

Renormalized Kinetic Theory of Classical Fluids in and out of Equilibrium

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Abstract We present a theory for the construction of renormalized kinetic equations to describe the dynamics of classical systems of particles in or out of equilibrium. A *closed, self-consistent* set of evolution equations is derived for the single-particle phase-space distribution function f , the correlation function $C = \langle \delta f \delta f \rangle$, the retarded and advanced density response functions $\chi^{R,A} = \delta f / \delta \phi$ to an external potential ϕ , and the associated memory functions $\Sigma^{R,A,C}$. The basis of the theory is an effective action functional Ω of external potentials ϕ that contains all information about the dynamical properties of the system. In particular, its functional derivatives generate successively the single-particle phase-space density f and all the correlation and density response functions, which are coupled through an infinite hierarchy of evolution equations. Traditional renormalization techniques (involving Legendre transform and vertex functions) are then used to perform the closure of the hierarchy through memory functions. The latter satisfy functional equations that can be used to devise systematic approximations that automatically imply the conservation laws of mass, momentum and energy. The present formulation can be equally regarded as (i) a generalization to dynamical problems of the density functional theory of fluids in equilibrium and (ii) as the classical mechanical counterpart of the theory of non-equilibrium Green's functions in quantum field theory. It unifies and encompasses previous results for classical Hamiltonian systems with any initial conditions. For equilibrium states, the theory reduces to the equilibrium memory function approach used in the kinetic theory of fluids in thermal equilibrium. For non-equilibrium fluids, popular closures of the BBGKY hierarchy (e.g. Landau, Boltzmann, Lenard-Balescu-Guernsey) are simply recovered and we discuss the correspondence with the seminal approaches of Martin-Siggia-Rose and of Rose and we discuss the correspondence with the seminal approaches of Martin-Siggia-Rose and of Rose.

Keywords Kinetic theory · Closure · Renormalization · Effective action · Schwinger closed-time contour

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1 Introduction

The present paper elaborates the foundations of a unifying approach for the construction of renormalized kinetic equations of classical systems of particles in and out of equilibrium. The statistical dynamics is formulated in terms of self-consistently determined single-particle phase-space distribution function, density response, correlation and memory functions. The memory functions satisfy a functional equation that can be used to devise systematic renormalized perturbative approximations in powers of the bare interparticle interaction. Important topical applications include the generalization of the Boltzmann equation to dense gases and liquids, the kinetic theory of strongly coupled plasmas and Hamiltonian systems in general, the proper macroscopic description of fluids beyond the Navier-Stokes equations, and the physics of plasma turbulence.

Before embarking on the detailed description of the theory, we recall a few of the most striking developments and unresolved issues in kinetic theory that motivated this work.

1.1 Background

Kinetic theory attempts to carry out a complete statistical description of the macroscopic dynamics of fluids in terms of the underlying microscopic interactions of its constituents. The foundation of modern kinetic theory dates back to 1872 when Boltzmann published his famous equation for the single-particle distribution function for dilute gases [1–3]. The solution of the Boltzmann equation, derived independently by Chapman and Enskog around 1915, achieved two basic goals of kinetic theory. That is, it (i) established the connection between the microscopic dynamics and the macroscopic equations of hydrodynamics and (ii) provided explicit expressions for the transport coefficients in terms of the molecular parameters. Unfortunately, since it is based on the assumption of uncorrelated binary collisions, the Boltzmann equation gives a satisfactory description of the behavior of sufficiently low density gases with short-range interactions only, and is inadequate to describe dense gases, liquids and plasmas.

The generalization of the Boltzmann equation to more dense fluids and to plasmas confronts the full complexity of a highly correlated many-body problem. This became very clear when, in the early 1960's,¹ it was realized that all the remarkable developments made until then, which were based on some form of perturbation theory of the Liouville equation or the BBGKY hierarchy, were plagued by unphysical divergences [7, 8].² Those findings, together with others permitted by the advent of computer simulations, shifted attention towards the development of a renormalization (regularization) procedure, which would encompass the “theoretical” divergences and take proper account of the correlated collisions, whereby particles interact via the effective (renormalized) potential that integrates the average effects

¹Detailed surveys and references to original publications of the post-war developments until the late 1960's and beyond can be found in [4–6] and in [7, 8].

²The search for the generalization of the Boltzmann equation has a long and rich history (see footnote 1). It is only after about 1946, under the impetus of Bogolyubov's ideas, that concentrated efforts to generalize the Boltzmann equation systematically to higher densities was undertaken. Starting with the Liouville equation, a method was worked out, notably by Bogolyubov, Choh and Uhlenbeck, Green and Cohen and others, which amounts to a systematic inclusion of many-body collisions through a density expansion similar to the virial expansion for computing equilibrium properties of dense gases. In the mid 60's, it was realized that the density expansion of the collision operator was plagued by divergences. While it may in principle be possible to deal with divergences by isolating and resumming the most secular terms of the virial expansion, the exceeding complexity of the procedure has severely restricted the usefulness of the density expansion in understanding the properties of even moderately dense gases—let alone dense gases and liquids.

of the medium on the bare interactions.^{3,4} Additionally, such a theory should yet retain the desirable properties of the Boltzmann equation and be tractable for practical calculations.

Such a renormalized kinetic theory was first presented by Mazenko in 1974 using the memory function approach [13]. His so-called “fully renormalized” theory applies only to fluids in or near thermal equilibrium by means of the fluctuation-dissipation theorem. At equilibrium, the distribution function f is known (the Maxwell-Boltzmann distribution) and the statistical dynamics is encoded in the equilibrium two-point time-correlation function $C_{eq}(1, 1')$ of the microscopic phase-space density. It was shown in the 1960's⁶ that an exact evolution equation for C_{eq} can be written in the form of a generalized Langevin equation in terms of a memory function kernel Σ_{eq} . Mazenko devised an iterative scheme that can be used to develop systematic renormalized approximations of Σ_{eq} .

The development of a renormalization procedure that can describe non-equilibrium states faces additional challenges.⁷ A first major development in that direction was done in 1973 by Martin, Siggia and Rose (MSR) [15]. MSR elaborated a procedure to derive self-consistent approximations for calculating the statistical dynamical properties of a classical random variable or field whose time dependence is governed by a nonlinear differential evolution equation. In other words, they devised a solution to the ubiquitous statistical closure problem, which occurs as a consequence of the statistical averages and the non-linearity of the fundamental evolution equation. Noting that satisfactory approaches to the closure problem had been successfully developed in quantum field theory, MSR recast the classical problem

³The appearance of such divergences has several remarkable consequences. Firstly, they imply that the density dependence of the transport coefficients is non-analytic (e.g. it has logarithmic contributions). Secondly, they suggest that the relation between applied gradients and induced hydrodynamic fluxes in non-equilibrium thermodynamics is non-analytic in character, which leads one to wonder on the proper macroscopic description of a fluid beyond the Navier-Stokes equations at large values of the gradients. Thirdly, they show that correlations in the particles positions and velocities play an important role in the physical properties even in low density gases. The slow, non-exponential decay of the equilibrium time-correlation functions associated with linear transport coefficients discovered around 1968 with molecular dynamics simulations is one of the dramatic effect of correlations in dense fluids. The physical origin of those so-called long time tails is sometimes referred to as vortex diffusion and occurs through so-called mode-coupling effects. The latter occurs when a tagged particle in the fluid creates, through collisions with and between the surrounding particles, a back flow of momentum through the fluid, which ultimately returns to the tagged particle. At liquid density, correlations lead to other dramatic effects. The concepts of mean-free path and of collision time cease to have a clear meaning, and the motion of individual particles is dominated by cage diffusion: owing to pronounced structural correlations, each particle finds itself trapped for some period of time in the cage formed by its immediate neighbors, rebounding against it and thereby slowing down the diffusive motion. Cage diffusion is key to understand the “universal” Stokes-Einstein relation between self-diffusion and viscosity or the Arrhenius law satisfied by the viscosity.

⁴The need for renormalization techniques was long recognized in plasmas physics, where the long-range character of the Coulomb interaction yields to screening of the interaction. While in 1936 Landau⁵ regularized the Boltzmann equation to deal with the Coulomb potential by introducing ad-hoc cutoffs, in 1960, Lenard, Balescu and Guernsey (LBG) independently derived [10–12] an equation from first principles using a systematic ordering of the correlation in terms of the plasma parameter. The Lenard-Balescu-Guernsey equation describes the dynamics of charges undergoing binary collisions in their screened interactions.

⁵Reference [9]: Landau derived his equation from the Boltzmann equation but the Landau equation can also be derived systematically by a perturbation theory [8].

⁶Very good introduction to the equilibrium kinetic theory of fluids with references to seminal papers can be found in [34, 35].

⁷Reference [14]: This review paper on plasma turbulence actually also contains a wealth of information on modern theories of statistical dynamics, renormalization and closures and its relationships to other fields of physics. It is also a very rich source of references to the literature on the subject. Both versions of MSR, namely the operator and functional integral formalisms are presented.

into a quantum-mechanical-looking problem and borrowed techniques of quantum field theory to derive a renormalized perturbation theory. To accomplish the recast, MSR introduced an additional field operator that does not commute with the fundamental field and allows the calculation of both correlation functions and response functions simultaneously, where the latter describe the response of the fluid to the injection of particles.

Although the basic problem in kinetic theory also amounts to a closure problem, it was then recognized that its specificities did not fit into the framework of MSR theory; in particular, its natural field variable, the microscopic single-particle phase-space density, is discrete, singular and its statistics is strongly non-Gaussian. In 1979, Rose [16] developed another approach specifically for dealing with kinetic theory. Like MSR, Rose also recast the basic problem in a quantum-mechanical form but this time using an occupation number representation in classical phase-space [17]. The response to the injection of particles included in MSR is naturally incorporated here. The implications of Rose's paper to kinetic theory have not yet been fully explored. In addition, Rose points out that the steps necessary to reduce his general formalism to Mazenko's theory of fluids in thermal equilibrium are not apparent.

Finally, very recently, Mazenko⁸ published a new fundamental "theory of statistical particle dynamics that solves the chronic problem of self-consistency". In that paper, the theory is presented for the Smoluchowski dynamics and the author announces that its extension to Newtonian dynamics is under way. From the information available in [18], it is likely that the approach presented here is still different from Mazenko's new theory.

1.2 Present Work

In this paper, we present an alternative, arguably simpler and elegant approach to the derivation of renormalized kinetic equations for classical fluids that applies to *both* equilibrium and non-equilibrium states and encompasses the previous works on this topic. For simplicity of the exposition, we shall consider a system of identical point particles mutually interacting via a pair-wise additive central potential; however, no peculiar assumption is made on its range and strength, so the theory can be applied to investigate systems ranging from neutral liquids with short-range interactions to classical plasmas with the Coulomb interaction. Moreover, the theory is derived independently of the nature of initial state of the system, and the influence of initial correlations on the system dynamics, usually neglected or difficult to include in the previous works, is treated explicitly.

A *closed, self-consistent* set of evolution equations for the phase-space density $f(\mathbf{r}, \mathbf{p}, t)$, the two-point correlation function C , and the retarded and advanced response functions $\chi^{R,A}$ is derived in terms of time history integrals that involve three memory functions $\Sigma^{R,A,C}$. Loosely speaking, the correlation and response functions describe the dynamics of emission and absorption of phase-space density fluctuations in the fluid, which in turn determine the effect of collisions on the dynamics of the distribution function f . The memory response functions describe how many-body effects affect, i.e. renormalize, the time-dependent propagation and lifetime of density fluctuations, and as such play a role similar to self-energies in quantum field-theory.

To obtain this closure, we construct an action functional $\tilde{\Omega}[\phi]$ of external potentials ϕ that contains all information about the dynamical properties of the fluid. In particular, its derivatives with respect to ϕ successively generate the phase-space density f and all the correlation and response functions. The latter are coupled through an infinite hierarchy of

⁸This paper also gives a very informative introduction to many other aspects of classical statistical dynamics.

evolution equations, which subsumes the traditional BBGKY equations. The hierarchy is formally closed using traditional closure (renormalization) techniques involving the Legendre transform $\tilde{\Gamma}[f] = -\tilde{\Omega}[\phi] + \int \phi f$ of the effective action $\tilde{\Omega}[\phi]$.

The basis of the present approach is the extension to classical systems of the closed-time contour idea originally introduced in 1961 by Schwinger [19] in his seminal paper on the Brownian motion of a quantum particle. Schwinger's idea was later fruitfully used to develop the theory of non-equilibrium Green's functions in quantum field theory [20, 21]. Two fully equivalent formulations of the theory are presented. In the first formulation, the theory is expressed in terms of time-dependent quantities taking their values on the closed-time contour. The effective action $\tilde{\Omega}[\phi]$ is a functional of external potentials ϕ that linearly couples along the closed-time contour to the single-particle phase-space density. The first functional derivative with respect to ϕ generates the phase-space distribution function $f = \delta\tilde{\Omega}/\delta\phi$ and the second derivative $\delta^2\tilde{\Omega}/\delta\phi^2$ equals a quantity that combines both the two-point correlation function C and the density response functions $\chi^{R,A}$. In the second formulation, the theory is recast into a form that *directly* generates the physical quantities of interest. The effective action is written as a functional of two external potentials, $\Omega[\phi_p, \phi_\Delta]$, of the physical time variable t and has the remarkable derivatives $f = \frac{\delta\Omega}{\delta\phi_\Delta}$, $C = \frac{\delta^2\Omega}{\delta\phi_\Delta\delta\phi_\Delta}$, $\chi^R = \frac{\delta^2\Omega}{\delta\phi_\Delta\delta\phi_p}$ and $\chi^A = \frac{\delta^2\Omega}{\delta\phi_p\delta\phi_\Delta}$.

The main purpose of this paper is to lay down the general foundations of the theory without reference to a specific physical system or model. Its application to physical problems would require substantial additional work, some of it being under way. The paper is organized as follows. In Sect. 2, the basic definitions and notations are introduced. To provide a self-contained presentation of the work, we recall several basic results of classical statistical mechanics that are used thereafter. The original contributions of this work really begin into Sect. 3 where we develop the closed-time formulation of our theory and continue in Sects. 4 and 5 where we recast the results into equations that involve quantities depending on the physical time. For clarity, the details of the proofs of the calculations are given in Appendices A–I. Throughout these sections, we discuss the implications and merits of the new approach presented. We study the special case of a fluid at equilibrium, make contact with Mazenko's renormalized theory, show the correspondence with popular kinetic equations (Landau, Boltzmann, Lenard-Balescu-Guernsey), and study the correspondence with MSR and Rose's theories. Also the present approach naturally shed light on analogies and differences between quantum and classical kinetic theory, which we highlight throughout the paper and in Appendices A–I. The comparison allows us (i) to comprehend the longer resistance of classical statistical mechanics to renormalization, and (ii) to justify some of the ingenious approaches used by previous works like MSR. For convenience, a summary of the main components of the theory is given in Sect. 6.

2 Basic Definitions

In this section, we introduce the physical systems under consideration and recall several basic notions of statistical dynamics used thereafter such as the correlation functions, the linear response functions to external perturbations, and the closure problem. Most of the material is discussed in textbooks, e.g. [8, 22], and is recalled here for completeness. The reader already familiar with these notions may wish to skip ahead to Sect. 3 where the original contribution of this paper begins.

2.1 Physical System

We consider a system consisting of N identical point-particles of mass m enclosed in a volume V of the d -dimensional space \mathbb{R}^d . We assume that the system dynamics is governed by the laws of classical mechanics under the total, possibly time-dependent Hamiltonian H_{tot} . Thus, the position $\mathbf{r}_j(t)$ and momentum $\mathbf{p}_j(t)$ of the j -th particle at a time t evolve according to the Hamilton equations,

$$\frac{d\mathbf{r}_j}{dt} = \frac{\partial H_{tot}(x, t)}{\partial \mathbf{p}_j}, \quad \frac{d\mathbf{p}_j}{dt} = -\frac{\partial H_{tot}(x, t)}{\partial \mathbf{r}_j}, \tag{1}$$

where $x = (\mathbf{r}_1, \dots, \mathbf{r}_N; \mathbf{p}_1, \dots, \mathbf{p}_N) \in V^N \times \mathbb{R}^{dN}$. These equations (1) are to be solved subject of $2dN$ initial conditions on the coordinates and momenta $x(t_0) = x_0$ at an initial time t_0 .

We assume that the initial state x_0 of the system is imperfectly known but can be characterized by a distribution $F_0(x_0)$ defined such that $F_0(x_0)dx_0$ is the probability that the system is initially in a microscopic state represented by a phase-space point of volume dx_0 around x_0 . Most importantly, the present theory is derived independently of the nature of initial distribution F_0 ; it is just assumed F_0 to be normalized, i.e. $\int dx_0 F_0(x_0) = 1$.

We are thus interested in the dynamics at time $t \geq t_0$ of a statistical ensemble of independent systems, each of which is a replica of the system defined above, and initially distributed according to a given F_0 ; the dynamics prior to the initial time t_0 is not of interest to us. The uncertainty on the initial conditions will be the only element of statistics in the present theory. Once the non-equilibrium initial state is specified, the time-evolution is deterministic and completely determined by the Hamiltonian.

As time increases, the initial distribution of states F_0 evolves into the distribution $F(x, t)$ at $t \geq t_0$ according to Liouville equation,

$$\frac{\partial}{\partial t} F(x, t) = [H_{tot}, F]_{PB}(x, t), \tag{2}$$

where $[A, B]_{PB}$ denotes the N -particle Poisson bracket

$$[A, B]_{PB} = \sum_{j=1}^N \left(\frac{\partial A}{\partial \mathbf{r}_j} \cdot \frac{\partial B}{\partial \mathbf{p}_j} - \frac{\partial A}{\partial \mathbf{p}_j} \cdot \frac{\partial B}{\partial \mathbf{r}_j} \right).$$

We assume that the total Hamiltonian can be written as

$$H_{tot}(x, t) = H_N(x) + H_{ext}(x, t). \tag{3}$$

The time-independent term H_N characterizes the system in the absence of external, time-dependent perturbations, and is of the form,

$$\begin{aligned} H_N(x) &= \sum_{j=1}^N \left(\frac{\mathbf{p}_j^2}{2m} + v_0(\mathbf{r}_j) \right) + \frac{1}{2} \sum_{i \neq j=1}^N v(|\mathbf{r}_i - \mathbf{r}_j|) \\ &= \sum_{j=1}^N h_0(\mathbf{r}_j, \mathbf{p}_j) + \frac{1}{2} \sum_{i \neq j=1}^N v(|\mathbf{r}_i - \mathbf{r}_j|). \end{aligned} \tag{4}$$

The particles interact according to a pair-wise additive central potential $v(r)$ and the whole system is possibly confined by a static potential $v_0(\mathbf{r})$. Throughout the paper, no peculiar

assumption is made on the range and strength of the interaction potential v other than being differentiable for $r > 0$. In particular, the theory applies to both short-range potentials as encountered in neutral liquids [23] and also to the long-range, Coulomb potential of importance to plasma physics; in the latter case, a background potential may be included in v_0 to ensure electrical neutrality [24].

The term H_{ext} in (3) represents the possible interaction to an external, time-dependent perturbation $\phi_0(\mathbf{r}, \mathbf{p}, t)$,

$$H_{ext}(x, t) = \sum_{j=1}^N \phi_0(\mathbf{r}_j, \mathbf{p}_j, t) = \iint d\mathbf{r} d\mathbf{p} N(\mathbf{r}, \mathbf{p}, t) \phi_0(\mathbf{r}, \mathbf{p}, t), \quad (5)$$

which linearly couples to the phase-space density $N(\mathbf{r}, \mathbf{p}, t)$ (see (7) below).

The general definitions given above encompass a large class of systems, including for instance (i) the dynamics of a fluid at equilibrium when $H_{ext} \equiv 0$ and $F_0 = f_{eq}$ is an equilibrium (Gibbs) distribution function, (ii) the relaxation dynamics to equilibrium when $F_0 \neq f_{eq}$ and $H_{ext} \equiv 0$, (iii) the out-of-equilibrium dynamics of a fluid in the presence of time-dependent fields when $H_{ext} \neq 0$.

2.2 Closure Problem, Correlation and Response Functions

2.2.1 Fundamental Field Variable and Correlation Functions

A dynamical variable is a quantity A that depends parametrically on the particles' trajectory $x(t)$, and therefore on the initial condition x_0 . As a consequence of the statistical description, A no longer has a definite value but is instead characterized by its average over all possible initial conditions weighted by F_0 ,

$$\langle A \rangle(y) = \int dx_0 F_0(x_0) A(x_0; y); \quad (6)$$

here y denotes the possible dependence on other parameters.

A fundamental dynamical variable in classical kinetic theory is the microscopic single-particle phase-space density

$$N(\mathbf{r}, \mathbf{p}, t) = \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j(t)) \delta(\mathbf{p} - \mathbf{p}_j(t)), \quad (7)$$

where $(\mathbf{r}, \mathbf{p}) \in V \times \mathbb{R}^d$. The density $N(\mathbf{r}, \mathbf{p}, t)$ plays a role similar to a field in field theory or of a random variable in the theory of stochastic processes; here $N(\mathbf{r}, \mathbf{p}, t)$ is random in that its value varies due to its sensitivity to initial conditions. The ensemble average of $N(\mathbf{r}, \mathbf{p}, t)$ defines the single-particle distribution function

$$f(\mathbf{r}, \mathbf{p}, t) = \langle N(\mathbf{r}, \mathbf{p}, t) \rangle, \quad (8)$$

and has the meaning of the probability distribution of particles at position \mathbf{r} with momentum \mathbf{p} at time t . For an unconfined fluid ($v_0 = 0$) in thermal equilibrium at temperature T , f is independent of space and time, and reduces to the Maxwell-Boltzmann distribution $f(\mathbf{p}) = ne^{-\mathbf{p}^2/2mk_B T} / (2\pi mk_B T)^{3/2}$ where $n = N/V$ is the particle density. In non-equilibrium fluids, f generally depends on both \mathbf{r} and t .

As is typical in a statistical theory of a random variable $N(1)$, an important role in the theory is played by the fluctuations around its averaged value,

$$\delta N(1) = N(1) - \langle N(1) \rangle = N(1) - f(1), \tag{9}$$

and by the associated n -point correlation functions (or cumulants)

$$C^{(n)}(1, \dots, n) = \langle \delta N(1) \dots \delta N(n) \rangle. \tag{10}$$

For the two-point correlation function, we write $C(1, 2) \equiv C^{(2)}(1, 2)$. Equal-time correlation functions, i.e. $t_1 = \dots = t_n$, will be denoted by a bar as $\bar{C}^{(n)}(x_1, \dots, x_n; t)$.

As was emphasized by Rose [16], a statistical theory based on a discrete (i.e., a sum of delta functions) random variable such as $N(1)$ presents a serious technical difficulty in that it is strongly non-Gaussian, even for non-interacting particles, since the equal-time cumulants $\bar{C}^{(n)}$ are all non-vanishing and singular. Indeed, in terms of the conventional n -particle correlation g_n introduced in kinetic theory from the cluster expansion of the reduced distribution functions (see Appendix A), we have

$$\bar{C}^{(2)}(X, X', t) = \delta(X - X')f(X, t) + g_2(X, X'; t) \tag{11}$$

and

$$\begin{aligned} \bar{C}^{(3)}(X, X', X''; t) &= \delta(X - X')\delta(X' - X'')f(X, t) \\ &+ [\delta(X - X')g_2(X', X''; t) + \text{cyclic permutations}] \\ &+ g_3(X, X', X''; t) \end{aligned} \tag{12}$$

and so on, with $X = (\mathbf{r}, \mathbf{p})$. Thus, even in the absence of three-particle correlations ($g_3 = 0$), the three-point cumulant is non-vanishing because of particle self-correlations, and this remains true at all times $t \geq t_0$. This result precludes the applicability the Wick theorem so useful in conventional statistical field theories.

2.2.2 Field Equation and Closure Problem

For convenience we introduce the shorthand notation in which a field point and the time variable are designated by a single number, i.e. $n \equiv (\mathbf{r}_n, \mathbf{p}_n, t_n)$ (not to be confused with the particle labels n); for $n = 1$, we often drop the subscript so that $1 = (\mathbf{r}, \mathbf{p}, t)$. The delta function $\delta(1 - 2)$ denotes $\delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2)\delta^{(3)}(\mathbf{p}_1 - \mathbf{p}_2)\delta(t_1 - t_2)$.

From the Hamilton equations (1), it is straightforward to show that the phase-space density evolves according to

$$\frac{\partial}{\partial t_1} N(1) = L_1 N(1) + \int d2 L_{12} N(1) N(2),$$

where the summation is defined as

$$\int d1 \dots = \int_V d\mathbf{r}_1 \int_{\mathbb{R}^d} d\mathbf{p}_1 \int_{t_0}^{\infty} dt_1 \dots$$

Here,

$$L_1 \bullet = \frac{\partial h(1)}{\partial \mathbf{r}_1} \cdot \frac{\partial \bullet}{\partial \mathbf{p}_1} - \frac{\partial h(1)}{\partial \mathbf{p}_1} \cdot \frac{\partial \bullet}{\partial \mathbf{r}_1} = \{h, \bullet\}(1) \tag{13}$$

is the single particle part of the Liouville operator with the total single-particle Hamiltonian $h = h_0 + \phi_0$. In the second line of (13), it is expressed in terms of the single-particle Poisson bracket

$$\{a, b\}(\mathbf{r}, \mathbf{p}) = \frac{\partial a}{\partial \mathbf{r}} \cdot \frac{\partial b}{\partial \mathbf{p}} - \frac{\partial a}{\partial \mathbf{p}} \cdot \frac{\partial b}{\partial \mathbf{r}}, \tag{14}$$

for any function $a(\mathbf{r}, \mathbf{p})$ and $b(\mathbf{r}, \mathbf{p})$ in R^{2d} (note the curly brackets notation to avoid confusion with the N -particle Poisson bracket $[\cdot, \cdot]_{PB}$ defined earlier). Finally,

$$L_{12}\bullet = \frac{\partial}{\partial \mathbf{r}_1} \tilde{v}_{12} \cdot \left(\frac{\partial \bullet}{\partial \mathbf{p}_1} - \frac{\partial \bullet}{\partial \mathbf{p}_2} \right) \tag{15}$$

is the interaction part of the Liouville operator with $\tilde{v}_{12} = v(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$. Those notations are in widespread use in the literature on classical kinetic theory. In the theory presented below, however, it will be more convenient to rewrite (13) as

$$\begin{aligned} \left(\frac{\partial}{\partial t_1} - L_1 \right) N(1) &= \frac{1}{2} \int d2 \int d3 \gamma_3(1, 2, 3) N(2) N(3) \\ &= \frac{1}{2} \gamma_3(1, 2, 3) N(2) N(3) \end{aligned} \tag{16}$$

in terms of the “bare interaction vertex”,

$$\begin{aligned} \gamma_3(1, 2, 3) &= \frac{\partial}{\partial \mathbf{p}_1} \cdot (\mathbf{w}_{12}\delta(1 - 3) + \mathbf{w}_{13}\delta(1 - 2)), \\ \mathbf{w}_{12} &= \frac{\partial}{\partial \mathbf{r}_1} \tilde{v}_{12} \end{aligned} \tag{17}$$

which is symmetric in its last two arguments. The second line of (16) illustrates the summation convention over repeated indices of dummy variables that we shall use throughout the paper.

Averaging (16) over the initial conditions, we obtain the equation of evolution of the phase-space distribution $f(1)$,

$$\left[\frac{\partial}{\partial t_1} - L_1 \right] f(1) - \{u^{mf}(1), f(1)\} = \frac{1}{2} \gamma_3(1, 2, 3) C(2, 3), \tag{18}$$

where u^{mf} is the mean-field (a.k.a. Vlasov) potential

$$u^{mf}(\mathbf{r}, t) = \int d2 f(2) \tilde{v}(1 - 2). \tag{19}$$

Equation (18) couples $f(1)$ to the (equal-time) two-point correlation function $C(1, 2)$, and corresponds to the first equation of the ordinary BBGKY hierarchy; the right-hand side (rhs) is usually referred to as the collision integral. Similarly, as a consequence of the quadratic non-linearity of the field equation (16), the evolution of $C^{(n)}$ at each order n involves the next higher-order correlation $C^{(n+1)}$; those equations can be straightforwardly derived using the equation for the density fluctuations δN obtained by subtracting (16) and (18). Thus, for the two-point correlation function, we find

$$\left[\frac{\partial}{\partial t_1} - L_1 \right] C(1, 1') - \Sigma^{mf}(1, 2) C(2, 1') = \frac{1}{2} \gamma_3(1, 2, 3) C^{(3)}(2, 3, 1')$$

Table 1 The most popular closures of classical statistical physics amount, among additional hypothesis, to replace (11)–(12) for $\bar{C}^{(2),(3)}$ by the terms displayed in the table. Those approximations usually neglect the n -particle correlation functions g_n with $n \geq 3$, which is inappropriate whenever correlations are strong. One of the challenge of kinetic theory is to incorporate the effects of those neglected terms in a self-consistent manner. For comparison, the term g_2 kept in the Lenard-Balescu-Guernsey (LBG) equation but discarded in the Boltzmann equation allows the renormalization of the bare interaction into a dynamically screened two-particle interaction between the particles of the plasma. On the contrary, the contribution to $\bar{C}^{(3)}$ kept in the Boltzmann approximation but discarded in the Lenard-Balescu-Guernsey equation, is responsible for the bare two-particle interactions (large-angle scattering) describing the two-body collision in a dilute gas

Closure	$\bar{C}^{(2)}$	$\bar{C}^{(3)}$
Vlasov	0	0
Landau	$\delta(x - x')f(x, t)$	0
Boltzmann	$\delta(x - x')f(x, t)$	$[\delta(x - x')g_2(x', x''; t) + c.p.]$ $+ \delta(x - x')\delta(x' - x'')f(x, t)$
LBG	$g_2(x, x'; t) + \delta(x - x')f(x, t)$	0
Book-Frieman [36]	$g_2(x, x'; t) + \delta(x - x')f(x, t)$	$[\delta(x - x')g_2(x', x''; t) + c.p.]$ $+ \delta(x - y)\delta(y - z)f(x, t)$

where

$$\Sigma^{mf}(1, 1') = \gamma_3(1, 2, 3)f(2)\delta(1' - 3). \tag{20}$$

The hierarchy of evolution equations for the $C^{(n)}$ is different from the ordinary BBGKY hierarchy, which instead involves the correlation functions g_n (a quick summary of BBGKY is given in Appendix A). The BBGKY can be recovered by considering the equal-time limit of the equations for the $C^{(n)}$'s. The “simplest” closures of the BBGKY hierarchy lead to the most famous kinetic equations, in particular the Vlasov equation, the Landau equation (see footnote 5) for so-called weakly-interacting gases, the Boltzmann equation [1] for dilutes gases, and the Lenard-Balescu-Guernsey equation [10–12] for weakly-coupled plasmas. Those closures rely, among additional hypothesis, on a systematic ordering of the correlations g_n in terms of an adequately chosen small parameter [8]. As summarized in Table 1, each closure amounts to keeping only certain contributions in (11)–(12). In particular, these popular closures neglect the n -particle correlation functions g_n with $n \geq 3$, which is inappropriate whenever correlations are strong. A major challenge of kinetic theory is to incorporate the effects of those neglected terms in a self-consistent manner. In Sect. 4.5, we shall see how the present theory addresses the problem.

2.2.3 Linear Response Functions and Fluctuation-Dissipation Theorem

We now consider the linear response of the system defined above to weak, external perturbations ϕ that couples linearly to the single-particle density $N(X, t)$ as

$$H_{pert}(\mathbf{r}, \mathbf{p}, t) = \int d\mathbf{r}d\mathbf{p}N(\mathbf{r}, \mathbf{p}, t)\delta\phi(\mathbf{r}, \mathbf{p}, t).$$

By linearizing with respect to $\delta\phi$ the Liouville equation (2) with H_{tot} replaced by $H_{tot} + H_{pert}$, we find that to first order in the external perturbation the phase-space distribution

$f(\mathbf{r}, \mathbf{p}, t)$ is modified from its value in the absence of perturbation by the amount,

$$\delta f(1) = \int d1' \chi^R(1; 1') \delta \phi(1'),$$

in term of the retarded response function,

$$\chi^R(1, 1') = \frac{\delta f(1)}{\delta \phi(1')} = \theta(t - t') \theta(t' - t_0) \langle [N(1), N(1')]_{PB} \rangle, \quad (21)$$

for all $t, t' \geq t_0$. The retarded response function is not symmetrical in its arguments but instead $\chi^R(1', 1) = \chi^A(1, 1')$, where χ^A is the *advanced* response function,

$$\chi^A(1; 1') = -\theta(t' - t) \theta(t - t_0) \langle [N(1), N(1')]_{PB} \rangle. \quad (22)$$

In the Poisson bracket, $N(1)$ is evaluated along the unperturbed trajectory governed by H_{tot} (interaction representation). Other useful properties of $\chi^{R,A}$ are given in Appendix B.

The two-point correlation C and response functions $\chi^{R,A}$ play a fundamental role in the present theory. The correlation function gives information about the likelihood of fluctuations in the fluid and determines the effect of particle encounters in the collision integral of (18). The response functions carry the dynamical information on how fluctuations are propagated in time. In classical mechanics, those functions are related to averages of dynamical variables of different nature, namely the averaged *product* of field variables for C and their averaged *Poisson bracket* for $\chi^{R,A}$. This result is to be contrasted with the equivalent result in quantum mechanics where both correlation and response functions are related to the average of products of the same dynamical variables, on which more is said later.

Only for the special case of a system in thermal equilibrium ($F_0 = f_{eq}$ and $H_{ext} \equiv 0$), the response and correlation function are simply related according to

$$\chi^R(1, 1') = \beta \theta(t - t') \theta(t' - t_0) \frac{d}{dt'} C(1, 1'),$$

with $\beta = 1/k_B T$. This result is known as the fluctuation-dissipation theorem.⁹

3 Renormalization on the Closed-Time Contour

The present theory is based on the definition of a generating functional $\tilde{\Omega}[\phi]$ that contains all the information about the dynamics under investigation. Here ϕ represents some external time-dependent potential, which perturbs the system and, just like ϕ_0 in (5), couples linearly to the microscopic phase-space density in the total Hamiltonian. The functional is designed such that its derivatives with respect to ϕ generate the phase-space distribution f , the correlation and response functions C and $\chi^{R/A}$ of the system.

The functional $\tilde{\Omega}[\phi]$ plays a role similar to the grand-potential $\Omega[v_0]$ in the density functional theory of classical fluids used to study their static properties [23]; in this case,

⁹With $t_0 \rightarrow -\infty$, all dynamical quantities are time-translational invariant, e.g. $\chi^R(1, 1') = \chi^R(X, t - t'; X', 0) \equiv \chi^R(X, X'; t - t')$ and the fluctuation-dissipation theorem reads

$$\chi^R(X, X'; t) = -\beta \theta(t) \frac{d}{dt} C(X, X'; t).$$

the first derivative with respect to the confining potential v_0 gives the particle density $\delta\Omega[v_0]/\delta v_0(\mathbf{r}) = \rho(\mathbf{r})$ and the second derivative equals the density correlation function $\delta\Omega[v_0]/\delta v_0(\mathbf{r})\delta v_0(\mathbf{r}') = \langle \delta\rho(\mathbf{r})\delta\rho(\mathbf{r}') \rangle_{eq}$ [23]. The existence of such a generating functional for the calculation of dynamical properties is far from obvious. For instance, if one imagines a straightforward extension of the static theory in which $\tilde{\Omega}[\phi_0(1)]$ is a functional of time-dependent external potentials $\phi_0(\mathbf{r}, \mathbf{p}, t)$ that generates the phase-space density $\delta\tilde{\Omega}/\delta\phi_0(1) = f(1)$, one is immediately led to a contradiction. Indeed, the symmetry of the second-order derivative requires

$$\frac{\delta}{\delta\phi_0(2)} \frac{\delta\tilde{\Omega}}{\delta\phi_0(1)} = \frac{\delta}{\delta\phi_0(1)} \frac{\delta\tilde{\Omega}}{\delta\phi_0(2)},$$

while causality requires

$$\frac{\delta}{\delta\phi_0(2)} \frac{\delta\tilde{\Omega}}{\delta\phi_0(1)} = \frac{\delta f(1)}{\delta\phi_0(2)} = \chi^R(1, 2) \neq \chi^R(2, 1)$$

since, say when $t_1 > t_2$, $\chi^R(1, 2) = \langle [N(1), N(2)]_{PB} \rangle$ and $\chi^R(2, 1) = 0$ (see (21)). Both requirements could never be satisfied together and therefore the search for such a functional is doomed to fail.

In order to cope with the problem, we shall define $\tilde{\Omega}$ over a wider set of dynamics using the idea of closed-time contour originally introduced by Schwinger in the early 1960's to deal with quantum systems [19]. Because quantum mechanics propagates probability amplitudes instead of probability densities, the mere notion of closed-time contour arises more manifestly in quantum than in classical mechanics. Thus, if at time $t \geq t_0$ a quantum system is in the state $|\Psi(t)\rangle$, the expectation value of an observable \hat{O} at that time can be expressed as

$$\langle O \rangle(t) = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle \tag{23}$$

$$= \langle \Psi(t_0) | U(t_0, t) \hat{O} U(t, t_0) | \Psi(t_0) \rangle \tag{24}$$

in terms of the propagator $\hat{U}(t, t')$ from time t' to t , and the initial state $|\Psi(t_0)\rangle$ at time t_0 . If we read the time arguments of the propagators in (24) from right to left we may say that the system evolves from t_0 to time t after which the operator \hat{O} acts; then the system evolves back along the real axis from time t to t_0 . Schwinger first noticed that one could imagine that the forward and backward time evolutions are governed by different dynamics (e.g., if a different external potential acts on each branch), and showed how this can be turned into an ingenious device to probe (generate) the properties of the physical system under investigation simply by suitably perturbing its dynamics along the closed-time contour that goes from t_0 to t back to t_0 . The closed-time contour approach was further developed by Keldysh [25] and many others to obtain an elegant and powerful treatment of non-equilibrium quantum systems in terms of non-equilibrium Green's functions [20, 21, 26].

By contrast, in classical mechanics, the expectation value (23) becomes

$$\langle O \rangle(t) = \int dx_0 F(x_0) O(x(t)),$$

and the concept of closed-time contour is much less apparent. Nevertheless, we shall show how a similar idea can be fruitfully developed to the classical case. First we shall define the notions of closed-time contour and extended dynamics. Then we shall use these concepts to define the action functional $\tilde{\Omega}[\phi]$ and investigate its generating properties. Finally we shall show how $\tilde{\Omega}[\phi]$ provides a formal solution to the closure problem.

Fig. 1 Schematic illustration of the closed-time contour. For any time $t \in [t_0, t_M]$, τ_+ is the time on the forward branch c_+ and τ_- is the time on the backward branch c_- of the closed-time contour such that $t = t(\tau_+) = t(\tau_-)$

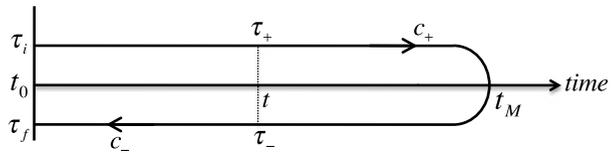
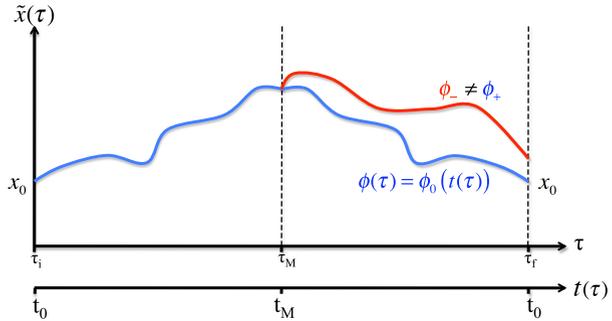


Fig. 2 Illustration of the extended dynamics $\tilde{x}(\tau)$ on the closed-time contour. For a physical potential, the dynamics retraces the forward trajectory on the return branch



3.1 Closed Time Contour

We shall extend the dynamics under investigation along a closed path in time that, as illustrated in Fig. 1, goes from the initial time t_0 to some time t_M in the future and back to the initial time t_0 . The value of t_M can be chosen arbitrarily as long as it is larger than the largest time of interest; for definiteness, we shall set $t_M = +\infty$ in the following. The closed-time contour can be conveniently defined by parameterizing the physical time $t = t(\tau)$ in terms of a time variable τ in such way that if τ runs from an initial τ_i to a final τ_f then $t(\tau)$ monotonically increases from the initial time t_0 to the maximum time t_M at τ_M and then monotonically decreases from t_M back to t_0 .¹⁰ In fact, the chosen parametrization is inconsequential since the final results are independent of it.

In the following, for any physical time $t \in [t_0, t_M]$, we will denote by τ_+ the unique time on the forward branch and τ_- the unique time on the backward branch of the closed-time contour such that $t = t(\tau_+) = t(\tau_-)$. We will also distinguish certain quantities defined on the closed-time contour variable τ by a tilde. Thus we write $\tilde{I} = (\mathbf{r}_1, \mathbf{p}_1, \tau_1) = (X_1, \tau_1)$ or simply $\tilde{I} = (X, \tau)$ when no confusion is possible. In these notations, $\delta(\tilde{I} - \tilde{2}) = \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2)\delta^{(3)}(\mathbf{p}_1 - \mathbf{p}_2)\delta(\tau_1 - \tau_2)$.

3.2 Dynamics on the Closed Time Contour

Let us first imagine that the dynamics $x(t) = \{\mathbf{r}_j(t), \mathbf{p}_j(t)\}_{j=1,N}$ under investigation over the physical time interval $t_0 \leq t \leq t_M$, or equivalently $\tau_i \leq \tau \leq \tau_M$, extends to the backward branch $\tau_M \leq \tau \leq \tau_f$ of the contour in such way that, as illustrated in Fig. 2, the extended

¹⁰A possible parametrization is given by

$$t(\tau) = \begin{cases} \alpha(\tau - \tau_i) + t_0, & \tau_i \leq \tau \leq \tau_M = \frac{\tau_i + \tau_f}{2}, \\ -\alpha(\tau - \tau_M) + t_M, & \tau_M \leq \tau \leq \tau_f \end{cases}$$

with $\alpha = 2(t_M - t_0)/(\tau_f - \tau_i)$.

dynamics retraces backward the *same* phase-space trajectory along $[\tau_M, \tau_f]$. In other words, if $\tilde{\mathbf{r}}_j(\tau)$ and $\tilde{\mathbf{p}}_j(\tau)$ denote the positions and momenta of this extended dynamics, we require that for all $\tau \in [\tau_i, \tau_f]$,

$$\tilde{\mathbf{r}}_j(\tau) = \mathbf{r}_j(t(\tau)), \quad \tilde{\mathbf{p}}_j(\tau) = \mathbf{p}_j(t(\tau)). \tag{25}$$

We stress that this operation is not equivalent to the traditional *time reversal transformation*. Indeed, in the latter case, both the propagation of time and the particles momenta are flipped, i.e. $\mathbf{p}_j \rightarrow -\mathbf{p}_j$, while here only the direction of time is reversed $\tilde{\mathbf{p}}_j(\tau_M^+) = \tilde{\mathbf{p}}_j(\tau_M^-) = \mathbf{p}_j(t_M)$.

By differentiation of (25) with respect to τ , we easily find that the extended dynamics is Newtonian and governed by the Hamiltonian,

$$\mathcal{H}_{\phi_0}(\tilde{\mathbf{x}}, \tau) = t'(\tau) H_{tot}(\tilde{\mathbf{x}}, t(\tau)) = t'(\tau) \left(H_N(\tilde{\mathbf{x}}) + \sum_{j=1}^N \phi_0(\tilde{\mathbf{r}}_j, \tilde{\mathbf{p}}_j, t(\tau)) \right) \tag{26}$$

with $\tilde{\mathbf{x}} = (\tilde{\mathbf{r}}_1, \dots, \tilde{\mathbf{r}}_N; \tilde{\mathbf{p}}_1, \dots, \tilde{\mathbf{p}}_N)$.

We then note that this extended dynamics can be regarded as a special case of a larger set of dynamics on the closed-time contour and characterized by the Hamiltonians

$$\begin{aligned} \mathcal{H}_\phi(\tilde{\mathbf{x}}, \tau) &= t'(\tau) \left(H_N(\tilde{\mathbf{x}}) + \sum_{j=1}^N \phi(\tilde{\mathbf{r}}_j, \tilde{\mathbf{p}}_j, \tau) \right) \\ &= t'(\tau) \left(H_N(\tilde{\mathbf{x}}) + \oint dx d\tau \mathcal{N}(\tilde{\mathbf{x}}, \tau) \phi(\tilde{\mathbf{x}}, \tau) \right) \end{aligned} \tag{27}$$

where ϕ is any external, time-dependent potential defined on the closed-time contour, and

$$\mathcal{N}(\mathbf{r}, \mathbf{p}, \tau) = \sum_{j=1}^N \delta(\mathbf{r} - \tilde{\mathbf{r}}_j(\tau)) \delta(\mathbf{p} - \tilde{\mathbf{p}}_j(\tau))$$

is the single-particle phase-space density. Just like in calculus it is often very useful to consider a real function of the real variable as a complex function of the complex variable, considering the physical dynamics under consideration as an element of the set of extended dynamics will allow us to derive properties of the physical dynamics that are difficult to obtain otherwise.

We can distinguish between two types of external potentials ϕ , namely physical and non-physical potentials; we shall denote physical potentials with a subscript p , e.g. ϕ_p . A *physical potential* is identical on both branches of the contour, i.e. $\phi_p(\tau_+) = \phi_p(\tau_-)$, while a non-physical potential is not. Any potential with real, physical origin such as ϕ_0 in (5), defines a physical potential through $\phi_p(\tau) = \phi_0(t(\tau))$. By construction, under the influence of a physical potential, the extended dynamics retraces its forward trajectory backwards on the return branch of the closed-time contour, while for a non-physical potential, forward and backward trajectories are generally different. Both cases are illustrated in Fig. 2.

3.3 Generating Action Functional

The extended dynamics governed by \mathcal{H}_ϕ can also be described by the Lagrangian

$$\mathcal{L}_\phi(\tilde{\mathbf{r}}, \tilde{\mathbf{v}}, \tau) = \tilde{\mathbf{p}} \cdot \tilde{\mathbf{v}} - \mathcal{H}_\phi(\tilde{\mathbf{r}}, \tilde{\mathbf{p}}, \tau), \tag{28}$$

with the velocity $\tilde{v} = d\tilde{r}/d\tau$ and the short-hand notation $\tilde{r} = (\tilde{\mathbf{r}}_1, \dots, \tilde{\mathbf{r}}_N)$.

Given an initial condition x_0 and the corresponding trajectory $(\tilde{r}(\tau), \tilde{v}(\tau))$, we define the total action over the closed-time contour as

$$\mathcal{S}[\phi; x_0] = \int_{\tau_i}^{\tau_f} d\tau \mathcal{L}_\phi(\tilde{r}(\tau), \tilde{v}(\tau), \tau) - \mathcal{S}_b[\phi, x_0] \quad (29)$$

$$= \int_{-\infty}^{+\infty} d\tau \Pi(\tau) \mathcal{L}_\phi(\tilde{r}(\tau), \tilde{v}(\tau), \tau) - \mathcal{S}_b[\phi, x_0], \quad (30)$$

with the boundary term,

$$\mathcal{S}_b[\phi, x_0] = \frac{1}{2} (\tilde{p}(\tau_i) + \tilde{p}(\tau_f)) (\tilde{r}(\tau_i) - \tilde{r}(\tau_f)).$$

The role of \mathcal{S}_b is to cancel boundary terms that arise when performing the variations of the first term with respect to ϕ . In the second line, we include the integration range $[\tau_i, \tau_f]$ in the integrand through the “window” function

$$\Pi(\tau) = \theta(\tau - \tau_i) \theta(\tau_f - \tau) = \theta(\tau - t_0) \quad (31)$$

where θ is the (Heaviside) step function¹¹ so that $\Pi(\tau) = 1$ when $\tau_i < \tau < \tau_f$ and $\Pi(\tau) = 0$ when $\tau < \tau_i$ or $\tau > \tau_f$. As we shall see, this apparently insignificant rewriting of (29) in fact allows us to self-consistently include the contribution of initial conditions within the theory.

We then define the effective action functional $\tilde{\Omega}[\phi]$ such as

$$e^{-\frac{i}{s} \tilde{\Omega}[\phi]} = \langle e^{\frac{i}{s} \mathcal{S}[\phi; x_0]} \rangle = \mathcal{Z}[\phi], \quad (32)$$

where we recall that $\langle \dots \rangle$ denotes the average of the initial conditions x_0 as in (6). Here s is a fixed parameter with the dimension of an action, or energy times time, to make the exponent dimensionless. Its value may be set to the quantum of action \hbar if one regards $e^{\frac{i}{\hbar} \mathcal{S}[\phi; x_0]}$ as the classical contribution to the total quantum amplitude to go from points $\tilde{x}(\tau_i) = x_0$ to $\tilde{x}(\tau_f)$ [27]. However the identification $s = \hbar$ is not required since (32) could also be defined without reference to its quantum origin. Accordingly, we find that the actual value of s is inconsequential since all the general results derived from (32) are independent of it. (The situation here is reminiscent of the problem encountered in the early days of classical statistical mechanics [28], where an arbitrarily chosen size h_0 of the unit cell in phase-space was introduced in order to count the accessible classical states; while the physical laws were not affected by the value of h_0 , the arbitrariness was later removed using the principles of quantum mechanics, leading to $h_0 = \hbar$.) It may for instance be useful to chose s to be purely imaginary, $s \rightarrow is$, and write

$$\tilde{\Omega}[\phi] = -s \ln \mathcal{Z}[\phi] = -s \ln \langle e^{\frac{1}{s} \mathcal{S}[\phi; x_0]} \rangle$$

in order to circumvent difficulties related to complex logarithms, to ensure nice properties of the effective action (e.g. convexity), etc.; we shall not delve into these technical points here.

¹¹The Heaviside step function is defined as

$$\Theta(\tau) = \begin{cases} 1 & \tau \geq 0, \\ 0 & \tau < 0. \end{cases}$$

We remark that the action functional vanishes at any physical potential ϕ_p ,

$$\tilde{\Omega}[\phi_p] = 0, \quad \forall \phi_p.$$

Indeed, the total action S vanishes

$$S[\phi_p; x_0] = 0, \quad \forall x_0,$$

since the contributions over both branches of the closed-time contour have opposite sign by construction,

$$\int_{\tau_i}^{\tau_M} d\tau \mathcal{L}_\phi(\tau) = - \int_{\tau_M}^{\tau_f} d\tau \mathcal{L}_\phi(\tau),$$

and $S_b = 0$ since $\tilde{r}(\tau_i) = \tilde{r}(\tau_f)$. As a consequence, $\mathcal{Z}[\phi_p] = \int dx_0 F(x_0) = 1$, and therefore $\tilde{\Omega}[\phi_p] = 0$. However, since $\tilde{\Omega}[\phi]$ generally takes on nonzero values outside the subset of physical potentials, its functional derivatives at a ϕ_p can take finite values.¹² As mentioned earlier, those functional derivatives are indeed quite remarkable since they are simply related to key physical quantities.

3.4 Functional Derivatives of $\tilde{\Omega}[\phi]$

3.4.1 Quick Comparison with Quantum Action Functionals

Action functionals of the form (32), i.e. the exponential of an action, play a fundamental role in field theory, which often deals with generating field integrals (i.e. traces) of the form [29],

$$\begin{aligned} e^{-i\tilde{\Omega}_Q[\phi]/\hbar} &= \left\langle \int \mathcal{D}\Psi e^{\frac{i}{\hbar}(S_Q[\Psi] + \int \phi \Psi)} \right\rangle \\ &= \iint d\psi_1 d\psi_2 \langle \psi_1 | \hat{\rho}_0 | \psi_2 \rangle \int_{\psi_1}^{\psi_2} \mathcal{D}\Psi e^{\frac{i}{\hbar}(S_Q[\Psi] + \int \phi \Psi)} \end{aligned} \tag{33}$$

where Ψ is the field, $S_Q[\Psi]$ is the action, $\hat{\rho}_0$ is the initial density matrix, and ϕ is an external source term that couples linearly to Ψ . In that case, the whole exponent in (33) is linear in ϕ , and the successive functional derivatives $\delta^{(n)}\tilde{\Omega}_Q[\phi]/\delta\phi(1) \dots \delta\phi(n)$ simply insert the field Ψ in the field integral and generate the averaged (time-ordered) products $\langle \delta\phi(1) \dots \delta\phi(n) \rangle$ of the field, alternatively referred to as the time-ordered correlation functions, propagators or Green's functions of the theory.

By contrast, the classical action functional (32) is highly non-linear on the external potential ϕ since the phase-space trajectory $\tilde{x}(\tau)$ in $S[\phi; x_0]$ implicitly depends on the external potential ϕ as well. If, as already mentioned in the previous paragraph, one regards $\tilde{S}[\phi; x_0]$ as the classical contribution to the total quantum amplitude to go from x_0 to $\tilde{x}(\tau_f)$, we see that the reduction of the quantum field integral from all possible field configurations to the classical path only is responsible for the non-linearity in the external perturbation of the

¹²The situation is analogous to a function, say $f(x, y) = e^x \sin(y)$, which is zero along the x -axis but takes non-zero values when leaving it, i.e. when $y \neq 0$, and therefore has differentials that are generally non-zero along the x -axis.

classical action (32). As a consequence, two types of quantities arise when differentiating the classical action functional $\tilde{\Omega}[\phi]$ instead of only one, namely the time-ordered correlation functions, in quantum field theory. The explicit linear dependence of \mathcal{S} on ϕ generates the correlations of the phase-space density as in field theory, while the implicit non-linearities generate terms involving the Poisson bracket $[\cdot, \cdot]_{PB}$ such as the response functions $\chi^{R,A}$, (21).¹³

3.4.2 First and Second Derivatives

In the neighborhood of the external potential ϕ_0 , $\tilde{\Omega}[\phi]$ can be expanded in the series,

$$\tilde{\Omega}[\phi_0 + \delta\phi] = \sum_{n=0}^{\infty} \frac{1}{n!} \oint d\tilde{1} \dots d\tilde{n} \Omega^{(n)}(\tilde{1}, \dots, \tilde{n}) \delta\phi(\tilde{1}) \dots \delta\phi(\tilde{n}), \tag{34}$$

where we introduce the short-hand notation,

$$\oint d\tilde{1} \dots = \int_{-\infty}^{+\infty} d\tau_1 t'(\tau_1) \int_V d\mathbf{q}_1 \int d\mathbf{p}_1 \dots$$

Here $\tilde{\Omega}^{(0)} = \tilde{\Omega}[\phi_0]$ and, for $n \geq 1$, $\tilde{\Omega}^{(n)}$ is the n -th functional derivative at potential ϕ_0 ,

$$\Omega^{(n)}(\tilde{1}, \dots, \tilde{n}) \equiv \left. \frac{\delta^{(n)} \tilde{\Omega}[\phi]}{\delta\phi(\tilde{1}) \dots \delta\phi(\tilde{n})} \right|_{\phi=\phi_0}.$$

The latter can be obtained by a systematic perturbation expansion in powers of the variations $\delta\phi$ around ϕ_0 . We are particularly interested in this work in the first two derivatives $n = 1, 2$. For clarity, we just report here the main results and give their proofs in Appendix C; in addition, the differentiability properties of $\tilde{\Omega}[\phi]$ are discussed more thoroughly in Appendix D.

The first functional derivative generates the phase-space distribution function f of the dynamics under investigation,

$$\left. \frac{\delta \tilde{\Omega}}{\delta\phi(\tilde{1})} \right|_{\phi=\phi_0} = \Pi(\tau) \langle \mathcal{N}(\mathbf{r}, \mathbf{p}, \tau) \rangle = \Pi(\tau) f(\mathbf{r}, \mathbf{p}, t(\tau)) \equiv \tilde{f}(\tilde{1}), \tag{35}$$

where we recall that $\Pi(\tau)$ is the window function defined by (31). Accordingly, its second functional derivative,

$$\left. \frac{\delta^{(2)} \tilde{\Omega}[\phi]}{\delta\phi(\tilde{1}) \delta\phi(\tilde{2})} \right|_{\phi=\phi_0} = \left. \frac{\delta \tilde{f}(\tilde{1})}{\delta\phi(\tilde{2})} \right|_{\phi=\phi_0} \equiv \chi(\tilde{1}, \tilde{2}) \tag{36}$$

can be regarded as the linear response function *along the closed-time contour* of the system's dynamics. The direct calculation of χ developed in Appendix C leads to

$$\chi(\tilde{1}, \tilde{2}) = \Pi(\tau_1) \Pi(\tau_2) \left(\mathcal{R}(\tilde{1}, \tilde{2}) - \frac{i}{s} C(\tilde{1}, \tilde{2}) \right), \tag{37}$$

¹³Another distinction between (33) and (32) is in the boundary conditions. In the quantum expression (33), the field integral is over all trajectories starting at $\phi(\tau_i) = \phi_1$ at τ_i and ending ϕ_2 at $\phi(\tau_f) = \tau_f$, independently of the source ϕ . In the classical expression (32), while initial the value $x(\tau_i) = x(\tau_i)$ is the same for all external potential ϕ , the final value $\tilde{x}(\tau_f)$ depends on the overall trajectory $\tilde{x}(\tau)$ and therefore on the potential ϕ . This saddle difference actually can not be discarded when considering the functional derivatives and the additional term \mathcal{S}_b in (30) was added to absorb such spurious boundary effects (see Appendix C).

and consist in the linear combination of two terms. The last term is the two-body correlation function

$$C(\tilde{1}, \tilde{2}) = \langle \delta \mathcal{N}(\tilde{1}) \delta \mathcal{N}(\tilde{2}) \rangle, \tag{38}$$

and, as discussed earlier, comes from the explicit linearity of the action S in the external potential. The first term in (37) originates from the non-linearity of the action and involves the many-body Poisson bracket $[\dots]_{PB}$,

$$\mathcal{R}(\tilde{1}, \tilde{2}) = \frac{1}{2} \langle \mathcal{T}_c [\mathcal{N}(\tilde{1}), \mathcal{N}(\tilde{2})]_{PB} \rangle. \tag{39}$$

In (39), we have introduced the chronologically ordered Poisson bracket of two dynamical variables $A(\tau)$ and $B(\tau)$ as

$$\mathcal{T}_c[A(\tau_1), B(\tau_2)]_{PB} = \theta(\tau_1 - \tau_2)[A(\tau_1), B(\tau_2)]_{PB} + \theta(\tau_2 - \tau_1)[B(\tau_2), A(\tau_1)]_{PB}.$$

Accordingly, χ can also be expressed as,¹⁴

$$\chi(\tilde{1}, \tilde{2}) = \theta(\tau_1 - \tau_2) \chi^>(\tilde{1}, \tilde{2}) + \theta(\tau_2 - \tau_1) \chi^<(\tilde{1}, \tilde{2}), \tag{40}$$

where for $\tau_1 > \tau_2$ (dropping the window functions for simplicity),

$$\chi^>(\tilde{1}, \tilde{2}) = \frac{1}{2} \langle [\mathcal{N}(\tilde{1}), \mathcal{N}(\tilde{2})]_{PB} \rangle - \frac{i}{s} C(\tilde{1}, \tilde{2}), \tag{41}$$

and for $\tau_2 > \tau_1$,

$$\chi^<(\tilde{1}, \tilde{2}) = -\frac{1}{2} \langle [\mathcal{N}(\tilde{1}), \mathcal{N}(\tilde{2})]_{PB} \rangle - \frac{i}{s} C(\tilde{1}, \tilde{2}). \tag{42}$$

3.5 Connection to Physical Response and Correlation Functions

Remarkably, the function χ contains information about both the physical correlations and response properties of the physical system, which can easily be extracted as follows.

The physical correlation function $C(1, 2)$ defined in Sect. 2 is easily extracted from χ by taking the sum of (41) and (42),¹⁵

$$C(1, 2) = \frac{is}{2} (\chi^>(1, 2) + \chi^<(1, 2)), \quad \forall t_1, t_2 \geq t_0. \tag{43}$$

The connection to the physical response can be seen by calculating the variation δf of the phase-space density due to a change in the external potential $\delta\phi_0$ around ϕ_0 . We have,

¹⁴We remark that, contrary to the functional defined on the real-time axis imagined at the beginning of Sect. 3, χ is fully symmetric in its arguments,

$$\chi(\tilde{1}, \tilde{2}) = \chi(\tilde{2}, \tilde{1}) \quad \forall \tilde{1}, \tilde{2}.$$

¹⁵For simplicity, we write $a(t) = a(\tau_+) = a(\tau_-)$ where (see Fig. 1) $t = t(\tau_+) = t(\tau_-)$, and $\chi^>(1, 1') = \chi^>(\mathbf{r}_1, \mathbf{p}_1, \tau_-; \mathbf{r}_1, \mathbf{p}_1, \tau'_+)$ and $\chi^<(1, 1') = \chi^>(\mathbf{r}_1, \mathbf{p}_1, \tau_+; \mathbf{r}_1, \mathbf{p}_1, \tau'_-)$.

$$\begin{aligned} \delta f(\mathbf{x}_1, t_1) &= \oint d\tilde{2} \chi(\tilde{1}, \tilde{2}) \delta\phi_0(\tilde{2}) \\ &= \int d\mathbf{x}_2 \int_{t_0}^{t_1} dt_2 \chi^>(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \delta\phi_0(\mathbf{x}_2, t_2) \\ &\quad + \int d\mathbf{x}_2 \int_{t_1}^{\infty} \chi^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \delta\phi_0(\mathbf{x}_2, t_2) \\ &\quad + \int d\mathbf{x}_2 \int_{-\infty}^{t_0} \chi^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \delta\phi_0(\mathbf{x}_2, t_2) \\ &= \int d\mathbf{x}_2 \int_{t_0}^{t_1} dt_2 [\chi^>(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) - \chi^<(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2)] \delta\phi_0(\mathbf{x}_2, t_2). \end{aligned}$$

Using (41)–(42), we find $\delta f(1) = \int d\mathbf{x}_2 \int_{-\infty}^{\infty} dt_2 \chi^R(1, 2) \delta\phi_0(2)$, with

$$\begin{aligned} \chi^R(1, 2) &= \theta(t_1 - t_2) [\chi^>(1, 2) - \chi^<(1, 2)] \\ &= \theta(t_1 - t_2) \theta(t_2 - t_0) \{ [N(1), N(2)]_{PB} \}, \end{aligned}$$

which is just the retarded response function (21) of traditional perturbation theory recalled in Sect. 2.2.

In conclusion, simple linear combinations of the second order derivatives χ yield to key dynamical properties of the physical system under investigation, namely C and $\chi^{R,A}$. The simultaneous occurrence of both C and χ^R , two quantities of different nature, is remarkable and further discussed in Appendix E with regard to its counterpart in quantum field theory.

3.6 Generalized BBGKY Hierarchy for the Extended Dynamics

We consider the statistical dynamics on the closed-time contour governed by \mathcal{H}_ϕ defined in (27). We assume that at the initial time τ_i , the initial positions and momenta $\tilde{x}(\tau_i)$ are distributed according to the same distribution $F_0(x_0)$ as the physical system under investigation (see Sect. 2). The notations used here for L_1, γ_3, \dots are those of Sect. 2.2 with the real time variables t_1, t_2, \dots simply replaced by τ_1, τ_2, \dots .

The microscopic phase-space density $\mathcal{N}(\tilde{1})$ evolves according to,

$$\left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau} - L_{\tilde{1}} \right] \mathcal{N}(\tilde{1}) = \frac{1}{2} \gamma_3(\tilde{1}, \tilde{2}, \tilde{3}) \mathcal{N}(\tilde{2}) \mathcal{N}(\tilde{3}). \tag{44}$$

By averaging over the initial state, we obtain the evolution equation for the phase-space density \tilde{f} defined by (35),

$$\left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau} - L_{\tilde{1}} \right] \tilde{f}(\tilde{1}) - \{u^{mf}(\tilde{1}), \tilde{f}(\tilde{1})\} = \frac{1}{2} \gamma_3(\tilde{1}, \tilde{2}, \tilde{3}) C(\tilde{2}, \tilde{3}) + \Delta(\tau) f(1), \tag{45}$$

in terms of the two-point correlation function C and of

$$\Delta(\tau) = \frac{1}{t'(\tau)} \frac{d\Pi(\tau)}{d\tau} = \frac{1}{t'(\tau)} [\delta(\tau - \tau_i) - \delta(\tau - \tau_f)] = \delta(t(\tau) - t_0). \tag{46}$$

Following the traditional BBGKY approach, the evolution equation (45) would be regarded as the first equation of the hierarchy of evolution equations between the successive equal-time cumulants $C^{(n)}$. Our approach allows us to instead regard (45) as the first equation of

a “larger” hierarchy in terms of the successive functional derivatives $\Omega^{(n)}(1, \dots, n)$, which combine information on both correlation and response functions. The advantage of this extended hierarchy is that it can be formally closed at second order $n = 2$ using the procedure discussed below.

To obtain this extended hierarchy, we note the equal-time property

$$\chi(X_1, \tau; X_2, \tau) = -\frac{i}{s}C(X_1, \tau; X_2, \tau),$$

as can simply be seen by setting $\tau_1 = \tau_2 = \tau$ in (40). The collision integral in (47) can then be rewritten in terms of χ and yields the evolution equation

$$\left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau} - L_{\tilde{1}} \right] \tilde{f}(\tilde{1}) - \{u^{mf}(\tilde{1}), \tilde{f}(\tilde{1})\} = \frac{1}{2}\gamma_3(\tilde{1}, \tilde{2}, \tilde{3})\chi(\tilde{2}, \tilde{3}) + \Delta(\tau)\tilde{f}(1), \tag{47}$$

which relates the first derivative $f = \delta\tilde{\Omega}/\delta\phi$ to the second derivative $\chi = \delta^2\tilde{\Omega}/\delta\phi^2$ of the generating functional. Successive functional differentiations of (47) with respect to ϕ generate the extended hierarchy between the $\Omega^{(n)}$'s. The first functional derivative yields the evolution equation for χ (see footnote 16 for details),

$$\begin{aligned} &\left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau} - L_1 \right] \chi(\tilde{1}, \tilde{1}') - \Sigma^{mf}(\tilde{1}, \tilde{2}) \cdot \chi(\tilde{2}, \tilde{1}') \\ &= s_2(\tilde{1}, \tilde{1}') + \frac{is}{2}\gamma_3(\tilde{1}, \tilde{2}, \tilde{3})\tilde{\Omega}^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}') + \Delta(\tau)\Pi(\tau')C(\tilde{1}, \tilde{1}')/is, \end{aligned} \tag{48}$$

where we define,¹⁶

$$s_2(\tilde{1}, \tilde{1}') \equiv \{\delta(\tilde{1} - \tilde{1}'), \tilde{f}(\tilde{1})\}(\tilde{1}).$$

The mean-field kernel is defined as in (20),

$$\Sigma^{mf}(\tilde{1}, \tilde{1}') = \gamma_3(\tilde{1}, \tilde{2}, \tilde{3})\tilde{f}(\tilde{2})\delta(\tilde{1}' - \tilde{3}). \tag{49}$$

In the rhs of (48), the second term comes from the direct differentiation of the collision integral in (47), and the last term includes the boundary conditions.

Similarly, functional differentiation of (48) yields the evolution equation for $\Omega^{(3)}$,

$$\begin{aligned} &\left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau'} - L_1 \right] \Omega^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}) - \Sigma^{mf}(\tilde{1}, \tilde{2}')\Omega^{(3)}(\tilde{2}', \tilde{2}, \tilde{3}) \\ &= s_3(\tilde{2}\tilde{3}\tilde{1}) + \frac{is}{2}\gamma_3(\tilde{1}\tilde{2}'\tilde{3}')\left(\Omega^{(4)}(\tilde{2}', \tilde{3}', \tilde{2}, \tilde{3}) + \frac{2}{is}\chi(\tilde{2}', \tilde{2})\chi(\tilde{3}', \tilde{3}) \right) \\ &+ \Delta(\tau')\Omega^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}), \end{aligned} \tag{50}$$

¹⁶Alternatively, of course, the same hierarchy could be obtained from a “direct calculation” using (44) and the explicit expressions of the $\Omega^{(n)}$'s in terms of the microscopic field \mathcal{N} . In this direct approach, the secular term s_2 in (48) arises from the time derivative of the Heaviside functions in (40),

$$\delta(\tau - \tau')\chi^>(1, 1') - \delta(\tau' - \tau)\chi^<(1, 1') = \delta(\tau - \tau')\{\mathcal{N}(1), \mathcal{N}(1')\} = s_2(1, 1').$$

The functional derivative of the boundary term in (47) yields $\Delta(\tau)\Pi(\tau')C(\tilde{1}, \tilde{1}')$ as can be seen by applying (131) with $A = \mathcal{N}$ and using $\delta\mathcal{N}(\tau_i)/\delta\phi(\tau') = 0$ since the initial value is fixed.

where

$$s_3(\tilde{2}\tilde{3}\tilde{1}) = \{\delta(\tilde{1} - \tilde{2}), \chi(\tilde{1}, \tilde{3})\}(\tilde{1}) + \{\delta(\tilde{1} - \tilde{3}), \chi(\tilde{1}, \tilde{2})\}(\tilde{1}), \tag{51}$$

and so on and so forth. The hierarchy thus obtained for the $\Omega^{(n)}$'s suffers from the closure problem whereby the equation for $\tilde{\Omega}^{(n)}$ depends on the next order response function $\tilde{\Omega}^{(n+1)}$. In the following we show that this hierarchy can be closed at the $n = 2$ level.

3.7 Formal Closure of the Hierarchy¹⁷

3.7.1 Effective Potential and Vertex Functions

The method uses a Legendre transformation of $\tilde{\Omega}[\phi]$ [29, 30], a functional of the external potentials ϕ , to obtain a function $\tilde{\Gamma}[f_\phi]$ of the phase-space densities f_ϕ given by

$$\tilde{\Gamma}[f_\phi] = -\tilde{\Omega}[\phi] + \oint d\tilde{1} f_\phi(\tilde{1})\phi(\tilde{1}). \tag{52}$$

We shall refer to $\tilde{\Gamma}$ as the *effective potential*; the latter can be regarded as the generalization of the Helmholtz free energy used in density functional theory [23]. The transformation (52) shifts attention from the potential that perturbs the system to the phase-space density that describes its effect.

The functional derivatives of the Legendre transform $\Gamma[f_\phi]$ at the phase-space distribution $f_\phi = f$ under investigation,

$$\Gamma^{(n)}(\tilde{1}, \dots, \tilde{n}) = \left. \frac{\delta^n \tilde{\Gamma}[f_\phi]}{\delta f_\phi(\tilde{1}) \dots \delta f_\phi(\tilde{n})} \right|_{f_\phi=f},$$

are intimately related to those of $\tilde{\Omega}[\phi]$. In statistical field theory, the functions $\Gamma^{(n)}$ are usually referred to as *vertex functions*. For $n = 2$, we shall write $\Gamma \equiv \Gamma^{(2)}$.

The first derivative simply equals the external potential,

$$\left. \frac{\delta \tilde{\Gamma}}{\delta f_\phi(\tilde{1})} \right|_{f_\phi=f} = \phi_0(\tilde{1}). \tag{53}$$

In the special case when $\phi_0 = 0$ as in equilibrium or relaxation problems, the previous relation shows that the physical density f under investigation is an extremum of the effective potential $\tilde{\Gamma}$. As such, $\tilde{\Gamma}$ plays a role similar to a thermodynamic potential in equilibrium statistical mechanics.

¹⁷Using $\Omega^{(3)} = \delta\chi/\delta\phi$ in (48), the latter can then be regarded as a functional differential equation for $\chi(1, 1')$. In principle, this equation could be used to generate approximate but closed relations for χ . Thus, following ordinary perturbation theory, we could for instance use (48) to expand χ in powers of the bare interaction vertex γ_3 and of its “non-interacting” limit solution χ_0 (solution of (48) with $\gamma_3 = 0$). Lowest order approximation obtained in this way would most certainly suffer from the common divergence and secular problems that often plague ordinary perturbation theory. These difficulties could in principle be cured by summing infinite classes of terms in the expansion, which would lead to excessively complicated calculations. In our approach, following the lessons of field theory, those issues are dealt with more efficiently by working directly with the so-called self-energy and vertex corrections; in the present work, the role of self-energy is played by the memory function.

The higher-order derivatives can be obtained by differentiation (53) with respect to ϕ and using the chain rule of differentiation. For instance, for the second-order derivative, we find

$$\oint d\tilde{2} \frac{\delta^2 \Gamma[\phi]}{\delta f_\phi(\tilde{1}) \delta f_\phi(\tilde{2})} \frac{\delta f_\phi(\tilde{2})}{\delta \phi(\tilde{1}')} = \oint d\tilde{2} \frac{\delta^2 \Gamma[\phi]}{\delta f_\phi(\tilde{1}) \delta f_\phi(\tilde{2})} \frac{\delta^2 \tilde{\Omega}[\phi]}{\delta \phi(\tilde{2}) \delta \phi(\tilde{1}')} = \delta_c(\tilde{1} - \tilde{1}') \quad (54)$$

where the δ_c -function $\delta_c(\tilde{1} - \tilde{1}') = \frac{1}{t'(\tau)} \delta(\tilde{1} - \tilde{1}')$ satisfies

$$\oint d\tilde{2} \delta_c(\tilde{1} - \tilde{2}) \tilde{f}(\tilde{2}) = \tilde{f}(\tilde{1}). \quad (55)$$

With short-hand notations, (54) writes as

$$\Gamma(\tilde{1}, \tilde{2}) \cdot \chi(\tilde{2}, \tilde{1}') = \chi(\tilde{1}, \tilde{2}) \cdot \Gamma(\tilde{2}, \tilde{1}') = \delta_c(\tilde{1} - \tilde{1}'), \quad (56)$$

and shows that Γ can be regarded as the inverse of the response function χ . Taking the derivative of (56) with respect to ϕ yields a relation between $\Gamma^{(3)}$ and $\Omega^{(3)}$,

$$\Omega^{(3)}(\tilde{1}, \tilde{2}, \tilde{3}) = -\chi(\tilde{1}, \tilde{1}') \chi(\tilde{2}, \tilde{2}') \chi(\tilde{3}, \tilde{3}') \Gamma^{(3)}(\tilde{1}', \tilde{2}', \tilde{3}'), \quad (57)$$

and so on and so forth [30].

3.7.2 Closure of the Hierarchy

The relation (57) provides the starting point for closing the extended BBGKY hierarchy linking the $\Omega^{(n)}$. Firstly, we can now express the collision integral (48) as

$$\begin{aligned} \frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3}) \Omega^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}') &= \frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3}) [-\chi(\tilde{2}, \tilde{2}) \chi(\tilde{3}, \tilde{3}) \chi(\tilde{1}', \tilde{1}') \Gamma^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}')] \\ &\equiv \Sigma(\tilde{1}, \tilde{2}) \cdot \chi(\tilde{2}, \tilde{1}'), \end{aligned}$$

in terms of the memory function kernel Σ ,

$$\Sigma(\tilde{1}, \tilde{1}') = -\frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3}) \chi(\tilde{2}, \tilde{2}) \chi(\tilde{3}, \tilde{3}) \Gamma^{(3)}(\tilde{2}, \tilde{3}, \tilde{1}') \quad (58)$$

$$= -\frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3}) \frac{\delta \chi(\tilde{2}, \tilde{3})}{\delta f_\phi(\tilde{1}')} \quad (59)$$

The equation of evolution (48) becomes

$$[G(\tilde{1}, \tilde{2}) - \Sigma^{mf}(\tilde{1}, \tilde{2}) - \Sigma(\tilde{1}, \tilde{2})] \cdot \chi(\tilde{2}, \tilde{1}') = s_2(\tilde{1}, \tilde{1}') + \Delta(\tau) \Pi(\tau') C(\tilde{1}, \tilde{1}') / is \quad (60)$$

where for convenience we have defined

$$G(\tilde{1}, \tilde{2}) = \left[\frac{1}{t'(\tau)} \frac{\partial}{\partial \tau} - L_1 \right] \delta(\tilde{1} - \tilde{2}).$$

Equation (60) for the closed-time contour response function χ will play here a role similar to the Dyson equation in quantum field theory [26, 30]. In the latter case, the equation describes the evolution of the time-dependent Green's functions, from which all other dynamical properties including correlation and response functions can be calculated. Here, in

contrast, (60) describes the evolution of the quantity χ , defined in (37), which combines in one single quantity, two properties of different nature in classical mechanics, namely the correlation and response functions (see also discussion in Appendix E).

Secondly, (60) allows us to derive another relation that expresses $\Gamma^{(3)}$ in terms of Σ . To this end, we multiply (60) on the right by the inverse $\chi^{-1} = \Gamma$, which leads to a relation between Σ and Γ ,

$$G(\tilde{1}, \tilde{1}') - \Sigma^{mf}(\tilde{1}, \tilde{1}') - \Sigma(\tilde{1}, \tilde{1}') \\ = \{\Gamma(\tilde{1}, \tilde{1}'), f(\tilde{1})\}(\tilde{1}) + \Delta(\tau)\Pi(\tau')C(\tilde{1}, \tilde{2})\Gamma(\tilde{2}, \tilde{1}')/is.$$

By taking the functional derivative of the previous equation with respect to f and combining the result with (58), we obtain the following integro-differential equation for the memory function kernel,

$$\{\Sigma(\tilde{1}, \tilde{1}'), \tilde{f}(\tilde{1}')\}(\tilde{1}') \\ = \frac{is}{2}\gamma_3(\tilde{1}23)s_3(23\tilde{1}') \tag{61a}$$

$$+ \frac{is}{2}\gamma_3(\tilde{1}23)\chi(2, \tilde{2})\chi(3, \tilde{3})\left(\gamma_3(\tilde{1}'2'3') + \frac{\delta\Sigma(\tilde{1}', \tilde{2})}{\delta f_\phi(\tilde{3})}\Big|_{f_\phi=f}\right) \tag{61b}$$

$$+ \Delta(\tau')\frac{1}{2}\gamma_3(\tilde{1}23)\chi(2, \tilde{2})\chi(3, \tilde{3})\frac{\delta}{\delta f(\tilde{3})}[C(\tilde{1}', \tilde{2}')\Gamma(\tilde{2}', \tilde{2})]. \tag{61c}$$

The set of equations consisting of the first two equations (47) and (60) of the hierarchy, together with (58) and (61a)–(61c) is closed and is fully equivalent to the hierarchy of evolution equations for the $\Omega^{(n)}$. Equations (61a)–(61c) are a functional equation for the memory function that can be used to generate self-consistent approximations in terms of γ_3 and χ (see also Appendix F).

3.8 The Memory Function Kernel

Equations (61a)–(61c) imply that the memory function Σ can be splitted into three parts as

$$\Sigma(1, 1') \equiv \Sigma^{(0)}(X_1, X'_1; \tau)\Delta(\tau') + \Sigma^\delta(X_1, X'_1; \tau)\delta(\tau - \tau') + \Sigma^{reg}(1, 1'). \tag{62}$$

The physical interpretation of the different components of Σ is discussed in detail in the following sections. We just give here a short description of their origin.

The first term

$$\{\Sigma^{(0)}(X_1, X'_1; \tau), f(\tilde{1}')\}(\tilde{1}') \\ = \frac{1}{2}\gamma_3(\tilde{1}\tilde{2}\tilde{3})\chi(\tilde{2}, \tilde{2})\chi(\tilde{3}, \tilde{3})\frac{\delta}{\delta f(\tilde{3})}[C(\tilde{1}', \tilde{2}')\chi^{-1}(\tilde{2}', \tilde{2})]$$

describes the effect of initial correlations in the initial state at time t_0 on the dynamics of the system at $t > t_0$. This term can be shown to vanish for Gaussian initial conditions but, as was recalled in Sect. 2.2, this simplification is always invalid here since the phase-space density \mathcal{N} is always strongly non-Gaussian [16]. The neglect of this term has deep consequences related to so-called *Bogolyubov's condition* of weakening (suppression) of the

initial correlations and to the transition from reversible to irreversible dynamical equations [31].

The second term, proportional to the delta function $\delta(\tau - \tau')$, is singular in time and satisfies,

$$\begin{aligned} \{\Sigma^{(\delta)}(X_1, X'_1; \tau), f(\tilde{1}')\}(\tilde{1}') &= \frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3})s_3(\tilde{2}\tilde{3}\tilde{1}') \\ &= \gamma_3(\tilde{1}\tilde{2}\tilde{3})\{\delta(\tilde{1}' - \tilde{2}), C(\tilde{1}', \tilde{3})\}(\tilde{1}'). \end{aligned} \tag{63}$$

This term is related the instantaneous effect of correlations on the effective interactions between particles (at equilibrium, those correlations are the so-called ‘static’ correlations [23]). This term naturally combines to the mean-field contribution Σ^{mf} , (49), such that

$$\Sigma_{tot}^{(\delta)} \equiv \Sigma^{mf} + \Sigma^{(\delta)},$$

renormalizes the instantaneous mean-field effect with instantaneous correlations effects beyond the mean-field. In the absence of particle correlations (Vlasov approximation), $\Sigma^{(\delta)}$ vanishes.

Finally, the last term describes memory, non-Markovian correlation effects in the dynamics and satisfies

$$\begin{aligned} &\{\Sigma^{(reg)}(\tilde{1}, \tilde{1}'), \tilde{f}(\tilde{1}')\}(\tilde{1}') \\ &= \frac{is}{2} \gamma_3(\tilde{1}\tilde{2}\tilde{3})\chi(\tilde{2}, \tilde{2})\chi(\tilde{3}, \tilde{3}) \left(\gamma_3(\tilde{1}'\tilde{2}\tilde{3}) + \frac{\delta\Sigma(\tilde{1}', \tilde{2})}{\delta f_\phi(\tilde{3})} \Big|_{f_\phi=f} \right). \end{aligned}$$

4 Real-Time Formalism (I)

The previous approach allowed us to derive a closed, self-consistent set of equations to describe the evolution of the single-particle phase-space distribution function f of the system. However, being expressed in terms of quantities defined along the closed-time contour, this formulation lacks physical transparency and does not appeal to intuition. In the next two sections, we shall re-express these exact results in terms of quantities defined on the real-time axis, namely the correlation C and response functions $\chi^{R,A}$ and a set of memory functions. In the following section, Sect. 5, we will recast the overall approach into a form that leads to the same results *directly* in terms of physical quantities defined on the real-time axis. In the present section, we focus on the evolution equations, discuss their physical content, and make contacts with previous works. The careful derivation of the evolution equations for $C, \chi^{R,A}$ done in the next subsection is somewhat lengthy; the reader uninterested in those details may safely skip ahead to (71a)–(71c) in Sect. 4.2, where the results are given and then discussed and compared with previous works.

4.1 From Closed-Time to Real-Time Representations

Throughout the section, we will use the (Pauli) matrices defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

4.1.1 Real-Time (Matrix) Representation of χ

The most straightforward transcription of the closed-time contour formalism is obtained by mapping the function $\chi(1, 1')$ onto the 2×2 -matrix [20],

$$\bar{\bar{\chi}}(1, 1') = \begin{pmatrix} \chi_{++}(1, 1') & \chi_{+-}(1, 1') \\ \chi_{-+}(1, 1') & \chi_{--}(1, 1') \end{pmatrix}, \quad (64)$$

defined such that the jk -component, $i, j = \pm$, is $\chi(1, 1')$ with 1 lying on c_i and $1'$ lying on c_j where c_+ (c_-) is the upper (lower) part of the closed-time contour (see Fig. 1). Explicitly, using (37), the matrix components are

$$\begin{aligned} \chi_{++}(1, 1') &= \frac{1}{2} \langle \mathcal{T}_c [N(1), N(1')]_{PB} \rangle - \frac{i}{s} C(1, 1'), \\ \chi_{--}(1, 1') &= \frac{1}{2} \langle \mathcal{T}_a [N(1), N(1')]_{PB} \rangle - \frac{i}{s} C(1, 1'), \\ \chi_{+-}(1, 1') &= -\frac{1}{2} \langle [N(1), N(1')]_{PB} \rangle - \frac{i}{s} C(1, 1'), \\ \chi_{-+}(1, 1') &= \frac{1}{2} \langle [N(1), N(1')]_{PB} \rangle - \frac{i}{s} C(1, 1') \end{aligned}$$

where \mathcal{T}_c and \mathcal{T}_a are the chronological and anti-chronological time-ordering operators on the real-time axis $[t_0, +\infty]$. This matrix representation has, however, the disadvantage that it does not explicitly take account of the linear dependence of its components; for instance,

$$\chi_{++} + \chi_{--} = \chi_{+-} + \chi_{-+}.$$

It is possible to choose another representation that not only removes this redundancy of information but also involves the physically relevant quantities. Indeed we note that simple linear combinations of the χ_{jk} 's yield the correlation and response functions of interest,

$$\begin{aligned} \chi^R &= \chi_{++} - \chi_{+-} = \chi_{-+} - \chi_{--}, \\ \chi^A &= \chi_{++} - \chi_{-+} = \chi_{+-} - \chi_{--}, \\ \frac{2}{is} C &= \chi_{+-} + \chi_{-+} = \chi_{++} + \chi_{--}. \end{aligned}$$

Using these relations, it is straightforward to show that the orthogonal transformation¹⁸ defined as $\hat{\chi} = Q \bar{\bar{\chi}} Q^\dagger$ with the orthogonal matrix $Q = (1 - i\sigma_y)/\sqrt{2}$ defines the equivalent real-time representation,

$$\hat{\chi} = Q \bar{\bar{\chi}} Q^\dagger = \begin{pmatrix} 0 & \chi^A \\ \chi^R & \frac{2}{is} C \end{pmatrix}, \quad (65)$$

which has the remarkable property that it depends on the correlation function C and response functions $\chi^{R,A}$ only.

¹⁸This transformation was used in the original article of Keldysh [25] on quantum non-equilibrium Green's functions.

4.1.2 From Closed-Time to Real-Time Integrals

The theory derived in Sect. 3 involves integrals over the closed-time contour of the form $\oint d2\Sigma(1, 2)\chi(2, 1')$. Here we provide useful identities to express such quantities in terms of integrals along the real axis (see e.g. [26]).

We remark that the quantities χ and Σ defined before belong to the class of functions of two closed-time variables of the form

$$f(\tau, \tau') = f^0(\tau')[\delta_c(\tau' - \tau_i) - \delta_c(\tau' - \tau_f)] + f^\delta(\tau)\delta_c(\tau - \tau') + \theta(\tau - \tau')f^>(\tau, \tau') + \theta(\tau' - \tau)f^<(\tau, \tau'), \quad (66)$$

where for simplicity we do not write the possible dependence on phase-space variables. In matrix form, f can be represented by \bar{f} as in (64) or by $\hat{f} = Q\bar{f}Q^\dagger$ as in (65), namely

$$\hat{f} = \begin{pmatrix} 0 & f^A \\ f^R & \frac{2}{iS}f^C \end{pmatrix}$$

where the direct calculation of the retarded (R), advanced (A) and correlation (C) components in physical time gives the following expressions,

$$f^R(t, t') = f^\delta(t)\delta(t - t') + \theta(t - t')[f^>(t, t') - f^<(t, t')], \quad (67a)$$

$$f^A(t, t') = f^\delta(t)\delta(t - t') - \theta(t' - t)[f^>(t, t') - f^<(t, t')], \quad (67b)$$

$$\frac{2}{iS}f^C(t, t') = 2f^{(0)}(t')\delta(t' - t_0) + (f^>(t, t') + f^<(t, t')). \quad (67c)$$

In the special case $f = \chi$, (67a)–(67c) give back $f^{R,A} = \chi^{R,A}$ and $f^C = C$. With $f = \Sigma$, the retarded and advanced terms $\Sigma^{A,R}$ contain the singular part Σ^δ that arises from static correlations, while Σ^C contains the part $\Sigma^{(0)}$ due to the initial conditions (see (72)–(73) below). Finally, for the delta function δ_c defined by (55), we obtain the matrix representation $\hat{\delta}_c(\bar{1}, \bar{1}') = \frac{1}{i'(\bar{\tau})}\delta(1 - 1')\sigma_z$.

We are interested in integrals of the kind

$$h(\tau, \tau') = \oint d\bar{\tau} f(\tau, \bar{\tau})g(\bar{\tau}, \tau'), \quad (68)$$

where f and g are of the form (66). It is easy to show that $h(\tau, \tau')$ also belongs to the class (66). By splitting the closed-time contour integral into integrals over the forward and backward branches, namely $\oint_c d\tau = \int_{t_0}^\infty dt - \int_0^\infty dt$, it is straightforward to derive the following relations,

$$\begin{aligned} h^R(t, t') &= f^R \cdot g^R(t, t') = \int_{t_0}^\infty dt'' f^R(t, t'')g^R(t'', t'), \\ h^A(t, t') &= f^A \cdot g^A(t, t') = \int_{t_0}^\infty dt'' f^A(t, t'')g^A(t'', t'), \\ h^C(t, t') &= f^C \cdot g^R(t, t') + f^R \cdot g^C(t, t'). \end{aligned} \quad (69)$$

In matrix form, those properties can be summarized as

$$\bar{h}(1, 1') = \bar{f}(1, 2)\sigma_z\bar{g}(2, 1'), \quad \hat{h}(1, 1') = \hat{f}(1, 2)\sigma_x\hat{g}(2, 1'),$$

with

$$\hat{h} = \begin{pmatrix} 0 & f^A \cdot g^A \\ f^R \cdot g^R & \frac{2}{is}(f^R \cdot g^C + f^C \cdot g^A) \end{pmatrix}.$$

4.2 Equations of Motion

With the help of the previous identities, we can easily re-express the evolution equation (60) of $\chi(\tilde{1}, \tilde{1}')$ into equations for the physically relevant quantities $C(1, 1')$ and $\chi^{R,A}(1, 1;)$ in real time. In matrix form, (60) writes

$$\begin{aligned} (\hat{G} - \hat{\Sigma}^{mf} - \hat{\Sigma})\sigma_z \hat{\chi}(1, 1') &= \begin{pmatrix} G - \Sigma^{mf} - \Sigma^A & 0 \\ -\frac{2}{is}\Sigma^C & G - \Sigma^{mf} - \Sigma^R \end{pmatrix} \cdot \hat{\chi}(1, 1') \\ &= \{\delta(1 - 1'), f(1)\}\sigma_x \end{aligned} \tag{70}$$

where we recall that the phase-space density $f(1)$ evolves according to (18). In (70), we introduced the short-hand notations,

$$\begin{aligned} G(1, 2) &= -\frac{\partial}{\partial t_2} \delta(1 - 2) + \{h_0(2) + \phi_0(2), \delta(1 - 2)\}(2), \\ \Sigma^{mf}(1, 1') &= \gamma_3(1, 2, 3) f(2) \delta(1' - 3). \end{aligned}$$

Explicitly in terms of the components, we obtain the coupled evolution equations for the correlation and response functions,¹⁹

$$\begin{aligned} \left[\frac{\partial}{\partial t} - L_1 \right] C(1, 1') - \int_{t_0}^{\infty} dt_2 \int dX_2 \Sigma_{tot}^R(1, 2) C(2, 1') \\ = \int_{t_0}^{\infty} dt_2 \int dX_2 \Sigma^C(1, 2) \chi^A(2, 1') + \delta(t - t_0) C(1, 1'), \end{aligned} \tag{71a}$$

$$\begin{aligned} \left[\frac{\partial}{\partial t} - L_1 \right] \chi^R(1, 1') - \int_{t_0}^{\infty} dt_2 \int dX_2 \Sigma_{tot}^R(1, 2) \chi^R(2, 1') \\ = \{\delta(1 - 1'), f(1)\}(1), \end{aligned} \tag{71b}$$

$$\begin{aligned} \left[\frac{\partial}{\partial t} - L_1 \right] \chi^A(1, 1') - \int_{t_0}^{\infty} dt_2 \int dX_2 \Sigma_{tot}^A(1, 2) \chi^A(2, 1') \\ = \{\delta(1 - 1'), f(1)\}(1). \end{aligned} \tag{71c}$$

Here we have combined the mean-field contribution Σ^{mf} to $\Sigma^{R,A}$,

$$\begin{aligned} \Sigma_{tot}^{R,A}(1, 1') &= \Sigma^{mf}(1, 1') + \Sigma^{R,A}(1, 1') \\ &= \Sigma_{tot}^{\delta} \delta(t - t') \pm \Theta(\mp(t - t')) (\Sigma^>(1, 1') - \Sigma^<(1, 1')) \\ &\equiv \Sigma_{tot}^{\delta} \delta(t - t') \pm \Theta(\mp(t - t')) \Sigma^{\Delta}(1, 1') \end{aligned} \tag{72}$$

¹⁹The equations for χ^R and χ^A are adjoint (C is symmetric so the adjoint equation is equivalent to (74a)).

and, according to (67c), Σ^C is given by

$$\begin{aligned} \Sigma^C(1, 1') &= is \Sigma^{(0)}(X_1, X'_1; t) \delta(t' - t_0) + \frac{is}{2} (\Sigma^>(t, t') + \Sigma^<(t, t')) \\ &\equiv \Sigma^{C,0}(X_1, X'_1; t) \delta(t' - t_0) + \Sigma^{C,reg}(t, t'), \end{aligned} \tag{73}$$

where in the last expression we introduce notations where is does not appear explicitly since indeed $is \Sigma^{(0)}$ and $is(\Sigma^> - \Sigma^<)$ are independent of s (see e.g. (43) for a similar property). With (72)–(73), the evolution equations (71a)–(71c) can be further details as follows: for all $t, t' \geq t_0$,

$$\begin{aligned} &\left[\frac{\partial}{\partial t} - L_1 \right] C(1, 1') \\ &\quad - \int dX_2 \Sigma_{tot}^\delta(X_1, X_2; t_1) C(X_2, t_1, 1') - \int_{t_0}^t dt_2 \int dX_2 \Sigma^\Delta(1, 2) C(2, 1') \\ &= \int dX_2 \Sigma^{C,0}(X_1, X_2; t_1) \chi^A(X_1, t_0; 1') + \int_{t_0}^{t'} dt_2 \int dX_2 \Sigma^{C,reg}(1, 2) \chi^A(2, 1') \\ &\quad + \delta(t - t_0) C(1, 1') \end{aligned} \tag{74a}$$

and for all $t_0 \leq t' \leq t$,

$$\begin{aligned} &\left[\frac{\partial}{\partial t} - L_1 \right] \chi^R(1, 1') \\ &\quad - \int dX_2 \Sigma_{tot}^\delta(X_1, X_2; t_1) \chi^R(X_2, t_1, 1') - \int_{t'}^t dt_2 \int dX_2 \Sigma^\Delta(1, 2) \chi^R(2, 1') \\ &= \{ \delta(1 - 1'), f(1) \} (1) \end{aligned} \tag{74b}$$

and for all $t_0 \leq t \leq t'$,

$$\begin{aligned} &\left[\frac{\partial}{\partial t} - L_1 \right] \chi^A(1, 1') \\ &\quad - \int dX_2 \Sigma_{tot}^\delta(X_1, X_2; t_1) \chi^A(X_2, t_1, 1') + \int_{t'}^t dt_2 \int dX_2 \Sigma^\Delta(1, 2) \chi^A(2, 1') \\ &= \{ \delta(1 - 1'), f(1) \} (1). \end{aligned} \tag{74c}$$

In the remaining of this section, we discuss general properties of (71a)–(71c) and make contact with previous approaches. The full closure of the set of equations for f , $\chi^{R,A}$ and C in real-time is completed in Sect. 5, where we transcribe the closure relation (61a)–(61c) in terms of $\Sigma^{R,A,C}$ and f , $\chi^{R,A}$, C .

4.3 Discussion

4.3.1 Initial Conditions

Equations (18) and (74a)–(74c) specify an initial-value problem for which $t = t' = t_0$ is the initial time. They require initial conditions for $f(X, t_0)$, $\chi^R(X, t_0; X', t_0) =$

$-\chi^A(X, t_0; X', t_0)$ and $C(X, t_0; X' t_0)$. Since $\chi^{R,A}$ must comply with (116), i.e.

$$\chi^{R/A}(X, t_0; X', t_0) = \mp\{\delta(X - X'), f(X, t_0)\}(X),$$

their initial value is fixed when $f(X, t_0)$ is given. Therefore, the initial conditions are completely specified by the given of $f(X, t_0)$ and $C(X, t_0; X' t_0)$.

4.3.2 Reversibility

Equations (74a)–(74c) form a set of causal equations with time history integrals. The presence of those memory integrals is a property of the exact statistical dynamics defined in Sect. 2 and, despite their formal resemblance with (generalized) Langevin equations, they should be distinguished from phenomenological non-equilibrium equations. Thus the complete information on time reversibility and other symmetries of the microscopic Hamilton dynamics resides in the time dependent, non-local memory kernels: the equations themselves do not single out a direction of time. The transition to irreversible dynamics can be induced by approximation, e.g., as alluded earlier, when neglecting the dependence on the initial conditions (Bogolyubov's condition).

4.3.3 Many-Body Effects

The original non-linearity of the microscopic equations (13) has become separated into several effects.²⁰ Given a certain level of fluctuations, $C(1, 1')$, the term Σ_{tot}^R can cause them to grow or decay, and when viewed as a matrix in its momentum indices, transfer fluctuations from one component of C to another. The singular part $\Sigma^{mf} + \Sigma^\delta$ is related to the instantaneous effect of the mean-field and of the correlations, respectively, while the regular part Σ^Δ describes non-Markovian (i.e. delayed) correlation effects. Another effect contained in Σ_{tot}^R is the renormalization of the spectrum of fluctuations by the many-body interactions.

The term on the left-hand side of (74a) can be interpreted as follows (a more complete discussion is given in Sect. 4.6). Given a fluctuation δN of the density around its average f , let $\delta\phi(1)$ be the potential defined such as

$$\delta N(1) = \chi^R(1, 2)\delta\phi(2).$$

In other words, we imagine that δN can be created by disturbing the system by the external potential $\delta\phi$. From (71a)–(71c), we have

$$(G - \Sigma^{mf} - \Sigma^R)(1, 2) \cdot \delta N(2) = \{\phi(1), f(1)\}.$$

Multiplying the previous equation by $\delta N(1') = \chi^R(1', 3)\delta\phi(3) = \chi^A(3, 1')\delta\phi(3)$ and ensemble averaging yields

$$(G - \Sigma^{mf} - \Sigma^R)(1, 2) \cdot C(1, 1') = \{\langle\phi(1)\phi(3)\rangle, f(1)\} \cdot \chi^A(3, 1').$$

Comparing this with (71a)–(71c), we may interpret Σ^C as an effective random source of potential fluctuations. Since, as we shall find later, Σ^C includes terms which are quadratic in C , this term can be interpreted as a source of non-linear noise which drives the fluctuations C , and couples modes of different wave numbers.

²⁰The analysis here follows closely that given by Rose [16].

More on those properties will be discussed in Sect. 4.6. In the next two subsections, we compare the results derived so far with previous works, starting with fluids at equilibrium and then with non-equilibrium kinetic theories. The comparison with those previous works is not thorough and would certainly deserve a more detailed analysis.

4.3.4 Conservation Laws

Remarkably, at every level of approximation of the memory functions $\Sigma^{R,A,C}$ consistent with our approximation procedure outlined in Sect. 3.7.2 and further discussed below in Sect. 5.2, the kinetic equations automatically agree for all times with the differential and global laws of conservation of mass, momentum and energy. This property is essential to predict the long-wavelength, low-frequency transport phenomena characteristic of the hydrodynamic regime and so well accounted for by the Boltzmann equation in the case of dilute gases.

The local mass and momentum conservation laws follow directly (18) for the distribution function $f(\mathbf{r}, \mathbf{p}, t)$, which is the well-known lowest-order equation of the BBGKY hierarchy (see, e.g., [32, 33]).

The evolution of the energy density $\rho_E(\mathbf{r}, t)$ is determined by not only by the evolution of $f(\mathbf{r}, \mathbf{p}, t)$ for the but also by the evolution of $\iint d\mathbf{p}d\mathbf{p}' C(1, 1')$ since (e.g., [33]),

$$\begin{aligned} \rho_E(\mathbf{r}, t) = & \int d\mathbf{p} [h_0(\mathbf{r}, \mathbf{p}) + \phi_0(\mathbf{r}, \mathbf{p}, t)] f(\mathbf{r}, \mathbf{p}, t) \\ & + \frac{1}{2} \iint d\mathbf{p}d\mathbf{p}' \int d\mathbf{r}' \int_0^1 d\lambda v(|\mathbf{r}'|) f_2(\mathbf{r} + (1 - \lambda)\mathbf{r}', \mathbf{p}; \mathbf{r} + \lambda\mathbf{r}', \mathbf{p}') \end{aligned} \quad (75)$$

where f_2 is the two-body distribution function (114). Since, as we shall see in Sect. 5, the expressions for any approximation of the memory functions Σ_{tot}^R and Σ^C have a leading factor given by the bare interaction vertex $\gamma_3(1, 2, 3)$ and hence by the divergence $\frac{\partial}{\partial \mathbf{p}_1}$, it is straightforward to show that the evolution equation of $\rho_E(\mathbf{r}, t)$ obtained combining (75) and (71a) is guaranteed to be a conservation equation, independently of the approximation used for the memory functions.

At that stage, we have not been able to rigorously prove something like an H-theorem that is satisfied at every level of approximation.

4.4 Equilibrium Limit, Fluctuation-Dissipation Theorem and Detailed Balance

When considering a system at equilibrium, we generally implicitly set the initial time $t_0 = -\infty$. As a consequence, statistical averages like the correlation and response functions are invariant under time translation, e.g. (see footnote 6)

$$C(t_1, t'_1) = C(t_1 + s, t'_1 + s), \quad \forall s \in \mathbb{R},$$

and are functions of the time difference $t = t_1 - t'_1$, i.e.

$$C(1, 1') \equiv C_{eq}(X_1, X'_1; t_1 - t'_1), \quad \forall t_1, t'_1.$$

As recalled in Sect. 2, a fundamental property of equilibrium fluids is the fluctuation-dissipation theorem, which simply relates C_{eq} and $\chi_{eq}^{R,A}$ as

$$\chi_{eq}^R(X, X'; t) - \chi_{eq}^A(X, X'; t) = -\beta \frac{\partial}{\partial t} C_{eq}(X, X'; t), \quad (76)$$

with the inverse temperature $\beta = 1/K_B T$. By rewriting the evolution equations (74a)–(74c) in terms of $t = t_1 - t'_1$, it is straightforward to show that these equations are consistent with the fluctuation-dissipation theorem if and only if the equilibrium memory function kernels satisfy a relation similar to (76)²¹

$$\Sigma_{eq}^R(X, X'; t) - \Sigma_{eq}^A(X, X'; t) = -\beta \frac{\partial}{\partial t} \Sigma_{eq}^{C, reg}(X, X'; t). \quad (77)$$

This relation describes detailed balance of the collision mechanisms that control the occurrence of spontaneous fluctuations and their damping.

It turns out that the evolution equations obtained by setting $t_0 = -\infty$ and $t = t_1 = t'_1$ in (74a)–(74c) are rather cumbersome to manipulate. In the study of the dynamics of equilibrium correlation functions, it is more customary to rather work with the following *explicit* expression of the correlation function,

$$C_M(X, X'; t) = C(X, t; X', 0) = \langle \delta N(X, t) \delta N(X', 0) \rangle. \quad (78)$$

This expression is one possible representation of $C_{eq}(X, X', t)$ (corresponding to $s = 0$ in $C(t + s, s) = C_{eq}(t)$); contrary to C_{eq} , C_M favors an initial time, $t_0 = t' = 0$. Previous works on the equilibrium kinetic theory of fluids and particular Mazenko's theory [13] discussed in the introduction are theories for $C_M(t)$. In our approach, the evolution equation for C_M can simply be obtained by setting both the initial time t_0 and the time t' to zero in (74a). We immediately obtain $\forall t > 0$,

$$\left[\frac{\partial}{\partial t} - L_1(X) \right] C_M(X, X'; t) - \int dX_2 \Sigma_{tot}^\delta(X; X_2; t) C_M(X_2, X', t) - \int_0^t d\bar{t} \int dX_2 \Sigma^\Delta(X, t; X_2, \bar{t}) C_M(X_2, X'; \bar{t}) = 0.$$

This evolution equation has the well-known form of memory function equations in the equilibrium theories (see footnote 6). In particular, it corresponds to Mazenko's memory function ϕ defined in [13] with the identification,

$$\begin{aligned} \Sigma_{tot}^\delta(X, \bar{X}; t) &= -\phi^s(X, \bar{X}), \\ \Sigma^\Delta(X, t; X', t') &= -\phi^c(X, X'; t - t'). \end{aligned}$$

4.5 Contact with Other Non-equilibrium Kinetic Theories

In this section, we explore the correspondence with previous non-equilibrium kinetic theories. First we make contact with some of the most popular closures of the BBGKY hierarchy. We shall see that those closures neglect the effects of the memory function kernels $\Sigma^{\Delta, C}$. Then we compare our results to the theory of Rose [16] mentioned in the introduction.

²¹To obtain (77) from (74a)–(74c), we set to zero the first term in the rhs of (74a), i.e. we assume that after the *infinite* duration separating $-\infty$ and the observation times, the initial correlations are fully damped.

Table 2 Left side: terms kept (×) and dropped (0) in the second BBGKY equation (79) for the Landau, Boltzmann, Lenard-Balescu-Guernsey and Book-Frieman closures. The latter, which was proposed to improve the close collisions in the Lenard-Balescu-Guernsey equation, simply amounts to setting the three-body correlation g_3 equal to zero. The same closures are expressed in terms of the cumulants $C^{(n)}$ in Table 1. Right side: in the approach developed in this paper, the approximations for C and D correspond to the approximations for the memory functions $\Sigma^{\delta, \Delta, C}$ given in the last three columns

Closure	A	B	C	D	Σ^δ	Σ^Δ	Σ^C
Landau	×	0	0	0	0	0	0
LBG	×	×	0	0	0	0	0
Boltzmann	×	0	×	0	(81)	0	0
Book-Frieman [36]	×	×	×	0	(81)	0	0

4.5.1 Reduction to Popular BBGKY Closures

The BBGKY hierarchy is a hierarchy for the equal-time correlation functions g_n (for convenience, we give a short reminder of the BBGKY hierarchy in Appendix A). Traditional closures of the BBGKY hierarchy are performed at the level of the evolution equation for g_2 , which reads

$$\begin{aligned}
 \left[\frac{\partial}{\partial t} - (L_1 + L_{1'}) \right] g_2(1, 1') &= \underbrace{L_{11'} f(1) f(1')}_A \\
 &+ \underbrace{\int d2 L_{12} f(1) g_2(1', 2) + L_{1'2} f(1') g_2(1, 2) + [L_{12} + L_{1'2}] f(2) g_2(1, 1')}_B \\
 &+ \underbrace{L_{11'} g_2(1, 1')}_C + \underbrace{\int d2 (L_{12} + L_{1'2}) g_3(1, 1', 2)}_D, \tag{79}
 \end{aligned}$$

where, throughout this sub-section, we write $1 = (\mathbf{r}, \mathbf{p})$ and all quantities are evaluated at the same time $t = t_1 = \dots = t_n$. They rely, among other hypothesis, on an assumed ordering of the correlations g_n in terms of an adequately chosen small parameter λ [8],

$$g_n = O(\lambda^n).$$

The Landau, Boltzmann and Lenard-Balescu-Guernsey closures give evolution equations for f that are second order in λ . The Landau closure is valid for so-called weakly coupled systems and λ is the dimensionless strength of the potential ($v(r) = \lambda \bar{v}(r)$ in (4)). The perturbation parameter in the Boltzmann equation is the density parameter $\lambda = nl_C^3$ where n is the particle density and l_C is the correlation length. The Lenard-Balescu-Guernsey equation is an equation for weakly-coupled plasmas and λ is the so-called plasma parameter $\lambda = q^2 / ak_B T$ (q is the particles charge, $a = n^{-1/3}$ is the interparticle spacing). In the Lenard-Balescu-Guernsey equation, the plasma is represented as a weakly coupled system in which the collisions are due to the interactions via an effective, dynamically screened potential. For those popular closures, Table 2 shows the terms that are kept (×) and dropped (0) in the evolution equation (79).

In our approach, the equation for $g_2(1, 1') = C(1, 1') - \delta(1 - 1')f(1)$ can be easily obtained from (74a) as

$$\left[\frac{\partial}{\partial t} - (L_1 + L_{1'}) \right] g_2(1, 1') = L_{11'} f(1) f(1') \quad (80a)$$

$$+ \int d2 L_{12} f(1) g_2(1', 2) + L_{1'2} f(1') g_2(1, 2) + [L_{12} + L_{1'2}] f(2) g_2(1, 1') \quad (80b)$$

$$+ \int d2 \Sigma^\delta(12) g_2(2, 1') + \Sigma^\delta(1'2) g_2(2, 1) \quad (80c)$$

$$+ \int d2 \Sigma^\Delta(12) g_2(2, 1') + g_2(1, 2) \Sigma^\Delta(21') \quad (80d)$$

$$+ \int d2 \Sigma^C(12) \chi^A(2, 1') + \chi^R(1, 2) \Sigma^C(21'), \quad (80e)$$

where $t = t' = t_2$ is implied. We note that in the rhs, the terms on lines (80a) and (80b), which are just the A and B terms of (79), come from the mean-field term Σ^{mf} , while all the other terms come from memory functions $\Sigma^{R,A,C}$. The term $C + D$ of (79) are replaced by the last three lines in (80a)–(80e).

In order to appreciate better the physics contained in those memory function terms, we translate the traditional closures discussed before in terms of approximations of (80a)–(80e); the results are summarized in Table 2.

Both the Landau and Lenard-Balescu-Guernsey closures discard all the terms involving the memory functions, which amounts to setting $\Sigma^{\delta,\Delta,C} = 0$ (Landau retains (80a) only and Landau-Balescu-Guernsey discards the terms (80c) through (80e)). This simply tells us that memory functions will account for effects not accounted in those closures, for instance by adding the effects of static (Σ^δ) and dynamic (Σ^Δ) correlations on the effective, dynamically screened interparticle potential through which particles mutually interact.

The Boltzmann and Book-Frieman equations are recovered by (i) discarding (80b), (ii) setting $\Sigma^\Delta = \Sigma^C = 0$, and (iii) using the following approximation for Σ^δ ,

$$\Sigma^\delta(11') = \gamma_3(123)\delta(1' - 2)\delta(1' - 3) = \frac{\partial \tilde{v}(1 - 1')}{\partial \mathbf{r}} \cdot \frac{\partial \delta(1 - 1')}{\partial \mathbf{p}}, \quad (81)$$

which, together with (80c) yields the term C of the second BBGKY equation (79) that describes bare two-particle interactions (uncorrelated binary collisions). The approximation (81) can be obtained using (63) together with the approximation $C(11') \approx \delta(1 - 1')f(1)$ (see Table 1). Indeed, we obtain

$$\begin{aligned} \{\Sigma^\delta(1, 1'), f(1')\}(1') &= \gamma_3(123)\{\delta(1' - 3), \delta(1' - 2)f(1')\}(1') \\ &= \gamma_3(123)\{\delta(1' - 3)\delta(1' - 2), f(1')\}(1'), \end{aligned}$$

which implies (81).

In summary, this quick comparison reveals that inclusion of any coherent approximation for the memory functions $\Sigma^{R,A,C}$ will bring in physics information that is neglected in traditional closures.

4.5.2 Connection with MSR and Rose’s Theories

General Remarks The present theory retains two main imprints of quantum mechanics, namely the classical amplitude $e^{\frac{i}{\hbar}S}$ with the action parameter s and the closed-time contour idea of Schwinger. In contrast, MSR [15] is based on the concepts of canonical quantization using field doubling via conjugate response field and, in Rose [16], on the second quantization using the occupation number representation in phase-space. Thus, MSR and Rose’s theories recast the classical problem in a form identical to quantum mechanics, while our approach should be seen as a classical limit of the quantum theory.

Another difference is in the nature of the external coupling. In MSR and Rose, as usually is the case in quantum field theory [29], the coupling corresponds to a source term in the evolution equation of the field, while here the coupling is an additional term in the Hamiltonian. The response function in MSR and Rose thus describes the response to an infinitesimal source of particles while in the present theory it describes the response to a disturbance produced by an externally applied force field. Since all three theories use similar renormalization techniques based on a generating functional and a Legendre transform, the equations obtained look alike. As we shall see, our results encompass the results of Rose’s renormalized kinetic theory [16] for any initial conditions. The ingenious formal devices introduced by MSR and Rose naturally arise in the present formalism.

Technical Comparison Briefly speaking, Rose’s theory is a theory for the correlation function C and the response function R that measures the linear response of the phase-space density to an infinitesimal source term η in the field equation (18), i.e.

$$\left[\frac{\partial}{\partial t_1} - L_1 \right] f(1) - \{u^{mf}(1), f(1)\} - \frac{1}{2} \gamma_3(1, 2, 3)C(2, 3) = \eta(1) \tag{82}$$

and

$$R(1, 1') = \left. \frac{\delta f(1)}{\delta \eta(1')} \right|_{\eta=0}.$$

The function R can also be regarded as the Green’s function of the linearized version of (18).

On the other hand, in our theory χ^R describes the linear response to a variation $\phi_0 + \delta\phi_0$ of the external potential. In the presence of $\delta\phi_0$, the evolution equation (18) can be regarded as (82) with the source term

$$\eta(1) = \{\delta\phi_0(1), f(1)\}$$

which has the particularity of conserving the number of particles (since the momentum integral vanishes). In the linear regime, we can write

$$\begin{aligned} \delta f(1) &= \chi^R(1, 2)\delta\phi_0(2) \\ &= R(1, 2)\eta(2) = -\{R(1, 2), f(2)\}(2)\delta\phi_0(2) \end{aligned}$$

and therefore,

$$\chi^R(1, 1') = -\{R(1, 1'), f(1')\}(1'). \tag{83}$$

When introduced into the evolution equations (71a)–(71c) for $\chi^{R,A}$ and C , we find

$$\left[\frac{\partial}{\partial t} - L_1(1) \right] R(1, 1') - \int d2 \Sigma_{tot}^R(1, 2) R(2, 1') = \delta(1 - 1') \tag{84}$$

and

$$\begin{aligned} & \left[\frac{\partial}{\partial t} - L_1(1) \right] C(1, 1') - \int d2 \Sigma_{tot}^R(1, 2) C(2, 1') \\ & = \int d2 \{ \Sigma^C(1, 2), f(2) \} (2) R(1', 2) + \delta(t - t_0) C(1, 1'). \end{aligned} \tag{85}$$

These equations are equivalent to the (Dyson) equations (63) and (64) of [16] derived by H. Rose, with the correspondence

$$\begin{aligned} \Sigma_{-+}(1, 2) &= \Sigma_{tot}^R(1, 2), \\ \Sigma_{--}(1, 2) &= \{ \Sigma^{C,reg}(1, 2), f(2) \} (2), \\ 0 &= \Sigma^{C,0}. \end{aligned} \tag{86}$$

The last equation is the consequence of the fact that Rose assumes Gaussian initial conditions. Although as noted by Rose in his Appendix A, formalisms developed by Deker [37] and more recently by Andersen [38] exist to extend their validity to general initial conditions, we have not performed the extension ourself yet. The closure relations, i.e. the functional equations for the memory functions, in Rose and our formalism (see Sect. 5) look quite different (simply because they involve different starting points and ingredients) and are thus difficult to compare. Moreover, Rose points out that the closure relations (52)–(62) of his paper are “exact if and only if the initial conditions satisfy a Wick-type theorem”, i.e. are Gaussian. Nevertheless, assuming Gaussian initial correlations in our formalism, the lowest order approximations in both approaches are the same (see Sect. 5). At this point, it is not clear which approach is more handy when it comes to practical calculations.

4.6 Formal Solution for $C(1, 1')$. Dependence on Initial Conditions

In this paragraph, we show that it is possible to solve at least formally the evolution equation (71a) for the correlation function $C(1, 1')$ in terms of the response functions $\chi^{R,A}$ and Green’s function R , respectively. When introduced in the collision integral (18), this solution may be used to build a kinetic equation for the distribution function f . In its simplest approximation, this approach corresponds to the quasi-linear theory used for instance in plasma physics to derive the Lenard-Balescu equation [39]. The solution given below is exact and takes care of the initial conditions.

General Expression Using the definitions of Sect. 4.1, it is straightforward to show that the inverse Γ of the closed-time response function χ defined by (56) can be represented as,²²

$$\hat{\Gamma} = \begin{pmatrix} 0 & \Gamma^A \\ \Gamma^R & \frac{2}{is} \Gamma^C \end{pmatrix},$$

²²Using the identity $Q\sigma_z Q^\dagger = \sigma_x$, we find the matrix representation of (56),

$$\hat{\Gamma} \hat{\sigma}_x \hat{\chi} \delta(1 - 1') = \hat{\sigma}_x \delta(1 - 1'), \tag{87}$$

where $\hat{\Gamma} = Q \bar{\Gamma} Q^\dagger$ and $\bar{\Gamma}$ is defined as in (64).

where the components Γ^R and Γ^A merely are the inverse of the retarded (advanced) response function χ^R and χ^A , respectively, i.e.

$$\begin{aligned} \Gamma^R(1, 2) \cdot \chi^R(2, 1') &= \chi^R(1, 2) \cdot \Gamma^R(2, 1') = \delta(1 - 1'), \\ \Gamma^A(1, 2) \cdot \chi^A(2, 1') &= \chi^A(1, 2) \cdot \Gamma^A(2, 1') = \delta(1 - 1'), \end{aligned} \tag{88}$$

and Γ^C is related to the correlation function as,

$$\Gamma^C(1, 1') = -\Gamma^R(1, 2)C(2, 3)\Gamma^A(3, 1'). \tag{89}$$

Equation (89) implies the following formal solution of its evolution equation (71a)

$$C(1, 1') = -\chi^R(1, 2)\Gamma^C(2, 3)\chi^A(3, 1') = -\chi^R(1, 2)\chi^R(1', 3)\Gamma^C(2, 3) \tag{90}$$

in terms of $\chi^{R,A}$ and of the quantity Γ^C . Another expression can be obtained using the relation (83) between χ^R and the Green's function R in (90) and yields

$$C(1, 1') = R(1, 2)R(1', 3)S(2, 3), \tag{91}$$

where we introduce the symmetric kernel,

$$S(1, 1') = -\{\{\Gamma^C(1, 1'), f(1)\}, f(1')\}. \tag{92}$$

Equation (89) can easily be verified by substitution into the evolution equation (71a), while (91) is solution of

$$\begin{aligned} \left[\frac{\partial}{\partial t} - L_1 \right] C(1, 1') - \int_{t_0}^{\infty} dt_2 \int dX_2 \Sigma_{tot}^R(1, 2)C(2, 1') \\ = \int_{t_0}^{\infty} dt_2 \int dX_2 S(1, 2)R(1', 2) + \delta(t - t_0)C(1, 1'), \end{aligned} \tag{93}$$

obtained by rewriting the rhs of (71a) with (83).²³ They may be considered as a generalized form of the fluctuation-dissipation theorem in the sense that they express the overall level of density fluctuations C as balance between forcing (through Γ^C or S) and dissipation (encapsulated in $\chi^{R,A}$ or R) [14]. In the next paragraph we show how (89)–(91) can be further split into more fundamental components.

Detailed expression Introducing (89) into (71a) leads to the following relation between Γ^C and Σ^C ,

$$\{\Gamma^C(1, 1'), f(1)\}(1') = \Sigma^C(1, 1') + \delta(t - t_0)C(1, 2)\Gamma^A(2, 1'), \tag{94}$$

which, as proved in details in Appendix G, imply the following structure for $\Gamma^C(1, 1')$,

$$\begin{aligned} \Gamma^C(1, 1') &= \Gamma^{reg}(1, 1') + \delta(t' - t_0)\Gamma^\delta(X_1, X'_1; t) + \delta(t - t_0)\Gamma^\delta(X'_1, X_1; t') \\ &\quad + \delta(t - t_0)\delta(t' - t_0)\Gamma^{(0)}(X_1, X'_1), \end{aligned} \tag{95}$$

²³In the approximation $\Sigma^{(0)} = 0$ (Gaussian initial conditions), S correspond to Σ_{--} in Rose's paper discussed in Sect. 4.5.2.

where $\Gamma^{reg,\delta,0}$ are given by

$$\{\Gamma^{reg}(1, 1'), f(1)\}(1') = \frac{iS}{2}(\Sigma^>(1, 1') + \Sigma^<(1, 1')) \quad (96a)$$

$$\{\Gamma^\delta(X_1, X'_1; t), f(1)\}(1') = iS\Sigma^{(0)}(X_1, X'_1; t) \quad (96b)$$

and

$$\{\{\Gamma^{(0)}(X_1, X'_1), f(X_1, t_0)\}, f(X'_1, t_0)\} = C_0(X_1, X'_1),$$

where $C_0(X_1, X'_1) = C(X_1, t_0; X'_1, t_0)$ is the initial value of the correlation function. Similarly, (92) implies

$$\begin{aligned} S(1, 1') &= S^{reg}(1, 1') + \delta(t' - t_0)S^\delta(X_1, X'_1; t) + \delta(t - t_0)S^\delta(X'_1, X_1; t') \\ &\quad + \delta(t - t_0)\delta(t' - t_0)S^0(X_1, X'_1) \end{aligned}$$

with

$$\begin{aligned} S^{reg}(1, 1') &= \frac{iS}{2}\{\Sigma^>(1, 1') + \Sigma^<(1, 1'), f(1')\}(1'), \\ S^\delta(X_1, X'_1; t) &= iS\{\Sigma^{(0)}(X_1, X'_1; t), f(1')\}(1'), \\ S^0(X_1, X'_1) &= C_0(X_1, X'_1). \end{aligned}$$

Substituting those expressions into (89)–(91), we obtain expressions that describe the temporal evolution of the correlation function from its initial value $C(X_1, t_0; X'_1, t_0)$ to $C(X_1, t; X'_1, t')$ at times $t, t' \geq t_0$,

$$\begin{aligned} C(1, 1') &= \iint dX_2 dX_3 \chi^R(1; X_2, t_0) \Gamma^{(0)}(X_2, X_3) \chi^A(X_3, t_0; 1') \\ &\quad + \int_{t_0}^t dt_2 \iint dX_2 dX_3 \chi^R(1, 2) \Gamma^\delta(X_2, X_3; t_2) \chi^A(X_3, t_0; 1') \\ &\quad + \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 \chi^R(1; X_2, t_0) \Gamma^\delta(X_2, X_3; t_3) \chi^A(3; 1') \\ &\quad + \int_{t_0}^t dt_2 \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 \chi^R(1, 2) \Gamma^{reg}(23) \chi^A(3, 1') \quad (97a) \end{aligned}$$

$$\begin{aligned} &= \iint dX_2 dX_3 R(1; X_2, t_0) R(1'; X_3, t_0) C_0(X_2, X_3) \\ &\quad + \int_{t_0}^t dt_2 \iint dX_2 dX_3 R(1, 2) R(1'; X_3, t_0) S^\delta(X_2, X_3; t_2) \\ &\quad + \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 R(1; X_2, t_0) R(1', 3) S^\delta(X_2, X_3; t_3) \\ &\quad + \int_{t_0}^t dt_2 \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 R(1, 2) R(1', 3) S^{reg}(23). \quad (97b) \end{aligned}$$

We can shed light on the different components of (97a)–(97b) by considering the dynamics of the density fluctuations $\Delta N(1)$. An equation of motion for $\Delta N(1) = N(1) - f(1)$ is easily obtained by subtracting (18) from (16). By subtracting the quantity $\Sigma^R(1, 2)\delta N(2)$ on both sides of the resulting equation, we find

$$\begin{aligned} &\left(\frac{\partial}{\partial t_1} - L_1\right)\delta N(1) - \Sigma^{mf}(1, 2)\delta N(2) - \Sigma^R(1, 2)\delta N(2) \\ &= \frac{1}{2}\gamma_3(1, 2, 3)(N(2)N(3) - C(2, 3)) - \Sigma^R(1, 2)\delta N(2) \equiv \delta\mathcal{F}(1), \end{aligned}$$

which can formally be integrated in terms of the Green’s function $R(1, 1')$ (recall (84)) as

$$\delta N(1) = \int dX_2 R(1; X_2, t_0)\delta N(X_2, t_0) + \int_{t_0}^t dt_2 \int dX_2 R(1, 2)\delta\mathcal{F}(2). \tag{98}$$

Thus the microscopic phase-space density fluctuation is written as the sum of two terms. The first term represents the propagation in the fluid of the density fluctuation that would be caused by a small initial perturbation $\delta N(X_2, t_0)$ in f . Roughly speaking, it describes how a microscopic fluctuation propagates in the fluid *on average and neglecting non-linear effects*. The second term in (98) describes the corrections to this interpretation that manifest in the equation of motion in the source term $\delta\mathcal{F}$ and in the solution (98) through non-local effects in both space and time. Using (98) to build the correlation function $C(1, 1') = \langle \delta N(1)\delta N(1') \rangle$ lead to the four contributions in (97b) with

$$\begin{aligned} \mathcal{S}^{reg}(1, 1') &= \langle \delta\mathcal{F}(1)\delta\mathcal{F}(1') \rangle, \\ \mathcal{S}^\delta(X_1, X'_1; t) &= \langle \delta\mathcal{F}(1)\delta N(X'_1, t_0) \rangle. \end{aligned} \tag{99}$$

Thus, the first term in (97b) describes the contribution obtained when propagating the initial fluctuations as if they were small, independent perturbations on the fluid. The three other terms represent the corrections to this picture, which allows us to express the components of the spectral function \mathcal{S} in terms of correlation functions between the noise term $\delta\mathcal{F}$ and the initial fluctuations δN : $\mathcal{S}^{reg}(1, 1')$ is the autocorrelation function of the noise term $\delta\mathcal{F}$ while \mathcal{S}^{reg} describes the influence the initial conditions.

Equation (97b) exhibits the influence of initial correlations in the initial state; the latter can be important when considering ultrafast relaxation processes when t, t' approach t_0 . The influence of initial correlations is often neglected in kinetic theory by invoking the condition of complete suppression of initial correlations (a.k.a. Bogolyubov’s condition [31]) according to which all initial correlations existing at t_0 are damped at a sufficiently large time $t - t_0 \gg t_{cor}$. Inspection of (97b) suggests that t_{cor} is determined by the decorrelation time of $\mathcal{S}^\delta(X_1, X'_1; t)$ in (99) and by the properties of $R(1, 1')$. Then for times $t - t_0 \gg t_{cor}$, we set $\mathcal{S}^\delta \equiv 0$ and

$$C_0(X_1, X'_1) = C_0^{ideal}(X_1, X'_1) = f_0(\mathbf{r}, \mathbf{p})\delta(\mathbf{r} - \mathbf{r}')\delta(\mathbf{p} - \mathbf{p}')$$

where $f_0(\mathbf{r}, \mathbf{p}) = \langle \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j)\delta(\mathbf{p} - \mathbf{p}_j) \rangle$ is the initial single-particle distribution function such that

$$\begin{aligned} C(1, 1') &= \iint dX_2 dX_3 R(1; X_2, t_0)R(1'; X_3, t_0)C_0^{ideal}(X_2, X_3) \\ &+ \int_{t_0}^t dt_2 \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 R(1, 2)R(1', 3)\mathcal{S}^{reg}(23). \end{aligned}$$

When dynamical correlations are altogether discarded ($\Sigma^{R,A,C} = 0$), then

$$C(1, 1') = \iint dX_2 dX_3 R^{mf}(1; X_2, t_0) R^{mf}(1'; X_3, t_0) C_0^{ideal}(X_2, X_3)$$

with $[\frac{\partial}{\partial t} - L_1(1)]R(1, 1') - \Sigma^{mf}(1, 2)R(2, 1') = \delta(1 - 1')$ corresponding to the linearized Vlasov equation, which in plasma physics is known as the quasi-linear theory and leads to the Lenard-Balescu-Guernsey equation.

5 Real-Time Formalism (II)

The previous section focused on the derivation of the coupled evolution equations for the correlation and response functions in terms of the $\Sigma^{R,A,C}$. Here we concentrate on translating to real time the closure relations (58) and (61a)–(61c) to obtain the equivalent relations for the real-time components $\Sigma^{R,A,C}$. Although it is possible to directly translate (59) in terms of the matrix components $\chi^{R,A,C}$, $\Sigma^{R,A,C}$ and of the components of the tensor obtained from the different components of the three-point vertex $\Gamma^{(3)}$ [40, 41], the manipulations are not trivial and we prefer the approach described below. A considerable advantage of this alternative approach is that it allows us to introduce an equivalent formulation of the closed-time contour approach, which directly generates the correlation C and response functions $\chi^{R,A}$.

5.1 Real-Time Representation of the Generating Functional

Given a potential $\phi(\tau)$ on the closed-time contour, we define the physical component $\phi_p(t)$ and non-physical $\phi_\Delta(t)$ on the real-time axis as

$$\begin{cases} \phi_p(X, t) = \frac{1}{2}[\phi(X, \tau_+) + \phi(X, \tau_-)], \\ \phi_\Delta(X, t) = \phi(X, \tau_+) - \phi(X, \tau_-), \end{cases} \quad (100)$$

where $t = t(\tau_+) = t(\tau_-)$. In this representation, physical potentials are simply characterized by $\phi_\Delta \equiv 0$. Similarly, we define the ‘physical’ and ‘non-physical’ components of the phase-space density as,²⁴

$$\begin{cases} \mathcal{N}_p(X, t) = \frac{1}{2}[\mathcal{N}(X, \tau_+) + \mathcal{N}(X, \tau_-)], \\ \mathcal{N}_\Delta(X, t) = \mathcal{N}(X, \tau_+) - \mathcal{N}(X, \tau_-). \end{cases} \quad (101)$$

For a physical potential, the phase-space density is equal on both sides of the contour and therefore $\mathcal{N}_\Delta(X, t) = 0$ and $\mathcal{N}_p(X, t)$ equals the phase-space density of the system under investigation in the external potential ϕ_p . With these definitions, the coupling term in the action (30) writes

$$\oint d\tilde{I} \tilde{\mathcal{N}}(\tilde{I}) \phi(\tilde{I}) = \int_{i_0}^{\infty} \int dX_1 \phi_p(1) \mathcal{N}_\Delta(1) + \phi_\Delta(1) \mathcal{N}_p(1), \quad (102)$$

which shows that ϕ_p linearly couples \mathcal{N}_Δ while ϕ_Δ couples to \mathcal{N}_p ; accordingly, variations with respect to ϕ_Δ will generate the physical phase-space distribution under investigation.

²⁴Interestingly, in quantum field theory, this splitting defines the classical and quantum components of the field, where the latter describes quantum fluctuations around the classical trajectory.

Equation (100) defines a one-to-one mapping between the potentials ϕ and the vector of potentials (ϕ_p, ϕ_Δ) . As a consequence, the generating functional $\tilde{\Omega}[\phi]$ can be replaced by the action functional $\Omega[\phi_p, \phi_\Delta]$ defined as

$$\Omega[\phi_p, \phi_\Delta] \equiv \tilde{\Omega}[\phi]. \tag{103}$$

In terms of the new variables, the Taylor expansion (34) around the external potential ϕ_0 becomes,

$$\begin{aligned} \Omega[\phi_0 + \delta\phi_p, \delta\phi_\Delta] &= \sum_{j,k=0}^{\infty} \frac{1}{j!k!} \int d1 \dots dj \int d1' \dots dk' \\ &\times \underbrace{\Omega_{1\dots 1}}_{j \text{ times}} \underbrace{2\dots 2}_{k \text{ times}}(1 \dots n; 1' \dots n') \delta\phi_p(1) \dots \delta\phi_p(j) \phi_\Delta(1') \dots \delta\phi_\Delta(k') \end{aligned} \tag{104}$$

where

$$\underbrace{\Omega_{1\dots 1}}_{j \text{ times}} \underbrace{2\dots 2}_{k \text{ times}}(1 \dots j; 1' \dots k') = \left. \frac{\delta^{j+k} \Omega}{\delta\phi_p(1) \dots \delta\phi_p(j) \delta\phi_\Delta(1') \dots \delta\phi_\Delta(k')} \right|_{\phi_p=\phi_0, \phi_\Delta=0}.$$

Explicit expressions for these derivatives can be obtained either from the $\tilde{\Omega}^{(n)}[\phi]$ or from a systematic perturbation expansion in the bare interaction as shown in Appendix C.²⁵

The first derivatives generate the phase-space density $f(\mathbf{r}, \mathbf{p}, t)$ under investigation,

$$\left. \frac{\delta \Omega}{\delta \phi_p(1)} \right|_{\phi_p=\phi_0, \phi_\Delta=0} = 0, \quad \left. \frac{\delta \Omega}{\delta \phi_\Delta(1)} \right|_{\phi_p=\phi_0, \phi_\Delta=0} = f(1).$$

²⁵ It is possible to derive explicit expressions for the higher-order derivatives $\Omega_{1\dots 1 2\dots 2}$ as ensemble average of combinations of products and Poisson brackets of the fundamental field $N(\mathbf{r}, \mathbf{p}, t)$, which exhaust all possible n -points functions [40]. In addition, we can also obtain the following properties. Firstly, from the normalization $\int dx_0 F_0(x_0) = 1$, $\Omega[\phi_p, 0] = 1$ and therefore, from (104),

$$\Omega_{1\dots 1}(1, \dots, n) = 0, \quad \forall n \geq 1.$$

Secondly, from $f_\Delta(1) = \delta\Omega/\delta\phi_p(1)|_{\phi_\Delta=0} = 0$, we find $\Gamma[f_p, 0] = 0$ and

$$\Gamma_{1\dots 1}(1, \dots, n) = 0, \quad \forall n \geq 1.$$

Third, it can be shown the causality property,

$$\begin{aligned} \underbrace{\Omega_{1\dots 1}}_{j \text{ times}} \underbrace{2\dots 2}_{k \text{ times}}(1 \dots j; 1' \dots k') &= 0, \\ \underbrace{\Gamma_{1\dots 1}}_{j \text{ times}} \underbrace{2\dots 2}_{k \text{ times}}(1 \dots j; 1' \dots k') &= 0 \end{aligned}$$

provided any unprimed time $t_i, i = 1, \dots, j$, is greater than a primed time $t'_i, i = 1, \dots, k$.

Most remarkably, the second (partial) derivatives directly generate the retarded and advanced response functions and correlation functions,

$$\begin{cases} \Omega_{11}(1, 2) = 0, \\ \Omega_{12}(1, 2) = \chi^A(1, 2), \\ \Omega_{21}(1, 2) = \chi^R(1, 2), \\ \Omega_{22}(1, 2) = \frac{1}{is}C(1, 2). \end{cases} \tag{105}$$

We therefore obtain the noteworthy result that a generating functional defined in terms of real-time quantities exists that generates the phase-space distribution, the correlation function C and response functions $\chi^{R,A}$.

We now continue the closure procedure by adapting the steps of Sect. 3 to the new action functional (103). We define the effective potential as the Legendre transform,

$$\Gamma[f_p, f_\Delta] = -\Omega[\phi_p, \phi_\Delta] + \int d1 f_p(1)\phi_\Delta(1) + f_\Delta(1)\phi_p(1). \tag{106}$$

Its derivatives at $f_p = f, f_\Delta = 0$ define the vertex functions

$$\Gamma_{\underbrace{1 \dots 1}_{j \text{ times}} \underbrace{2 \dots 2}_{k \text{ times}}}(1 \dots j; 1' \dots k') = \frac{\delta^{j+k}\Gamma}{\delta f_p(1) \dots \delta f_p(j)\delta f_\Delta(1') \dots \delta f_\Delta(k')} \Big|_{f_p=f, f_\Delta=0}.$$

The first derivative generates the external potential ϕ_0 ,

$$\frac{\delta\Gamma}{\delta f_p(1)} \Big|_{f_p=f, f_\Delta=0} = 0, \quad \frac{\delta\Gamma}{\delta f_\Delta(1)} \Big|_{f_p=f, f_\Delta=0} = \phi_0(1),$$

while, as shown in the Appendix H.1, the second-order derivatives directly yield the $\Gamma^{R,A,C}$, i.e.²⁶

$$\begin{cases} \Gamma_{11}(1, 1') = 0, \\ \Gamma_{12}(1, 1') = \Gamma^A(1, 1'), \\ \Gamma_{21}(1, 1') = \Gamma^R(1, 1'), \\ \Gamma_{22}(1, 1') = \frac{1}{is}\Gamma^C(1, 1'). \end{cases} \tag{107}$$

Higher order vertex functions can be obtained by taking the successive derivatives with respect to the potentials with the chain rule of differentiation. The direct calculations become rapidly cumbersome with the growing number of indices and variables and, in Appendix H, we present a graphical method that allows their calculation in a much more economical manner. We just give here the results for those derivatives of importance in the present work, namely

$$-\Omega_{221}(123) = \Omega_{22}(1\bar{1})\Omega_{21}(2\bar{2})\Omega_{12}(3\bar{3})\Gamma_{121}(\bar{1}\bar{2}\bar{3})$$

²⁶We thus find that the matrix representations $\hat{\chi}$ and $\hat{\Gamma}$ defined in Sect. 4.1 are simply given by

$$\hat{\chi} = \begin{pmatrix} 0 & \Omega_{12} \\ \Omega_{21} & 2\Omega_{22} \end{pmatrix}, \quad \hat{\Gamma} = \begin{pmatrix} 0 & \Gamma_{12} \\ \Gamma_{21} & 2\Gamma_{22} \end{pmatrix}.$$

$$\begin{aligned}
 & + \Omega_{21}(1\bar{1})\Omega_{22}(2\bar{2})\Omega_{12}(3\bar{3})\Gamma_{211}(\bar{1}\bar{2}\bar{3}) \\
 & + \Omega_{21}(1\bar{1})\Omega_{21}(2\bar{2})\Omega_{12}(3\bar{3})\Gamma_{221}(\bar{1}\bar{2}\bar{3}), \tag{108a}
 \end{aligned}$$

$$\begin{aligned}
 -\Omega_{222}(123) & = [\Omega_{21}(1\bar{1})\Omega_{22}(2\bar{2})\Omega_{22}(3\bar{3})\Gamma_{211}(\bar{1}\bar{2}\bar{3}) + c.p.] \\
 & + [\Omega_{21}(1\bar{1})\Omega_{21}(2\bar{2})\Omega_{22}(3\bar{3})\Gamma_{221}(\bar{1}\bar{2}\bar{3}) + c.p.] \\
 & + \Omega_{21}(1\bar{1})\Omega_{21}(2\bar{2})\Omega_{21}(3\bar{3})\Gamma_{222}(\bar{1}\bar{2}\bar{3}) \tag{108b}
 \end{aligned}$$

where c.p. stands for cyclic permutation of the triplet $(1\bar{1}, 2\bar{2}, 3\bar{3})$. These equations are the transcription in terms of real-time quantities of (57) derived before.

5.2 Real-Time Representation of the Closure

The same steps described in Sects. 3.6–3.7 to derive the closure can be followed with the evolution equations for $\mathcal{N}_{p,\Delta}$ as a starting point. The main steps are given in Appendix I and can be summarized as follows. From the evolution equation for $\mathcal{N}_{p,\Delta}$, we first obtain the evolution equation for $f_{p,\Delta}$ by averaging and for $\chi^{R,A}$ and C by functional differentiation using (105). The collision operators in those equations involve the third order derivatives Ω_{ijk} and are reexpressed in terms of memory function $\Sigma^{R,A,C}$ using (108a)–(108b). The overall procedure directly leads to the evolution equations (71a)–(71c) for $\chi^{R,A}$ and C together with the following closure relations

$$\Sigma^R(1, 1') = \frac{1}{2}\gamma_3(123) \left. \frac{\delta C(2, 3)}{\delta f_p(1')} \right|_{f_p; f_\Delta=0}, \tag{109a}$$

$$\Sigma^A(1, 1') = is\gamma_3(123) \left. \frac{\delta \chi^R(2, 3)}{\delta f_\Delta(1')} \right|_{f_p; f_\Delta=0}, \tag{109b}$$

$$\Sigma^C(1, 1') = \frac{is}{2}\gamma_3(123) \left. \frac{\delta C(2, 3)}{\delta f_\Delta(1')} \right|_{f_p; f_\Delta=0} \tag{109c}$$

or, after performing the functional differentiations,

$$\begin{aligned}
 \Sigma^R(1, 1') & = -\frac{is}{2}\gamma_3(123)[\Omega_{21}(2\bar{2})\Omega_{21}(3\bar{3})\Gamma_{221}(\bar{2}, \bar{3}, 1') \\
 & + 2\Omega_{22}(2\bar{2})\Omega_{21}(3\bar{3})\Gamma_{121}(\bar{2}, \bar{3}, 1')], \tag{110a}
 \end{aligned}$$

$$\begin{aligned}
 \Sigma^A(1, 1') & = -is\gamma_3(123)[\Omega_{12}(2\bar{2})\Omega_{21}(3\bar{3})\Gamma_{122}(\bar{2}, \bar{3}, 1') \\
 & + \Omega_{12}(2\bar{2})\Omega_{22}(3\bar{3})\Gamma_{112}(\bar{2}, \bar{3}, 1')], \tag{110b}
 \end{aligned}$$

$$\begin{aligned}
 \Sigma^C(1, 1') & = -\frac{(is)^2}{2}\gamma_3(123)[\Omega_{22}(2\bar{2})\Omega_{22}(3\bar{3})\Gamma_{112}(\bar{2}, \bar{3}, 1') \\
 & + 2\Omega_{21}(2\bar{2})\Omega_{22}(3\bar{3})\Gamma_{212}(\bar{2}, \bar{3}, 1') + \Omega_{21}(2\bar{2})\Omega_{21}(3\bar{3})\Gamma_{222}(\bar{2}, \bar{3}, 1')]. \tag{110c}
 \end{aligned}$$

These equations for $\Sigma^{R,A,C}$ are the transcription in real-time of the closed-time contour formulas (59) and (58). The set of equations consisting of the evolution equations (18) and (71a)–(71c) together with (109a)–(109c) is formally closed.

As in Sect. 3.7, the evolution equations (71a)–(71c) can be used to derive additional relations between the memory and vertex functions to derive functional equations for the

memory functions $\Sigma^{R,A,C}$. The details of the calculations are given in Appendix I. The resulting closure relations can be expressed in a variety of equivalent forms in terms of the quantities $C, \chi^{R,A}, R, \Sigma^{R,A,C}$ and \mathcal{S} encountered before, and we choose to give them in the following form (which is most directly comparable with previous works, e.g. [16]):

$$\begin{aligned} \Sigma^R(1, 1') &= \gamma_3(123)\gamma_3(\bar{2}\bar{3}1')R(\bar{2}\bar{2})C(\bar{3}\bar{3}) + \gamma_3(123)R(\bar{2}\bar{2})C(\bar{3}\bar{3})\frac{\delta\Sigma^R(\bar{2}\bar{3})}{\delta f_p(1')} \\ &\quad + \frac{1}{2}\gamma_3(123)R(\bar{2}\bar{2})R(\bar{3}\bar{3})\frac{\delta\mathcal{S}(\bar{2}\bar{3})}{\delta f_p(1')} \end{aligned} \tag{111}$$

and (see Sect. 4.6),

$$\begin{aligned} \mathcal{S}^{reg}(1, 1') &= \frac{1}{2}\gamma_3(123)\gamma_3(1'\bar{2}\bar{3})C(\bar{2}\bar{2})C(\bar{3}\bar{3}) + \frac{1}{2}\gamma_3(123)C(\bar{2}\bar{2})C(\bar{3}\bar{3})\frac{\delta\Sigma^R(1'\bar{3})}{\delta f_p(\bar{2})} \\ &\quad + is\gamma_3(123)\chi^R(\bar{2}\bar{2})C(\bar{3}\bar{3})\frac{\delta\Sigma^R(1'\bar{3})}{\delta f_\Delta(\bar{2})} + is\gamma_3(123)\chi^R(\bar{2}\bar{2})\chi^R(\bar{3}\bar{3})\frac{\delta\Sigma^C(1'\bar{3})}{\delta f_\Delta(\bar{2})} \end{aligned} \tag{112}$$

and

$$\mathcal{S}^\delta(X_1, X'_1; t) = \frac{1}{2}\gamma_3(123)\chi^R(\bar{2}\bar{2})\chi^R(\bar{3}\bar{3})\left[is\frac{\delta}{\delta f_\Delta(\bar{3})}C(X'_1, t_0; 4)\Gamma^A(4\bar{2})\right].$$

In the lowest order approximation,

$$\begin{aligned} \Sigma^R(1, 1') &= \gamma_3(123)\gamma_3(\bar{2}\bar{3}1')R(\bar{2}\bar{2})C(\bar{3}\bar{3}), \\ \mathcal{S}^{reg}(1, 1') &= \frac{1}{2}\gamma_3(123)\gamma_3(1'\bar{2}\bar{3})C(\bar{2}\bar{2})C(\bar{3}\bar{3}), \\ \mathcal{S}^\delta &= 0, \end{aligned}$$

we recover the famous Direct Interaction Approximation (DIA) derived by Kraichnan [42] in the context of fluid turbulence and later extended to the Klimontovich equations by Dubois and Espedal [14, 43]. Further discussions on the application of those closure relations to physical problems would certainly require substantial additional work, which is beyond the scope of the present paper.

6 Summary

We have presented the foundations of a theory to derive closed, self-consistent approximations for calculating the statistical dynamics of classical Hamiltonian systems, which can describe both equilibrium and non-equilibrium states. The theory, which unifies and encompasses previous results for classical Hamiltonian systems with any initial conditions, can be regarded (i) as the classical mechanical counterpart of the theory of non-equilibrium Green's functions in quantum field theory and (ii) as a generalization to dynamical problems of the density functional theory of fluids in equilibrium. The present approach avoids many of the complications inherent to previous works [38]; in particular the theory is valid for any initial

state and treats equilibrium and non-equilibrium states in a unified manner. Interestingly, several of the key ideas and tricks of the previous theories (e.g., the need for both correlation and response functions, operator doubling, imposed commutation relations and other causality constraints. . .) arise naturally here albeit in a different form (e.g., the operator doubling in MSR is replaced by the coupling to physical and non-physical phase-space densities $\mathcal{N}_{p,\Delta}$, which generate both response and correlation functions. . .)

The main ingredients of the present approach are the following. Given a Hamiltonian system in an external potential ϕ_0 and in the statistical state described by F_0 at initial time t_0 , the effective action functional (103) defined as

$$\Omega[\phi_p, \phi_\Delta] = -s \ln \mathcal{Z}[\phi_p, \phi_\Delta],$$

where s is a fixed parameter with the dimension of an action, contains all information about the dynamical properties of the system at times $t \geq t_0$. In particular, its first derivative at $\phi_p = \phi_0, \phi_\Delta = 0$ gives the single-particle phase-space distribution function,

$$\frac{\delta \Omega}{\delta \phi_\Delta(1)} = f(1),$$

with $1 = (\mathbf{r}, \mathbf{p}, t)$, and its second derivatives generate the correlation function and retarded and advanced response functions,

$$\begin{aligned} \frac{\delta^2 \Omega}{\delta \phi_\Delta(1) \delta \phi_p(2)} &= \chi^R(1, 2), \\ \frac{\delta^2 \Omega}{\delta \phi_p(1) \delta \phi_\Delta(2)} &= \chi^A(1, 2), \\ \frac{\delta^2 \Omega}{\delta \phi_\Delta(1) \delta \phi_\Delta(2)} &= C(1, 2)/is. \end{aligned}$$

Higher-order derivatives systematically generate combinations of products and Poisson brackets of the fundamental field $N(1)$. Using traditional renormalization techniques involving the Legendre transform of the action function $\Omega[\phi_p, \phi_\Delta]$, a closed, self-consistent set of equations of motion is derived for the single-particle phase-space distribution function f , the correlation function $C = \langle \delta f \delta f \rangle$, the retarded and advanced density response functions $\chi^{R,A}$ to external potentials, and the associated memory functions $\Sigma^{R,A,C}$,

$$\left[\frac{\partial}{\partial t_1} - L_1 \right] f(1) - \{u^{mf}(1), f(1)\} = \frac{1}{2} \gamma_3(1, 2, 3) C(2, 3),$$

and

$$\begin{aligned} \left[\frac{\partial}{\partial t} - L_1 \right] \chi^R(1, 1') - \int_{t_0}^\infty \int d2 \Sigma_{tot}^R(1, 2) \chi^R(2, 1') &= \{\delta(1 - 1'), f(1)\}(1), \\ \left[\frac{\partial}{\partial t} - L_1 \right] \chi^A(1, 1') - \int_{t_0}^\infty \int d2 \Sigma_{tot}^A(1, 2) \chi^A(2, 1') &= \{\delta(1 - 1'), f(1)\}(1), \\ \left[\frac{\partial}{\partial t} - L_1 \right] C(1, 1') - \int_{t_0}^\infty \int d2 \Sigma_{tot}^R(1, 2) C(2, 1') &= \int_{t_0}^\infty \int d2 \Sigma^C(1, 2) \chi^A(2, 1'), \end{aligned}$$

with the memory function kernels satisfying

$$\begin{aligned} \Sigma^R(1, 1') &= \frac{1}{2} \gamma_3(123) \frac{\delta C(2, 3)}{\delta f_p(1')} \Big|_{f_p; f_\Delta=0}, \\ \Sigma^A(1, 1') &= i s \gamma_3(123) \frac{\delta \chi^R(2, 3)}{\delta f_\Delta(1')} \Big|_{f_p; f_\Delta=0}, \\ \Sigma^C(1, 1') &= \frac{i s}{2} \gamma_3(123) \frac{\delta C(2, 3)}{\delta f_\Delta(1')} \Big|_{f_p; f_\Delta=0}. \end{aligned} \tag{113}$$

Moreover, the memory functions satisfy functional differential equations, e.g. (111), that may be used to obtain systematic renormalized approximations in powers of the bare inter-particle interaction. The kinetic equations thus obtained automatically agree with the laws of conservation of mass, momentum and energy.

In conclusion, the purpose of the present paper was to lay down the foundations of a theory for the construction of renormalized kinetic equations of classical systems of particles in and out of equilibrium. We hope that these results will serve to (re)stimulate further research on this challenging topic. Of course further works calls for applications of the approach to realistic problems; work along those lines is under way.

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Appendix A: BBGKY Hierarchy

The BBGKY hierarchy [8] is an hierarchy of equations coupling the *equal-time* reduced distribution function f_n ,

$$f_n(X_1, \dots, X_n) = \frac{N!}{(N-s)!} \int dX_{n+1} \dots dX_N F(X_1, \dots, X_N; t).$$

The latter can also be expression as ensemble average of microscopic fields, e.g.

$$\begin{aligned} f_1(X, t) &= \left\langle \sum_{j=1}^N \delta(x - \mathbf{x}_j(t)) \right\rangle, \\ f_2(X, X'; t) &= \left\langle \sum_{j=1}^N \sum_{k \neq j}^N \delta(x - \mathbf{x}_j(t)) \delta(x' - \mathbf{x}_k(t)) \right\rangle \end{aligned} \tag{114}$$

and

$$f_3(x, x', x''; t) = \left\langle \sum_{j=1}^N \sum_{k \neq j}^N \sum_{l \neq j, k}^N \delta(x - \mathbf{x}_j(t)) \delta(x' - \mathbf{x}_k(t)) \delta(x'' - \mathbf{x}_l(t)) \right\rangle,$$

and so forth.

The equations of the BBGKY hierarchy can be obtained by direct integration of the Liouville equation (2). The n -particle reduced distribution $f_n(X_1, \dots, X_n)$ represents—up

to the factor $N!/(N - s)!$ —the probability density of finding simultaneously n particles in the specified phase-space positions X_1, \dots, X_n . In practice, those equations are often recast in terms of the correlation functions defined from the cluster representation of the reduced distribution functions for $n \geq 2$,

$$\begin{aligned}
 f_2(x, x'; t) &= g_2(x, x', t) + f_1(x, t)f_1(x', t), \\
 f_3(x, x', x''; t) &= g_3(x, x', x'', t) + [f_1(x; t)g_2(x', x''; t) + c.p.] \\
 &\quad + f_1(x, t)f_1(x', t)f_1(x'', t)
 \end{aligned}$$

and so on, where c.p. means cyclic permutation. In terms of the standard notations (13) and (15), the first two equations are

$$\left[\frac{\partial}{\partial t} - L_1 \right] f_1(1) = \int d2 L_{12} f_1(1) f_1(2) + L_{12} g_2(12)$$

and

$$\begin{aligned}
 \left[\frac{\partial}{\partial t} - (L_1 + L_{1'}) \right] g_2(1, 1') &= L_{11'} f_1(1) f_1(1') \\
 &\quad + \int d2 [L_{12} f_1(1) g_2(1', 2) + L_{1'2} f_1(1') g_2(1, 2)] \\
 &\quad + \int d2 (L_{12} + L_{1'2}) f_1(2) g_2(1, 1') \\
 &\quad + L_{11'} g_2(1, 1') + \int d2 (L_{12} + L_{1'2}) g_3(1, 1', 2).
 \end{aligned}$$

Appendix B: Useful Properties

We gather here some basic properties that are often used in the remainder of the paper:

- Equal-time Poisson bracket:

$$\begin{aligned}
 &[N(X, t), N(X', t)]_{PB} \\
 &= \left(\frac{\partial}{\partial \mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{p}'} - \frac{\partial}{\partial \mathbf{r}'} \cdot \frac{\partial}{\partial \mathbf{p}} \right) [\delta(X - X') \mathcal{N}(X, t)] \\
 &= \{\delta(X - X'), N(X, t)\}(X).
 \end{aligned} \tag{115}$$

Therefore,

$$\chi^{R/A}(X, t; X', t) = \mp \{\delta(X - X'), f(X, t)\}(X). \tag{116}$$

- From rotational symmetry,

$$\int dX_2 L_{12} \delta(X_1 - X_2) = 0. \tag{117}$$

- Unlike their quantum counterparts, the n -point correlation functions $C^{(n)}$ are fully symmetric with respect to there arguments.

Appendix C: First and Second Derivatives of $\tilde{\Omega}[\phi]$

In this section, we present the main steps leading to (35) and (37). Since $\tilde{\Omega}[\phi]$ depends on ϕ through $S[\phi; x_0]$, its functional derivatives are combinations of the total action's derivatives. For instance, we easily find,

$$\left. \frac{\delta \tilde{\Omega}}{\delta \phi(\tilde{1})} \right|_{\phi_0} = - \left\langle \left. \frac{\delta S}{\delta \phi(\tilde{1})} \right|_{\phi_0} \right\rangle, \quad (118)$$

and

$$\begin{aligned} \left. \frac{\delta^2 \tilde{\Omega}}{\delta \phi(\tilde{1}) \delta \phi(\tilde{1}')} \right|_{\phi_0} &= - \left\langle \left. \frac{\delta^2 S}{\delta \phi(\tilde{1}) \delta \phi(\tilde{1}')} \right|_{\phi_0} \right\rangle \\ &\quad - \frac{i}{s} \left\langle \left(\left. \frac{\delta S}{\delta \phi(\tilde{1})} \right|_{\phi_0} - \left. \frac{\delta S}{\delta \phi(\tilde{1}')} \right|_{\phi_0} \right) \left(\left. \frac{\delta S}{\delta \phi(\tilde{1}')} \right|_{\phi_0} - \left. \frac{\delta S}{\delta \phi(\tilde{1})} \right|_{\phi_0} \right) \right\rangle. \end{aligned} \quad (119)$$

When S is linear in the external potential, the term in $\delta^2 S / \delta \phi(\tilde{1}) \delta \phi(\tilde{1}')$ vanishes and (119) equals the two-point correlation of $\delta S / \delta \phi(\tilde{1})$; this is the typical situation in field theory as discussed before. In the present theory, the action is non-linear in ϕ , $\delta^2 S / \delta \phi(\tilde{1}) \delta \phi(\tilde{1}')$ is nonzero and generates, in addition to the correlation function, the term $\mathcal{R}(1, 1')$ related to the response functions χ^R .

The derivatives of $S[\phi; x_0]$ at a given potential ϕ_0 can be obtained by a systematic perturbation expansion in powers of the variations $\delta\phi$ around ϕ_0 . To this end, we introduce the following notations. With $\phi = \phi_0 + \delta\phi$, we write the total Hamiltonian as

$$\mathcal{H}_\phi = \mathcal{H}_{\phi_0} + \delta\mathcal{H},$$

with $\delta\mathcal{H} = \int dX \mathcal{N}(X, \tau) \delta\phi(X, \tau)$. We denote by $x(\tau) = (q(\tau), p(\tau))$ and $x_0(\tau) = (q_0(\tau), p_0(\tau))$ the closed-time trajectories starting at x_0 and governed by the Hamiltonian \mathcal{H}_ϕ and \mathcal{H}_{ϕ_0} , respectively. Given a dynamical variable A , we denote by $A = A_0 + \delta A = A_0 + A_1 + A_2 + \dots$ its expansion in power of $\delta\phi$, where A_n is the term of order n in $\delta\phi$. For instance, $\delta\mathcal{H} = \delta\mathcal{H}_1 + \delta\mathcal{H}_2 + \dots$ with

$$\begin{aligned} \delta\mathcal{H}_1 &= i'(\tau) \int dX \mathcal{N}_0(X, \tau) \delta\phi(X, \tau), \\ \delta\mathcal{H}_2 &= i'(\tau) \int dX \mathcal{N}_1(X, \tau) \delta\phi(X, \tau) \\ &= q_1 \cdot \partial_q \delta H_1(q_0, p_0, \tau) + p_1 \cdot \partial_p \delta H_1(q_0, p_0, \tau). \end{aligned} \quad (120)$$

With these notations, we rewrite the Lagrangian as

$$\begin{aligned} \mathcal{L}_\phi(q, \dot{q}, \tau) &= [p_0 \cdot \dot{q}_0 - \mathcal{H}_\phi(x_0)] + [\delta p \cdot \dot{q}_0 - \dot{p}_0 \cdot \delta q + \mathcal{H}_\phi(x_0) - \mathcal{H}_\phi(x)] \\ &\quad + [p_0 \cdot \delta \dot{q} + \dot{p}_0 \cdot \delta q] + \delta p \cdot \delta \dot{q} \end{aligned}$$

so that by time integration and integrations by parts of the last line, we obtain

$$S[\phi] = S_0 + \oint d\tau (\delta p \cdot \dot{q}_0 - \dot{p}_0 \cdot \delta q + \mathcal{H}_\phi(x_0) - \mathcal{H}_\phi(x))$$

$$\begin{aligned}
 & + \frac{1}{2} \oint d\tau \delta p \cdot \delta \dot{q} - \delta \dot{p} \cdot \delta q \\
 & + p_0(\tau_f) \cdot \delta q(\tau_f) + \frac{1}{2} \delta p(\tau_f) \cdot \delta q(\tau_f) - \mathcal{S}_b(\phi).
 \end{aligned} \tag{121}$$

The boundary term is

$$\mathcal{S}_b[\phi_0 + \delta\phi, x_0] = p_0(\tau_f) \cdot \delta q(\tau_f) + \frac{1}{2} \delta p(\tau_f) \cdot \delta q(\tau_f) \tag{122}$$

so that, with $\phi = \phi_0 + \delta\phi$, the last line of (121) vanishes

$$\delta\mathcal{S} = \oint d\tau (\delta p \cdot \dot{q}_0 - \dot{p}_0 \cdot \delta q - \mathcal{H}_\phi(x_0) - \mathcal{H}_\phi(x)) + \frac{1}{2} \oint d\tau \delta p \cdot \delta \dot{q} - \delta \dot{p} \cdot \delta q. \tag{123}$$

Using the Hamilton equations for the unperturbed trajectories, the Taylor expansion of the Hamiltonian around the unperturbed trajectory gives

$$\mathcal{H}_\phi(x) - \mathcal{H}_{\phi_0}(x_0) = -\dot{p}_0 \cdot \delta q + \delta p \cdot \dot{q}_0 + \mathcal{H}_{\phi_0}^{(2)}(\delta x) + \dots, \tag{124}$$

and where the second order term is

$$\mathcal{H}_{\phi_0}^{(2)}(\delta x) = \frac{\delta q^2}{2} \cdot \partial_{qq} \mathcal{H}_{\phi_0}(x_0) + \delta q \cdot \delta p \cdot \partial_{qp} \mathcal{H}_{\phi_0}(x_0) + \frac{\delta p^2}{2} \cdot \partial_{pp} \mathcal{H}_{\phi_0}(x_0). \tag{125}$$

Using (124) and (125) in (123), the total variation of the action writes

$$\delta\mathcal{S} = \oint d\tau \left[\frac{1}{2} (\delta p \cdot \delta \dot{q} - \delta \dot{p} \cdot \delta q) - \mathcal{H}_{\phi_0}^{(2)}(\delta x) - \delta\mathcal{H}(x) \right] + \dots.$$

At this stage, we have removed all the terms that cancel irrespective of $\delta\phi$. We now proceed with the expansion in orders of $\delta\phi$. To third order in $\delta\phi$, the integral in the last expression is

$$\oint d\tau \left[\frac{1}{2} (p_1 \cdot \dot{q}_1 - \dot{p}_1 \cdot q_1) - \mathcal{H}_{\phi_0}^{(2)}(x_1) - \delta\mathcal{H}_1 - \delta\mathcal{H}_2 \right] + O(\delta\phi^3).$$

The first order variation $(q_1(\tau), p_1(\tau))$ of the trajectory satisfies

$$\begin{cases} \dot{q}_1 = q_1 \cdot \partial_{qp} H_{\phi_0}(x_0) + p_1 \cdot \partial_{pp} H_{\phi_0}(x_0) + \partial_p \delta H_1(x_0), \\ \dot{p}_1 = -q_1 \cdot \partial_{qq} H_{\phi_0}(x_0) - p_1 \cdot \partial_{pq} H_{\phi_0}(x_0) - \partial_q \delta H_1(x_0) \end{cases} \tag{126}$$

and therefore

$$\frac{1}{2} \oint d\tau [p_1 \cdot \dot{q}_1 - q_1 \cdot \dot{p}_1] = \oint d\tau \mathcal{H}_{\phi_0}^{(2)}(x_1) + \frac{1}{2} \oint \delta\mathcal{H}_2. \tag{127}$$

Combining (127) and (126), to second-order in $\delta\phi$, the total variation of the action is

$$\begin{aligned}
 \delta\mathcal{S} = & - \oint d\tau t'(\tau) \int dX \mathcal{N}_0(X, \tau) \delta\phi(X, \tau) \\
 & - \frac{1}{2} \oint d\tau t'(\tau) \int dX \mathcal{N}_1(X, \tau) \delta\phi(X, \tau) + O(\delta\phi^3).
 \end{aligned} \tag{128}$$

In order to express the second term in (128), we first note that, using the results of linear response theory recalled Sect. 2, the density variation \mathcal{N}_1 can be written as

$$\mathcal{N}_1(\tilde{\Gamma}) = \oint d\tilde{\Gamma}' R(\tilde{\Gamma}, \tilde{\Gamma}') \delta\phi(\tilde{\Gamma}'),$$

in terms of the response function over the closed-time contour,

$$R(\tilde{\Gamma}, \tilde{\Gamma}') = \theta(\tau - \tau') \{ \mathcal{N}_0(\tilde{\Gamma}), \mathcal{N}_0(\tilde{\Gamma}') \}.$$

Therefore

$$\begin{aligned} \oint d\tilde{\Gamma} \mathcal{N}_1(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}) &= \oint d\tilde{\Gamma} d\tilde{\Gamma}' \mathcal{R}(\tilde{\Gamma}, \tilde{\Gamma}') \delta\phi(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}') \\ &= \frac{1}{2} \oint d\tilde{\Gamma} \oint d\tilde{\Gamma}' [\mathcal{R}(\tilde{\Gamma}, \tilde{\Gamma}') + \mathcal{R}(\tilde{\Gamma}', \tilde{\Gamma})] \delta\phi(\tilde{\Gamma}') \delta\phi(\tilde{\Gamma}) \\ &= \oint d\tilde{\Gamma} \oint d\tilde{\Gamma}' \chi(\tilde{\Gamma}, \tilde{\Gamma}') \delta\phi(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}'), \end{aligned} \quad (129)$$

with

$$\chi(\tilde{\Gamma}, \tilde{\Gamma}') = \frac{1}{2} \langle \mathcal{T}_c \{ \mathcal{N}_0(\tilde{\Gamma}), \mathcal{N}_0(\tilde{\Gamma}') \} \rangle.$$

The power expansion of the total action (128) becomes

$$S[\phi_0 + \delta\phi] = S[\phi_0] - \oint d\tilde{\Gamma} \mathcal{N}_0(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}) - \frac{1}{2} \oint \oint d\tilde{\Gamma} d\tilde{\Gamma}' \chi(\tilde{\Gamma}, \tilde{\Gamma}') \delta\phi(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}') + O(\delta\phi^3).$$

Therefore the first two functional derivatives of the action are

$$\left. \frac{\delta S}{\delta\phi(\tilde{\Gamma})} \right|_{\phi=\phi_0} = -\mathcal{N}_0(\tilde{\Gamma}),$$

and

$$\left. \frac{\delta^2 S}{\delta\phi(\tilde{\Gamma}) \delta\phi(\tilde{\Gamma}')} \right|_{\phi=\phi_0} = -\frac{1}{2} \mathcal{T}_c \{ \mathcal{N}_0(\tilde{\Gamma}), \mathcal{N}_0(\tilde{\Gamma}') \},$$

which, combined with (118) and (119), yield the desired results.

Appendix D: On the Differentiability of the Action Functional

Although it is not at all the purpose of this paper to be concerned with mathematical details, we feel that a word of caution regarding the differentiability of $\tilde{\Omega}[\phi]$ and the derivatives $\Omega^{(n)}$ is in order. Strictly speaking, the effective action functional $\tilde{\Omega}[\phi]$ is not (Fréchet) differentiable everywhere. It is however infinitely differentiable at any physical potentials ϕ_p . In that case, the term \mathcal{S}_b in (30) cancels the boundary terms resulting from the variations of $\tilde{x}(\tau_f)$ in the first term $\int_{\tau_i}^{\tau_f} d\tau \mathcal{L}_\phi(\tilde{q}(\tau), \tilde{v}(\tau), \tau)$, which allows for the definition of the functional derivatives. For a non-physical potential, the cancellation does not necessarily occur and the

definition of the functional derivatives is not always possible. As a consequence, the quantities $\Omega^{(n)}$ can not be regarded as functional of ϕ and expressions like $\Omega^{(n+1)} \neq \delta\Omega^{(n)}/\delta\phi$ are not correct, and therefore using it could give wrong results. This is unfortunate since such recurrence relation is very useful to derive by simple differentiation the hierarchy of properties satisfied by all the successive derivatives from a single starting relation.

To regain the benefits of such recurrence properties, we define the following formal device. Given the ensemble average $\langle A(X, t) \rangle$ of a dynamical variable A , we define the generalized ensemble average as

$$\langle\langle A(\tilde{1}) \rangle\rangle_\phi = \frac{1}{\mathcal{Z}[\phi]} \left(e^{\frac{i}{s} S[\phi]} A(\tilde{1}) \right), \tag{130}$$

for any potential ϕ . At $\phi = \phi_0$, the generalized average reduces to the physical ensemble average (6),

$$\langle\langle A(X, \tau) \rangle\rangle_{\phi=\phi_0} = \langle A(X, t(\tau)) \rangle.$$

The generalized average is a functional of ϕ , which, like S , is differentiable at any physical potential ϕ_p . Using results of the previous sections, we find its functional derivative at ϕ_0 ,

$$\left. \frac{\delta}{\delta\phi(1')} \langle\langle A(1) \rangle\rangle \right|_{\phi_0} = -\frac{i}{s} \left\langle \delta A(1) \delta \mathcal{N}(1') \right\rangle + \left\langle \left. \frac{\delta A(1)}{\delta\phi(1')} \right|_{\phi_0} \right\rangle, \tag{131}$$

in terms of the fluctuations $\delta A = A - \langle A \rangle$. Since, using the results of linear response theory,

$$\frac{\delta A(1)}{\delta\phi(1')} = \frac{1}{2} \mathcal{T}_c \{ A(1), \mathcal{N}(1') \} \tag{132}$$

we find

$$\left. \frac{\delta \langle\langle A(1) \rangle\rangle_\phi}{\delta\phi(1')} \right|_{\phi_0} = \frac{1}{2} \langle \mathcal{T}_c \{ A(1), \mathcal{N}(1') \} \rangle - \frac{i}{s} \langle \delta A(1) \delta \mathcal{N}(1') \rangle. \tag{133}$$

For instance, with $A = \mathcal{N}$, we shall write

$$f_\phi(\tilde{1}) \equiv \langle\langle \mathcal{N}(\tilde{1}) \rangle\rangle_\phi.$$

The phase-space distribution is

$$f(X, t(\tau)) = f_{\phi=\phi_0}(X, \tau)$$

and from (133) and (37)

$$\begin{aligned} \left. \frac{f_\phi(\tilde{1})}{\delta\phi(\tilde{1}')} \right|_{\phi_0} &= \frac{1}{2} \langle \mathcal{T}_c \{ \mathcal{N}(\tilde{1}), \mathcal{N}(\tilde{1}') \} \rangle - \frac{i}{s} \langle \delta \mathcal{N}(\tilde{1}) \delta \mathcal{N}(\tilde{1}') \rangle \\ &= \Omega^{(2)}(\tilde{1}, \tilde{1}'). \end{aligned}$$

Therefore we can obtain the successive derivatives of $\tilde{\Omega}[\phi]$ by writing the n -th derivative as

$$\Omega^{(n)} = \langle \omega^{(n)} \rangle \tag{134}$$

in terms of the dynamical variable $\omega^{(n)}$, and obtain the $(n + 1)$ -th derivative by functional derivative of its generalized average at $\phi = \phi_0$,

$$\Omega^{(n+1)}(\tilde{1}, \dots, \widetilde{n+1}) = \frac{\delta \langle \langle \omega^{(n)}(\tilde{1}, \dots, \tilde{n}) \rangle \rangle_{\phi}}{\delta \phi(\tilde{1}')} \Big|_{\phi_0}. \quad (135)$$

This scheme can be used to systematically generate explicit expressions of the derivatives of the effective action [40] as combinations of products and Poisson brackets of the fundamental field. The steps (134) and (135) can be schematically written as

$$\Omega^{(n+1)}(\tilde{1}, \dots, \widetilde{n+1}) = \frac{\delta}{\delta \phi(\widetilde{n+1})} \Omega^n(\tilde{1}, \dots, \tilde{n}),$$

with the understanding of the caveats discussed before. In this work, successive functional derivatives are obtained according to the scheme just defined.

Appendix E: On the Occurrence of the Linear Combination of Correlation and Response Functions

As shown in Appendix D, for any dynamical variable $A(X, t)$ we have

$$\frac{\delta \langle A(1) \rangle}{\delta \phi(1')} \Big|_{\phi_0} = \frac{1}{2} \langle \mathcal{T}_c \{ A(1), \mathcal{N}(1') \} \rangle - \frac{i}{s} \langle \delta A(1) \delta \mathcal{N}(1') \rangle. \quad (136)$$

From the expression emerges a fundamental operation between dynamical variables, which we find interesting to highlight. For any dynamical variables A and B defined on the closed-time contour, we define with square brackets $[\cdot, \cdot]$ the symmetric operation,

$$\begin{aligned} [A(\tau), B(\tau')] &:= \frac{1}{2} \langle \mathcal{T}_c \{ A(\tau), B(\tau') \} \rangle - \frac{i}{s} \langle \delta A(\tau) \delta B(\tau') \rangle \\ &= [B(\tau'), A(\tau)]. \end{aligned} \quad (137)$$

In term of this operation, (136) reads

$$\frac{\delta}{\delta \phi(1')} \langle \langle A(1) \rangle \rangle \Big|_{\phi_0} = [A(1), \mathcal{N}(1')] \quad (138)$$

and

$$\chi(1, 1') = [\mathcal{N}(1), \mathcal{N}(1')].$$

The operation (137) combines two fundamental quantities of classical statistical mechanics, namely the Poisson bracket $[\cdot, \cdot]_{PB}$ and the product of dynamical variables, which are intimately related to the response and correlation functions. It obviously respects the dimensions thanks to the action parameter s (the Poisson bracket $[A, B]_{PB}$ has the dimension of the product AB divided by the product of a length times a momentum, i.e. by an action). The Poisson bracket carries the dynamical information on how fluctuations are propagated in time, while the correlation function gives information about the likelihood of fluctuations (occupation number). At equilibrium, both quantities are simply related by the fluctuation-dissipation theorem and only one is useful (one usually works with the phase-space density

correlation functions). The emergence of the linear combination provides a justification of the fact recognized by MSR and others [15] that a time-dependent theory of classical dynamics should be expanded to involve not only correlation functions but also response functions in order to be amenable to a systematic renormalization.

We can shed some light on the occurrence of that particular combination by regarding the action function as the classical limit discussed above (see discussion after (32)). In a quantum system, both fluctuation statistics (correlation) and response effects can be characterized by products of the same quantum field operator; the intensity of fluctuations involve the anti-commutator $[\cdot, \cdot]_+$ and the response is related to the commutator $[\cdot, \cdot]_-$. In practice, both properties are contained in the time-ordered Green's functions, say $G(\tau, \tau') = \langle \mathcal{T} \hat{\Psi}(\tau) \hat{\Psi}(\tau') \rangle$, where $\hat{\Psi}(\tau)$ is the field operator (for simplicity, we do not write the other degrees of freedom). We can re-express the Green's function in terms of the averaged commutator and anti-commutator of the field,

$$G(\tau, \tau') = \langle \hat{\Psi}(\tau) \hat{\Psi}(\tau') \rangle \theta(\tau - \tau') + \langle \hat{\Psi}(\tau') \hat{\Psi}(\tau) \rangle \theta(\tau' - \tau) \\ = \frac{1}{2} \langle [\hat{\Psi}(\tau), \hat{\Psi}(\tau')]_- \rangle \text{sign}(\tau - \tau') + \frac{1}{2} \langle [\hat{\Psi}(\tau), \hat{\Psi}(\tau')]_+ \rangle.$$

From the correspondence relations, in the classical limit, the anti-commutator $[\cdot, \cdot]_+$ becomes a product, the commutator becomes the Poisson bracket $i\hbar\{\Psi(\tau), \Psi(\tau')\}$ and therefore

$$G(\tau, \tau') \rightarrow \frac{is}{2} \langle \mathcal{T} [\Psi(\tau), \Psi(\tau')]_{PB} \rangle + \langle \Psi(\tau) \Psi(\tau') \rangle \\ = is \left(\frac{1}{2} \langle \mathcal{T} [\Psi(\tau), \Psi(\tau')]_{PB} \rangle - \frac{i}{s} \langle \Psi(\tau) \Psi(\tau') \rangle \right),$$

where we recognize the bracket (137) introduced earlier.

Appendix F: Closed vs Unclosed Expressions for $\Sigma(\tilde{\mathbf{I}}, \tilde{\mathbf{I}}')$

The previous closed expression for $\{\Sigma(\tilde{\mathbf{I}}, \tilde{\mathbf{I}}'), f(\tilde{\mathbf{I}}')\}$, (61a)–(61c), should be compared to its “unclosed” version, which can straightforwardly obtained by using the equations of evolution (48) and (50) for χ and $\Omega^{(3)}$ on both sides of (58) for Σ . We obtain,

$$\{\Sigma(\tilde{\mathbf{I}}, \tilde{\mathbf{I}}'), f(\tilde{\mathbf{I}}')\}(\tilde{\mathbf{I}}') = \frac{is}{2} \gamma_3(\tilde{\mathbf{I}}23)s_3(2\tilde{3}\tilde{\mathbf{I}}') \tag{139a}$$

$$+ \left(\frac{is}{2}\right)^2 \gamma_3(\tilde{\mathbf{I}}23)\gamma_3(\tilde{\mathbf{I}}'2'3')[\chi^{(4)}(232'3')] \\ - \frac{2}{is} \chi(22')\chi(33') - \chi^{(3)}(234)\chi^{-1}(45)\chi^{(3)}(52'3')] \tag{139b}$$

$$+ \Delta(\tau') \frac{1}{2} \gamma_3(\tilde{\mathbf{I}}23)\chi(2, \tilde{2})\chi(3, \tilde{3}) \frac{\delta}{\delta f(\tilde{3})} [C(\tilde{\mathbf{I}}', \tilde{2}')\chi^{-1}(\tilde{2}', \tilde{2})] \tag{139c}$$

thus establishing the correspondence between (61b) and (139b).

In his “fully renormalized” kinetic theory of equilibrium liquids, Mazenko [13] uses as a starting point an expression for the memory function equivalent to the equilibrium limit of (139a)–(139c).

Appendix G: Derivation of (95)

Equation (94), namely

$$\{\Gamma^C(1, 1'), f(1)\}(1') = \frac{is}{2}(\Sigma^>(t, t') + \Sigma^<(t, t')) + is\Sigma^{(0)}(X_1, X_1; t)\delta(t' - t_0) + \delta(t - t_0)C(1, 2)\Gamma^A(2, 1')$$

implies that Γ^C is of the form

$$\Gamma^C(1, 1') = \Gamma^{reg}(1, 1') + \delta(t' - t_0)\Gamma^\delta(X_1, X'_1; t) + \delta(t - t_0)\Gamma^{(1)}(X_1, X'_1; t') \tag{140}$$

where Γ^{reg} and Γ^δ are given by (96a)–(96a) and $\Gamma^{(1)}$ is a regular function of time variables satisfying,

$$\{\Gamma^{(1)}(X_1, X'_1; t'), f(X_1, t_0)\} = C(X_1, t_0; 2)\Gamma^A(2, 1'). \tag{141}$$

$\Gamma^{(1)}$ can be related to Γ^δ and the initial correlation function C_0 as follows. Introducing (140) into (90) yields

$$\begin{aligned} C(1, 1') &= \int_{t_0}^t dt_2 \int_{t_0}^{t'} dt_3 \iint dX_2 dX_3 \chi^R(1, 2)\Gamma^{reg}(2, 3)\chi^A(3, 1') \\ &\quad + \int_{t_0}^t dt_2 \iint dX_2 dX_3 \chi^R(1, 2)\Gamma^\delta(X_2, X_3; t_2)\chi^A(X_3, t_0; 1') \\ &\quad + \int dX_2 \int dX_3 \chi^R(1; X_2, t_0)\Gamma^{(1)}(X_2, X_3; t_3)\chi^A(3; 1'). \end{aligned}$$

Setting $t' = t_0$ in the previous expression, the resulting expression is used to calculate the rhs of (141), which gives

$$\begin{aligned} &\{\Gamma^{(1)}(X_1, X'_1; t'), f(X_1, t_0)\} \\ &= \{\Gamma^\delta(X'_1, X_1; t'), f(1, t_0)\} + \delta(t' - t_0) \int dX_2 \chi^R(X_1, t_0; 2)\Gamma^{(1)}(X'_1, X_2, t_2). \end{aligned}$$

Using $\chi^R(X_1, t_0; X_2, t_0) = \{f(X_1), \delta(X_1 - X_2)\}$, the previous relation implies the following expression for $\Gamma^{(1)}$

$$142\Gamma^{(1)}(X_1, X'_1; t') = \Gamma^\delta(X'_1, X_1; t') + \delta(t' - t_0)\Gamma^{(0)}(X_1, X'_1), \tag{142}$$

with $\Gamma^{(0)}$ given by (97). Combining (142) and (140) yield the desired result (95).

Appendix H: Diagrammatic Representation

H.1 Derivation of (107)

From the chain rule of differentiation, we have

$$\begin{aligned} \frac{\delta f_p(3)}{\delta f_p(1)} &= \delta(1 - 3) = \int d2\Gamma_{12}(12)\Omega_{12}(23) + \Gamma_{11}(12)\Omega_{22}(23), \\ \frac{\delta f_\Delta(3)}{\delta f_p(1)} &= 0 = \int d2\Gamma_{22}(12)\Omega_{12}(23) + \Gamma_{21}(12)\Omega_{22}(23) \end{aligned}$$

Fig. 3 Representation of derivatives of the effective action Ω and effective potential Γ . An inward (outward) arrow indicates derivative with respect to the physical (non-physical) component

$$\begin{aligned}
 & \begin{array}{c} 1' \quad 2' \quad \dots \quad n' \\ \nearrow \quad \nearrow \quad \nearrow \quad \nearrow \\ \textcircled{\Omega} \\ \searrow \quad \searrow \quad \searrow \quad \searrow \\ 1 \quad 2 \quad \dots \quad n \end{array} = \frac{\delta^{n+n'} \Omega}{\delta \phi_p(1) \dots \delta \phi_p(n) \delta \phi_\Delta(1') \dots \delta \phi_\Delta(n')} \\
 & = \Omega_{\underbrace{1 \dots 1}_n \underbrace{2 \dots 2}_{n'}}(1 \dots n; 1' \dots n') \\
 \\
 & \begin{array}{c} 1' \quad 2' \quad \dots \quad n' \\ \searrow \quad \searrow \quad \searrow \quad \searrow \\ \textcircled{\Gamma} \\ \nearrow \quad \nearrow \quad \nearrow \quad \nearrow \\ 1 \quad 2 \quad \dots \quad n \end{array} = \frac{\delta^{n+n'} \Gamma}{\delta f_p(1) \dots \delta f_p(n) \delta f_\Delta(1') \dots \delta f_\Delta(n')} \\
 & = \Gamma_{\underbrace{1 \dots 1}_n \underbrace{2 \dots 2}_{n'}}(1 \dots n; 1' \dots n')
 \end{aligned}$$

and

$$\frac{\delta f_\Delta(3)}{\delta f_p(1)} = 0 = \int d2 \Gamma_{11}(12) \Omega_{21}(23), \tag{143}$$

$$\frac{\delta f_\Delta(3)}{\delta f_\Delta(1)} = \delta(1-3) = \int d2 \Gamma_{21}(12) \Omega_{12}(21) \tag{144}$$

where we used $\Omega_{11} = 0$. We deduce $\Gamma_{11} = 0$, and therefore

$$\delta(1-3) = \int d2 \Gamma_{12}(12) \Omega_{12}(23), \tag{145a}$$

$$\delta(1-3) = \int d2 \Gamma_{21}(12) \Omega_{12}(21), \tag{145b}$$

$$0 = \int d2 \Gamma_{22}(12) \Omega_{12}(23) + \Gamma_{21}(12) \Omega_{22}(23). \tag{145c}$$

Combining (145a)–(145c) with (105) leads to (107).

H.2 Higher-Order Derivatives with Diagrams

We define here an economical graphical representation for deriving relations between the correlation and response functions with the vertex functions. We define the graphical notations as shown in Fig. 3.

Using the chain rule, the functional derivative $\delta/\delta f_p$ and $\delta/\delta f_\Delta$ of $\Omega_{1\dots n1'\dots n'}$ add an additional two-point vertex to the diagram as illustrated in Figs. 4 and 5. Using $\Gamma_{11} = 0$ and the rules in Fig. 4, we can evaluate the successive derivatives by letting $\delta/\delta f_{p,\Delta}$ act of the diagrams of Fig. 5. We illustrate the calculations leading to the third-order derivatives (108a) used in the body of the paper. $\delta/\delta f_p$ of the first diagram in Fig. 5 yields the diagram in Fig. 6, and $\delta/\delta f_p$ of last diagram in Fig. 5 yields the diagram in Fig. 7. Combining the diagrams in Figs. 6 and 7 yields the diagrammatic representation of (108a) shown in Fig. 8.

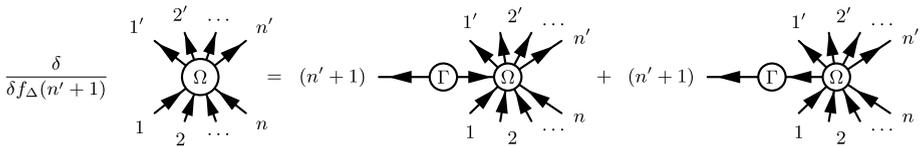
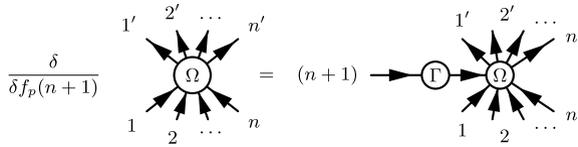


Fig. 4 Graphical representation of chain rule

Fig. 5 Graphical representations of (145a), (145b) and (145c)

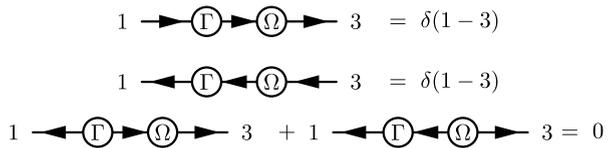
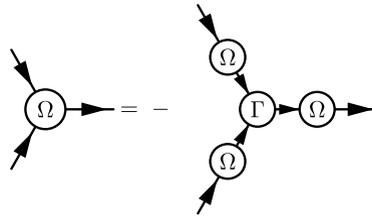


Fig. 6 $\delta/\delta f_p$ of the first diagram in Fig. 5



Appendix I: Details on the Derivation of the Real-Time Formalism

By considering the equation of motion (44) for $\mathcal{N}(\tau)$ in an external potential ϕ on both sides on the closed-time consider, it is straightforward to extract the evolution equation for the classical and non-classical components $\mathcal{N}'_{p,\Delta}$ as

$$\left[\frac{\partial}{\partial t_1} - L_1^p \right] N_p(1) - \frac{1}{4} L_1^\Delta N_\Delta(1) = \frac{1}{2} \gamma_3(1, 2, 3) \left(N_p(2) N_p(3) + \frac{1}{4} N_\Delta(2) N_\Delta(3) \right),$$

$$\left[\frac{\partial}{\partial t_1} - L_1^p \right] N_\Delta(1) - L_1^\Delta N_p(1) = \gamma_3(1, 2, 3) N_p(2) N_\Delta(3)$$

with the single particle Liouville operators,

$$L_1^p \bullet = \{h_0(1) + \phi_p(1), \bullet\},$$

$$L_1^\Delta \bullet = \{\phi_\Delta(1), \bullet\}.$$

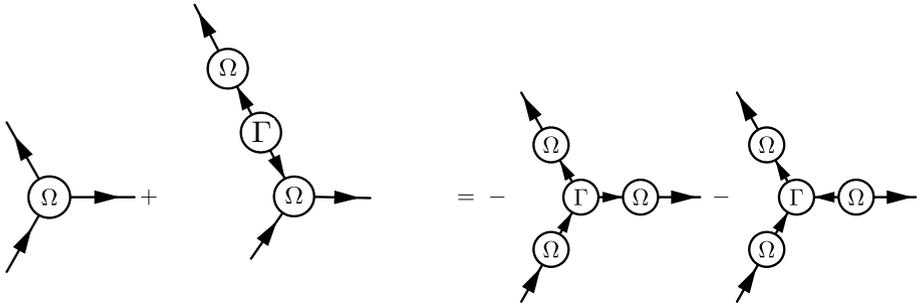


Fig. 7 $\delta/\delta f_p$ of last diagram in Fig. 5

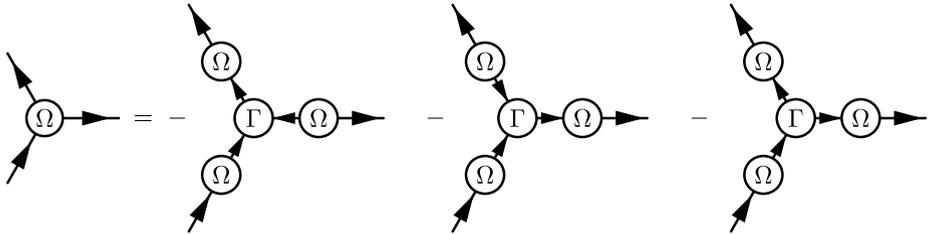


Fig. 8 Figures 6 and 7 can be combined to lead to this diagram

By averaging these equations over the initial conditions, we obtain the evolution equation of for the averaged densities $f_{p,\Delta} = \langle \mathcal{N}_{p,\Delta} \rangle$,

$$\begin{aligned} & \left[\frac{\partial}{\partial t_1} - L_1^p \right] f_p(1) - \frac{1}{4} L_1^\Delta f_\Delta(1) \\ &= \frac{1}{2} \gamma_3(1, 2, 3) \left(f_p(2) f_p(3) + \frac{1}{4} f_\Delta(2) f_\Delta(3) \right) + \frac{is}{2} \gamma_3(123) \Omega_{22}(23) + \delta(t - t_0) f_p(1) \end{aligned} \tag{146}$$

and

$$\left[\frac{\partial}{\partial t_1} - L_1^p \right] f_\Delta(1) - L_1^\Delta f_p(1) = \gamma_3(1, 2, 3) f_p(2) f_\Delta(3) is \gamma_3(123) \Omega_{21}(23). \tag{147}$$

As in Sect. 3.6, equations of evolutions for the second-order derivatives Ω_{ij} , i.e. for C and $\chi^{R,A}$, can be obtained by differentiation of (146)–(147). The terms involving the third-order derivatives Ω_{ijk} in the resulting equations (not shown here) can be expressed in terms of memory function kernels $\Sigma^{R,A,C}$ such as

$$\begin{aligned} & \frac{is}{2} \gamma_3(123) \begin{pmatrix} 0 & 2\Omega_{212}(231') \\ \Omega_{221}(231') & 2\Omega_{222}(231') \end{pmatrix} \\ &= \begin{pmatrix} 0 & \Sigma^A \cdot \Omega_{12} \\ \Sigma^R \cdot \Omega_{21} & \frac{2}{is} (is \Sigma^R \cdot \Omega_{22} + \Sigma^C \cdot \Omega_{12}) \end{pmatrix} (1, 1') \\ &= \begin{pmatrix} 0 & \Sigma^A \cdot \chi^A \\ \Sigma^R \cdot \chi^R & \frac{2}{is} (\Sigma^R \cdot C + \Sigma^C \cdot \chi^A) \end{pmatrix} (1, 1'), \end{aligned}$$

which leads to (109a)–(109c) and (110a)–(110c). Following the same steps as in Sect. 3.7, using (88)–(89), the evolution equations for $\chi^{R,A}$ and C yield the following (non-trivial) relations between $\Sigma^{R,A,C}$ and $\Gamma^{R,A,C}$,

$$\begin{aligned} \{\Gamma_{211}(123), f(1)\} &= \{\Gamma_{12}(32), \delta(1-2)\} - \{\Gamma_{21}(12), \delta(1-3)\} - \gamma_{123} - \frac{\delta\Sigma^R(12)}{\delta f_p(3)}, \\ \{\Gamma_{121}(123), f(1)\} &= \{\Gamma_{12}(32), \delta(1-2)\} - \{\Gamma_{12}(12), \delta(1-3)\} - \gamma_{123} - \frac{\delta\Sigma^A(12)}{\delta f_p(3)}, \\ \{\Gamma_{221}(123), f(1)\} &= -\{\Gamma_{22}(12), \delta(1-3)\} - \frac{1}{iS} \frac{\delta\Sigma^C(12)}{\delta f_p(3)} \\ &\quad - \delta(t_1 - t_0) \frac{\delta}{\delta f_p(3)} [\Omega_{22}(14)\Gamma_{12}(42)], \\ \{\Gamma_{222}(123), f(1)\} &= \frac{1}{4} \{\Gamma_{21}(32), \delta(1-2)\} - \frac{1}{4} \{\Gamma_{12}(12), \delta(1-3)\} - \frac{1}{4} \gamma_{123} \\ &\quad - \frac{1}{iS} \frac{\delta\Sigma^C(12)}{\delta f_\Delta(3)} - \delta(t_1 - t_0) \frac{\delta}{\delta f_\Delta(3)} [\Omega_{22}(14)\Gamma_{12}(42)] \\ \{\Gamma_{122}(123), f(1)\} &= \{\Gamma_{22}(32), \delta(1-2)\} - \{\Gamma_{22}(12), \delta(1-3)\} - \gamma_{123} - \frac{\delta\Sigma^A(12)}{\delta f_\Delta(3)}, \\ \{\Gamma_{212}(123), f(1)\} &= \{\Gamma_{22}(32), \delta(1-2)\} - \gamma_{123} - \frac{\delta\Sigma^R(12)}{\delta f_\Delta(3)}. \end{aligned}$$

Those relations are then combined with (110a)–(110c) to close the hierarchy through the functional differential equations (111) and (112) for the memory function kernels.

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