1} \sigma \Phi_{N+1} = \Phi_N \sigma \Phi_N + 2\phi^{(N+1)} \sigma \Phi_N = \Phi_N \sigma \Phi_N + 2F^{N+1} \Phi_N \quad (A3) \]

where we have defined \( F^{(N+1)} = \sigma \phi^{(N+1)} \). Therefore we have

\[ \frac{1}{2} \Phi_{N+1} \sigma \Phi_{N+1} = \frac{1}{2} \Phi_N \sigma \Phi_N + F^{(N+1)} \Phi_N \quad (A4) \]

Now consider

\[ Z_N(H + F_{N+1}) = T_T^N e^{H + F^{(N+1)} \cdot \Phi_N + \frac{1}{2} \Phi_N \sigma \Phi_N} \quad (A5) \]

\[ = T_T^N e^{H \Phi_N + \frac{1}{2} \Phi_{N+1} \sigma \Phi_{N+1}} \quad (A6) \]

Multiplying by \( e^{H \phi_{N+1}} \) gives the result

\[ e^{H \phi_{N+1}} Z_N(H + F^{(N+1)}) = T_T^N e^{H \Phi_{N+1} + \frac{1}{2} \Phi_{N+1} \sigma \Phi_{N+1}} \quad (A7) \]

This is the canonical form of the central identity. We now Trace over the degrees of freedom of the \((N+1)\)-th particle (which we denote by the label 0, \( i.e., N + 1 \rightarrow 0 \))

\[ \tilde{T}_r(0) e^{H \phi(0)} Z_N(H + F(0)) = T_T^{N+1} e^{H \Phi_{N+1} + \frac{1}{2} \Phi_{N+1} \sigma \Phi_{N+1}} \equiv Z_{N+1}(H) \quad (A8) \]

where \( \tilde{T}_r(0) \) implies the trace taken over the phase space coordinates of the \('0'\)-th particle. We now multiply the above equation by \( \frac{x^N}{N!} \) and sum over all \( N \).
$$\tilde{T}_N^{(0)} e^{H \cdot \phi(0)} Z_T(H + F(0)) = \sum_{N=0}^{\infty} \frac{x^N}{N!} Z_{N+1}(H) = \sum_{N=1}^{\infty} \frac{x^{N-1}}{(N-1)!} Z_N(H)$$

$$= \frac{\partial}{\partial x} \sum_{N=0}^{\infty} \frac{x^N}{N!} Z_N(H) = \frac{\partial}{\partial x} Z_T[H; x] . \quad (A9)$$

Divide the above equation by $Z_T[H; x]$ to obtain

$$\frac{\partial}{\partial x} W[H; x] = \tilde{T}_N^{(0)} e^{H \cdot \phi(0) + \Delta W[H + F(0); x]} \quad (A10)$$

where $\ln Z_T[H; x] = W[H; x]$ and we have defined

$$\Delta W[H + F; x] = W[H + F(0); x] - W[H; x] . \quad (A11)$$

Integrating the relation $\text{(A9)}$ we obtain

$$W(H; \rho_0) = \int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0) + \Delta W[H + F(0); x]} . \quad (A12)$$

We use this result to generate the one-point quantity

$$G_{\alpha} = \frac{\delta W}{\delta H_{\alpha}} = \frac{\delta}{\delta H_{\alpha}} \int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0) + \Delta W[H + F(0); x]}$$

$$= \int_0^{\rho_0} dx \tilde{T}_N^{(0)} \phi_{\alpha} e^{H \cdot \phi(0) + \Delta W[H + F(0); x]}$$

$$+ \int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0) + \Delta W[H + F(0); x]} \left[ G_{\alpha}(H + F(0); x) - G_{\alpha}(H; x) \right] . \quad (A13)$$

Substituting $H' = H + F(0)$ the integral in the second term on the RHS is written as

$$\int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0) + \Delta W[H'; x]} [G_{\alpha}(H'; x) - G_{\alpha}(H; x)] . \quad (A14)$$

Consider first the first part as,

$$I_2 = \int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0)} e^{\Delta W[H'; x]} G_{\alpha}(H'; x)$$

$$= \int_0^{\rho_0} dx \tilde{T}_N^{(0)} e^{H \cdot \phi(0)} Z_T[H'; x] G_{\alpha}(H'; x) \quad (A15)$$

We want to show self-consistently that
\[ G_\alpha(H'; x) = T r^{(1)} \phi_\alpha^{(1)} e^{H' \phi^{(1)} + \Delta W[H' + F^{(1)}]; x} \]
\[ \equiv x T r^{(1)} \phi_\alpha^{(1)} e^{H' \phi^{(1)} + \Delta W[H' + F^{(1)}]} \]  
(A16)

satisfies the eqn. (A13) above. Substituting eqn. (A16) in eqn. (A15) we obtain

\[ I_2 = x T r^{(0)} e^{H \phi^{(0)}} \frac{Z_T(H')}{Z_T(H)} T r^{(1)} \phi_\alpha^{(1)} e^{H \phi^{(1)} \frac{Z_T(H + F^{(1)})}{Z_T(H')}} \]
\[ = x T r^{(1)} \frac{\phi_\alpha^{(1)}}{Z_T(H)} e^{H \phi^{(1)}} T r^{(0)} e^{H \phi^{(0)}} Z_T(H + F^{(0)} + F^{(1)}) \]
\[ = x T r^{(1)} \frac{\phi_\alpha^{(1)}}{Z_T(H)} e^{H \phi^{(1)}} T r^{(0)} e^{(H + F^{(1)}) \phi^{(0)}} Z_T(H + F^{(1)} + F^{(0)}) \]  
(A17)

where in getting the last equality we have used the result

\[ H' \cdot \phi^{(1)} = H \cdot \phi^{(1)} + F^{(0)} \phi^{(1)} = H \cdot \phi^{(1)} + \sigma \phi^{(0)} \phi^{(1)} = H \cdot \phi^{(1)} + F^{(1)} \phi^{(0)} \]

Using the last relation (A9), we obtain from eqn. (A17)

\[ I_2 = x T r^{(1)} \frac{\phi_\alpha^{(1)}}{Z_T(H)} e^{H \phi^{(1)}} \frac{\partial}{\partial x} Z_T[H + F^{(1)}] \]

(A18)

The expression for \( I_2 \) is put back into the expression (A13) for \( G_\alpha \).

\[ G_\alpha = \int_0^{\rho_0} dx T r^{(0)} e^{H \phi^{(0)} \phi_\alpha^{(0)}} \frac{Z_T[H + F^{(0)}]}{Z_T[H; x]} \]
\[ + \int_0^{\rho_0} dx x T r^{(1)} \phi_\alpha^{(1)} e^{H \phi^{(1)}} \frac{1}{Z_T[H; x]} \frac{\partial}{\partial x} Z_T[H + F^{(1)}] - \frac{Z_T[H + F^{(1)}]}{Z_T[H; x]} \frac{\partial}{\partial x} Z_T[H] \]
\[ = T r^{(1)} \phi_\alpha^{(1)} e^{H \phi^{(1)}} \int_0^{\rho_0} dx \left[ x Z_T[H + F^{(1)}; x] \frac{Z_T[H + F^{(1)}]}{Z_T[H; x]} \right] \]
\[ = T r^{(1)} \phi_\alpha^{(1)} \rho_0 e^{H \phi^{(1)}} \frac{Z_T[H + F^{(1)}; \rho_0]}{Z_T[H; \rho_0]} \equiv T r^{(1)} \phi_\alpha^{(1)} e^{H \phi^{(1)} + \Delta W[H + F^{(1)}]} \]  
(A19)
Thus we have established the fundamental result

\[ G_\alpha = Tr(1) e^{H_\phi + \Delta W[H + E(1) + i \phi]} \]  

(A20)

**Appendix B: Single-particle Gaussian Problem**

We want to construct the generating functional associated with single-particle noninteracting dynamics. The single-particle problem is governed by the phase-space coordinates \( \psi_i \) with response variables \( \hat{\psi}_i \). The action governing these variables is quadratic

\[
A_0 = \sum_{ij} \int_{t_0}^{\infty} dt \hat{\psi}_i(t) \bar{D}_{ij} \psi_j(t) + \sum_i \int_{t_0}^{\infty} dt \left[ i \hat{\psi}_i(t) \left( \psi_i(t) + \sum_j K_{ij} \psi_j(t) \right) \right] 
- \sum_i \int_{t_0}^{\infty} dt \left[ h_i(t) \psi_i(t) + \hat{h}_i(t) \hat{\psi}_i(t) \right]
\]

(B1)

where \( \bar{D}_{ij} \) is the damping matrix, \( K_{ij} \) is a force matrix, and \( h_i(t) \) and \( \hat{h}_i(t) \) are the detailed external fields that couple to particle \( \psi \) and \( \hat{\psi} \). Newtonian dynamics corresponds to the special case where the damping matrix vanishes \( \bar{D}_{ij} = 0 \).

We proceed using the identities that hold in the range \( t_0 < t < \infty \):

\[
\int \mathcal{D}(\psi) \mathcal{D}(\hat{\psi}) \frac{\delta}{\delta \psi_i(t)} e^{-A_0} = 0
\]

\[
\int \mathcal{D}(\psi) \mathcal{D}(\hat{\psi}) \frac{\delta}{\delta \hat{\psi}_i(t)} e^{-A_0} = 0
\]

which leads to the set of equations where we sum over repeated indices labeled by \( j \) and we suppress the local time label:

\[
2 \bar{D}_{ij} \dot{G}_j + i \dot{G}_i + iK_{ij} G_j = \dot{h}_i
\]

\[
- i \frac{\partial}{\partial t} \dot{G}_i + iK^T_{ij} \dot{G}_j = h_i
\]

where \( K^T \) is the transpose of the matrix \( K \). We have defined the functions \( G_i \) and \( \hat{G}_i \) as

\[
G_i = \langle \psi_i \rangle
\]

\[
\hat{G}_i = \langle \hat{\psi}_i \rangle
\]
The $G$s depend on initial data which we must eventually average over. We must now solve these equations, at least formally, to obtain the generating functional.

Let us treat $G_i(t)$ and $\hat{G}_i(t)$ as inner products spanned by a complete and orthonormal set of states $|i>$ such that

$$G_i(t) = <i|G(t)>$$
$$\hat{G}_i(t) = <i|\hat{G}(t)>$$
$$K_{ij} = <i|K|j>$$
$$\hat{D}_{ij} = <i|\hat{D}|j>$$
$$h_i(t) = <i|h(t)>$$
$$\hat{h}_i(t) = <i|\hat{h}(t)>$$

which introduces the operators and vectors $G, \hat{G}, K, \hat{D}, h, \hat{h}$. We then have the operator equations

$$2\hat{D}\hat{G}(t) + i\left(\frac{\partial}{\partial t} + K\right)G(t) = \hat{h}(t)$$
$$-i\left(\frac{\partial}{\partial t} + K^T\right)\hat{G}(t) = h(t).$$

We first solve the eqn. (B3) for $\hat{G}$, obtaining

$$\hat{G}(t) = \int_{-\infty}^{\infty} d\tau g^T(t,\tau)h(\tau)$$

where

$$g^T(t,t') = -ie^{-K^Tt}\theta(t'-t)e^{K^Tt'}.$$

The solution for $\hat{G}$ is put back in the eqn. (B2) for $G$ to obtain

$$\left[\frac{\partial}{\partial t} + K\right]\hat{G}(t) = -i\left(\hat{h}(t) - 2\hat{D}\int_{-\infty}^{\infty} dt' g^T(t,t')h(t')\right).$$

It is straightforward to obtain the corresponding solution for $G(t)$ as

$$G(t) = ig(t,t_0)\psi^{(0)} + \int_{-\infty}^{\infty} dt'[g(t,t')\hat{h}(t') + c(t,t')h(t')]$$
where the functions $g$ and $c$ are given by

$$
g(t, t') = -ie^{-Kt\theta(t-t')}e^{Kt'} \quad (B8)$$

$$
c(t, t') = -\int_{-\infty}^{\infty} d\bar{t}g(t, \bar{t})2\bar{D}g^T(\bar{t}, t') \quad (B9)$$

and $\psi(0)$ is the initial value of the phase-space coordinates. Notice that $g$ satisfies the Green’s function equation

$$\left[ \frac{\partial}{\partial t} + K \right] g(t, t') = -i\delta(t - t') \quad (B10)$$

Putting in complete sets of states we obtain

$$\hat{G}_i(t) = \sum_j \int dt'h_j(t')g_{ji}(t' - t) \quad (B11)$$

$$G_i(t) = \sum_j \int_{-\infty}^{\infty} dt'[g_{ij}(t - t')\hat{h}_j(t') + c_{ij}(t - t')h_j(t')] + ig_{ij}(t - t_0)\psi_j(0) \quad (B12)$$

where the kernel matrix $c_{ij}$ is obtained as

$$c_{ij}(t, t') = -\sum_{k, \ell} \int_{-\infty}^{\infty} d\bar{t}g_{ik}(t, \bar{t})2\bar{D}g^T_{\ell j}(\bar{t}, t')$$

$$= -\sum_{k, \ell} \int_{-\infty}^{\infty} d\bar{t}g_{jk}(t', \bar{t})2\bar{D}g^T_{k \ell}(\bar{t}, t') = c_{ji}(t', t) \quad . \quad (B13)$$

In getting the last equality we have used the symmetry $\bar{D}_{ij} = \bar{D}_{ji}$ of the damping matrix.

The function $g_{ij}$ is now obtained from the solution of eqn. (B10) with labels restored:

$$\frac{\partial}{\partial t}g_{ij}(t, t') + \sum_k K_{ik}g_{kj}(t, t') = -i\delta(t - t')\delta_{ij} \quad (B14)$$

We then have the results for the generating functional

$$\hat{G}_i(t) = \frac{\delta}{\delta \hat{h}(t)} \ln Z_0(h, \hat{h}) \quad (B15)$$

$$G_i(t) = \frac{\delta}{\delta h(t)} \ln Z_0(h, \hat{h}) \quad (B16)$$

The solution to this set of equations, Eqs.(B11), (B12), (29) and (B16) for the generating functional is given by
\[
\ln Z_0(h, \hat{h}; \psi^{(0)}) = \frac{1}{2} \sum_{ij} \int dt \int dt' \left[ \frac{1}{2} h_i(t)c_{ij}(t - t') h_j(t') + h_i(t)g_{ij}(t - t') \hat{h}_j(t') \right] \\
+ \sum_{ij} \int dt h_i(t) i g_{ij}(t - t_0) \psi_j^{(0)} \\
\equiv \frac{1}{2} h \cdot c \cdot h + h \cdot g \cdot \hat{h} + h \cdot i g \cdot \psi^{(0)}. \tag{B17}
\]

The last short-hand representation is useful. The full generator requires averaging over the initial conditions

\[
Z_0[h, \hat{h}] = \int d^4\psi^{(0)} P_0(\psi^{(0)}) \exp \left[ \frac{1}{2} h \cdot c \cdot h + h \cdot g \cdot \hat{h} + h \cdot i g \cdot \psi^{(0)} \right] \\
= e^{\frac{1}{2} h \cdot c \cdot h + h \cdot g \cdot \hat{h}} \int d\psi^{(0)} P_0(\psi^{(0)}) e^{h \cdot i g \cdot \psi^{(0)}}. \tag{B18}
\]

This is the solution to a rather general gaussian problem.
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$$\lim_{t \to \infty} G_{\rho \rho}(q, t) = F(q)$$

then if the system is ergodic and $F(q) = 0$, while if the system is nonergodic $F(q)$ is nonzero.

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