Nonlinear Higher-Order Thermo-Hydrodynamics: Generalized Approach in a Nonequilibrium Ensemble Formalism

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Abstract

Construction of a nonlinear higher-order thermo-hydrodynamics, including correlations, in the framework of a Generalized Nonequilibrium Statistical Grand-Canonical Ensemble is presented. In that way it is provided a particular formalism for the coupling and simultaneous treatment of the kinetics and hydrodynamic levels of description. It is based on a complete thermostatistical approach in terms of the densities of energy and of matter and their fluxes of all orders, as well as on their direct and cross correlations, covering systems arbitrarily driven-away-from equilibrium. The set of coupled nonlinear integro-differential hydrodynamic equations is derived. Illustrations of the application of the theory are described in the follow up article.
I. INTRODUCTION

It has been noticed that one of the complicated problems of the nonequilibrium theory of transport processes in dense gases and liquids is the fact that their kinetics and hydrodynamics are intimately coupled and must be treated simultaneously (E.g. see Refs.[1-5]). Moreover, on this we may say that microscopic descriptions of hydrodynamics, that is, associated to derivation of the kinetic equations from classical or quantum mechanics and containing kinetic (transport) coefficients written in terms of correlation functions, is a traditional problem of long standing. An important aspect is the derivation of constitutive laws which express thermodynamic fluxes (or currents as those of matter and energy) in terms of appropriate thermodynamic forces (typically gradients of densities as those of matter and energy). In their most general form these laws are nonlocal in space and noninstantaneous in time. The nonlocality is usually dealt with in terms of spatial Fourier transforms, and then the laws - now expressed in reciprocal space - become dependent on wave-vector $Q$. A first kinetic-hydrodynamic approach can be considered to be the so-called classical (or Onsagerian) thermo-hydrodynamics; it gives foundations to, for example, the classical Fourier’s and Fick’s diffusion laws. But it works under quite restrictive conditions, namely, local equilibrium; linear relations between fluxes and thermodynamic forces (meaning weak amplitudes in the motion) with Onsager’s symmetry laws holding; near homogeneous and static movement (meaning that the motion can be well described with basically Fourier components with long wavelengths and low frequencies, and then involves only smooth variation in space and time); weak and rapidly regressing fluctuations [6, 7].

Hence, more advanced approaches require to lift these restrictions. Consider first near homogeneity, which implies validity in the limit of long wavelengths (or wavenumber $Q$ approaching zero), and to go beyond it is necessary to introduce a proper dependence on $Q$ valid, in principle, for intermediate and short wavelengths (intermediate to large wavenumbers). In phenomenological theories this corresponds to go from classical irreversible thermodynamics to extended irreversible thermodynamics [8, 9]. This is what has ben called generalized hydrodynamics, a question extensively debated for decades by the Statistical Mechanics community. Several approaches have been used, and a description can be consulted in Chapter 6 of the classical book on the subject by Boon and Yip [10]. Introduction of nonlocal effects for describing motions with influence of ever decreasing wavelengths, going
towards the very short limit, has been done in terms of expansions in increasing powers of the wavenumber, which consists in what is nowadays sometimes referred to as higher-order hydrodynamics (HOH). Attempts to perform such expansions are the so-called Burnett and super-Burnett approaches in the case of mass motion, and Guyer-Krumhansl approach in the case of propagation of energy (see for example Refs.[11] and [12]). An usual approach has been based on the moments solution procedure of Boltzmann equation, as in the work of Hess [13], using a higher-order Chapman-Enskog solution method. The Chapman-Enskog method provides a solution to Boltzmann equation consisting of a series in powers of the Knudsen number, $K_n$, given by the ratio between the mean-free path of the particles and the scale of change (relevant wavelengths in the motion) of the hydrodynamic fields. Retaining the term linear in $K_n$ there follows Navier-Stokes equation, the term in $K_n^2$ introduces Burnett-like contributions, and the higher-order ones ($K_n^3$ and up) the super-Burnett contributions.

A satisfactory development of a HOH being also nonlinear and including fluctuations is highly desirable for covering a large class of hydrodynamic situations, and, besides its own scientific interest, also for obtaining insights into technological-industrial processes having an associated economic interest. Also we can mention its fundamental relevance in Oceanography and Meteorology, as for example, the study of quite relevant phenomena as thermohaline circulation and ENSO (El Niño Southern Oscillation); see for example Refs.[14] and [15] respectively. Moreover, it has been stated [16] that the idea of promoting hydraulics by statistical inference is appealing because the complete information about phenomena in hydraulics seldom exists; for example sediment transport, also the more fundamental problem in fluid mechanics of describing the velocity distribution in fluids under flow. This latter question shall be approached in a future contribution. Indeed, the nonlocal terms become specially important in miniaturized devices at submicronic lengths [17], or in the design of stratospheric planes, which fly in rarefied gases in a density regime between the independent particle description and the purely continuous description. Another particular problem to it related is the one of obtaining the structures of shock waves in fluids for wide ranges of Mach numbers [18]. Moreover, Burnett approximation of hydrodynamics has been shown to provide substantial improvement on many features of the flow occurring in several problems in hydrodynamics, e.g. the case of Poiseuille flow [19] and others [20].

The microscopic derivation of a HOH, together with the analysis of the validity of existing theories, is still a point in question. It has been shown [21] that for the case of Maxwellian
molecules, whereas Navier-Stockes approximation yields equations which are stable against small perturbations, this is not the case when are introduced Burnett contributions to the equations. It follows that small perturbations to the solutions, which are periodic in the space variable with a wavelength smaller than a critical length, are exponentially unstable. This fact has been called Bobylev's instability. More recently, Garcia-Colin and collaborators [22] have extended Bobylev's analysis for the case of any interaction potential, and have argued that one can interpret the fact as to give a bound for a Knudsen number above which the Burnett equations are not valid. Moreover, Karlin [23] reconsidered the question looking for exact solutions to simplified models: when a linearized ten-moment Grad-method is used, and the Chapman-Enskog method is applied to the model, in fact there follow instabilities in the higher-order approximations. On the other hand, resorting to the Chapman-Enskog solution for linearized Grad ten-moment equations resummed exactly, solutions are obtained for which the stability of higher-order hydrodynamics, in various approximations, can be discussed.

Furthermore, inclusion of nonlinearity in the theory, in a Nonlinear Higher-Order Thermo-Hydrodynamics (NLHOTH for short and meaning thermal physics of fluid continua), leads to additional possible singularities, called hydrodynamic singularities, as, for example, described in Refs.[24] and [25]. A satisfactory construction of a NLHOTH is highly desirable for covering a large class of hydrodynamic situations obtaining an understanding of the physics involved from the microscopic level, and in the last instance gaining insights into technological and industrial processes as in, for instance, hydraulic engineering, food engineering, soft-matter engineering, etc., which have an associated economic interest. We do present here a description of the derivation of a NLHOTH which is based on a formalism in Statistical Mechanics shown to be quite appropriate for dealing with systems in far-from-equilibrium conditions.

II. THEORETICAL BACKGROUND

For building a nonlinear higher-order (generalized) thermo-hydrodynamics on mechanical-statistical basis, one needs a nonequilibrium ensemble formalism for open systems. In Ref.[26] has been described an information-theoretic approach to the construction of nonequilibrium ensembles. It involves a variational method which codifies the derivation of proba-
bility distributions - which are also obtained by heuristic approaches or projection operator techniques - [27], systematizing the work on the subject of a number of renowned scientists published along the past century.

According to theory, immediately after the open system of \( N \) particles, in contact with external sources and reservoirs, has been driven out of equilibrium to describe its state requires to introduce all its observables. But this is equivalent to have access to the so-called one-particle (or single-particle), \( \hat{n}_1 \), and two-particle, \( \hat{n}_2 \), dynamical operators for any subset of the particles involved: This is so because all usual observable quantities can be expressed at the microscopic mechanical level in terms of these operators (e.g. Refs.[28] and [29]), what is described in Appendix A.

On the basis of the construction of the nonequilibrium statistical operator [26, 27], and taking into account the fact that a complete description of the nonequilibrium state of the system follows from the knowledge of the single- and two-particle density operators [or equivalently the density matrix operator, cf. Eqs.(A1) and (A2)], the most complete statistical distribution is the one built in terms of the auxiliary ("instantaneously frozen") statistical operator

\[
\overline{\rho}(t, 0) = \bar{\rho}(t, 0) \times \rho_R,
\]

where

\[
\bar{\rho}(t, 0) = \exp\left\{ -\phi(t) - \sum_\lambda \int d^3r \int d^3p F_{1\lambda}(r, p; t) \hat{n}_{1\lambda}(r, p) \\
- \sum_\lambda \int d^3r \int d^3p \int d^3r' \int d^3p' F_{2\lambda}(r, p, r', p'; t) \hat{n}_{2\lambda}(r, p, r', p') \right\},
\]

in the classical case (the quantum one is given in Appendix B). Index \( \lambda (= 1, 2, \ldots, s) \) refers to the possible different \( s \) subsystems of particles (say, different chemical species in a multicomponent fluid, different classes of quasi-particles in a solid, namely, electrons in Bloch bands, phonons, etc.); \( r \) and \( p \) are the so-called position and momentum field variables. Moreover, we have simplified the matter considering the case of contact and interaction of the system of interest with ideal reservoir in stationary states, characterized by the statistical operator \( \rho_R \), so that the complete statistical operator can be factorized in the form of Eq.(1). Hence, \( \bar{\rho}(t, 0) \) depends on the variables of the system of interest and \( \rho_R \) on the variables of the reservoir; both distributions are taken as normalized - as it should -, with \( \phi(t) \) ensuring the
normalization of $\bar{\rho}$, meaning that

$$\phi(t) = \int d\Gamma \exp\left\{-\sum_\lambda \int d^3r \int d^3p F_{1\lambda}(r, p; t) \hat{n}_{1\lambda}(r, p) - \sum_\lambda \int d^3r \int d^3p \int d^3r' \int d^3p' F_{2\lambda}(r, p, r', p'; t) \hat{n}_{2\lambda}(r, p, r', p')\right\},$$

(3)

and $F_{1\lambda}$ and $F_{2\lambda}$ are the intensive nonequilibrium variables conjugated to $\hat{n}_1$ and $\hat{n}_2$ (the Lagrange multipliers in the variational approach). Moreover, $d\Gamma$ is the element of the volume in the phase space of the system, and for simplicity we have omitted to indicate the dependence on $\Gamma$ of $\hat{n}_1$, $\hat{n}_2$, $\bar{\rho}$, $\bar{R}$, and that $\rho_R$ depends on the point phase $\Gamma_R$ in the phase space of the reservoir.

We recall that $\bar{\rho}$ of Eq.(2) is not the statistical operator of the nonequilibrium system, but an auxiliary one - as noticed called the ”instantaneously frozen quasiequilibrium” statistical operator -, but which allows to built the proper nonequilibrium statistical operator (cf. Eq.(4) below), which needs to include historicity and irreversibility effects not present in $\bar{\rho}$, which does not account for dissipative processes, besides not providing correct average values in the calculation of transport coefficients and response functions.

Finally, the statistical operator explicitly written is given by

$$\mathcal{R}_\varepsilon(t) = \exp\left\{\ln \bar{\rho}(t, 0) - \int_{-\infty}^{t} dt' e^{\varepsilon(t' - t)} \frac{d}{dt'} \ln \bar{\rho}(t', t' - t)\right\} \times \rho_R,$$

(4)

with $\bar{\rho}(t, 0)$ of Eq.(2), and we recall that

$$\bar{\rho}(t', t' - t) = \exp\left\{i(t - t')\mathcal{L}\right\} \bar{\rho}(t', 0),$$

(5)

($\mathcal{L}$ is the Liouvillian operator of the system meaning $i\mathcal{L}\hat{A} = \{\hat{A}, \hat{H}\}$), which is the auxiliary operator carrying on the mechanical evolution of the system under Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{W} = \hat{H}_0 + \hat{H}'$, where we have introduced $\hat{H}' = \hat{H}_1 + \hat{W}$; with $\hat{H}_0$ being the kinetic energy operator, $\hat{H}_1$ contains the internal interactions and $\hat{W}$ accounts for the interaction of the system with reservoirs and sources. Finally, $\varepsilon$ is an infinitesimal positive real number which is taken going to zero after the traces in the calculation of averages have been performed (it is present in a kernel that introduces irreversibility in the calculations, in a Krylov-Bogoliubov sense). We stress that the second contribution in the exponent in Eq.(4) accounts for historicity and irreversible behavior from the initial time (taken in the
remote past, \( t_0 \rightarrow -\infty \), implying in adiabatic coupling of correlations, (see for example Ref.[26]), or alternatively, can be seen as the adiabatic coupling of the interactions responsible for relaxation processes \([30]\). Moreover we notice that the time derivative in Eq.(4) takes care of the change in time of the thermodynamic state of the system (in the first term on the argument i.e. \( t' \) ) and of the microscopic mechanical evolution [second term in the argument, i.e. \( t' - t \) and see Eq.(6)], and that the initial value condition is \( R_x(t_0) = \bar{\rho}(t_0, 0) \) for \( t_0 \rightarrow -\infty \).

But, as shown elsewhere \([26]\) it is quite convenient, and intuitively more satisfactory, to work in an alternative description than the one in Eq.(2), namely, the so-called generalized nonequilibrium grand-canonical ensemble. In words, it consists into introducing as basic variables independent linear combinations of \( \hat{n}_1 \) and \( \hat{n}_2 \). This can be done along several ways \([27]\), but once we are here working within the framework of classical mechanics, we present a simple derivation in Appendix C. According to the results presented in the latter, and once for simplicity we are considering the case of the presence of only one kind of particles in the system [i.e. \( \lambda = 1 \) in Eq.(2)], the auxiliary generalized classical nonequilibrium grand-canonical statistical operator is given by

\[
\bar{\rho}(t, 0) = \exp \left\{ -\hat{S}(t, 0) \right\},
\]

where \( \hat{S}(t, 0) \) is the so-called informational entropy operator \([31]\), which we write as composed of two contributions, namely

\[
\hat{S}(t, 0) = \hat{S}_1(t, 0) + \hat{S}_2(t, 0),
\]

with \( \hat{S}_1 \) and \( \hat{S}_2 \) given by

\[
\hat{S}_1(t, 0) = \phi_1(t) + \int d^3r \left\{ A(r, t) \hat{n}(r) + F_h(r, t) \hat{h}(r) + V(r, t) \cdot \hat{I}_n(r) + F_h(r, t) \cdot \hat{I}_h(r) \right. \\
+ \sum_{\geq 2} \left[ F_h^{[r]}(r, t) \otimes \hat{I}_h^{[r]}(r) + F_n^{[r]}(r, t) \otimes \hat{I}_n^{[r]}(r) \right] \right\},
\]

\[
\hat{S}_2(t, 0) = \phi_2(t) + \int d^3r \int d^3r' \sum_{p, p'} \sum_{r, r'} F_{pp'}^{[r+r']}(r, r', t) \otimes \hat{C}_{pp'}^{[r+r']}(r, r'),
\]

where \( p \) and \( p' \) stands for indexes \( n \) or \( h \), and \( r \) and \( r' \) are equal to zero (the densities), 1 (the vectorial fluxes), and 2, 3, \ldots \ (higher order fluxes). In the last two equations we have
introduce the definitions

\[ \hat{h}(\mathbf{r}) = \int d^3p \frac{p^2}{2m} \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(10)

\[ \hat{n}(\mathbf{r}) = \int d^3p \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(11)

\[ \hat{\mathbf{x}}_h(\mathbf{r}) = \int d^3p \frac{p^2}{2m} \mathbf{u} \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(12)

\[ \hat{\mathbf{x}}_n(\mathbf{r}) = \int d^3p \mathbf{u} \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(13)

\[ \hat{j}_h^{[r]}(\mathbf{r}) = \int d^3p \frac{p^2}{2m} u^{[r]} \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(14)

\[ \hat{j}_n^{[r]}(\mathbf{r}) = \int d^3p u^{[r]} \hat{n}_1(\mathbf{r}, \mathbf{p}), \]  

(15)

where [cf. Eqs.(C8) and (C9)]

\[ u^{[r]} = [\mathbf{u} \ldots r - times \ldots \mathbf{u}], \]  

(16)

with [...] being the tensorial product of \( r \) times the generating velocity (a vector)

\[ \mathbf{u} = p/m, \]  

(17)

which is the group velocity of the particle with energy-dispersion realtion \( \varepsilon(p) = p^2/2m \), but the present formalism also encompasses the case of systems with any kind of energy-dispersion relation, as, for example, electrons in quantum states \(|k\rangle\) of Bloch bands (when we take \( p = h \mathbf{k} \)), or phonons associated to lattice vibrations (for acoustic phonons in Debye model \( \varepsilon(p) = s |q| \) (taking \( p = h \mathbf{q} \) with \( \mathbf{q} \) running in Brillouin zone, and where \( s \) is the velocity of propagation), and similarly for photons in black-body radiation with \( \varepsilon(p) = c |k| \) (for \( p = h \mathbf{k} \), and \( c \) is the velocity of light): the general case is briefly summarized in Appendix D.

The operators in Eqs.(10) and (11) are, respectively, the density of kinetic energy and of particles, whose integration in space provides the kinetic energy Hamiltonian and the number of particles. The vector operators of Eqs.(12) and (13) are the fluxes of the two
previous densities, called first-order fluxes or currents, and those of Eqs.(14) and (15), with
\( r \geq 2 \), are the higher-order (tensorial) fluxes of kinetic energy and of matter (or particles).
All of them are present in \( \hat{S}_1 \), while in \( \hat{S}_2 \) we find the tensorial operators (of rank \( r + r' \))
\[ \hat{C}_{pp'}^{[r+r']}(\mathbf{r}, \mathbf{r}') = \left[ \hat{I}_k^{[r]}(\mathbf{r}) \, \hat{I}_{k'}^{[r']}(\mathbf{r}') \right], \tag{18} \]
where, we recall, \([\ldots]\) stands for the tensorial product, \( p \) and \( p' \) for \( h \) or \( n \) (referring to energy
and particle densities), and \( r \) and \( r' \) are \( 0, 1, 2, \ldots \).

The average values of the operators of Eqs.(10) to (15) - associated to the single-particle
dynamical operator -, and those of Eq.(18) - associated to the two-particle dynamical oper-
ator -, define the set of basic macrovariables for the thermo-hydrodynamics, namely
\[ I_p^{[r]}(\mathbf{r}, t) = \int d\Gamma \, \hat{I}_p^{[r]}(\mathbf{r}) \, \mathcal{R}_\epsilon(t), \tag{19} \]
for \( r = 0 \) (the densities), \( r = 1 \) (the vectorial fluxes or currents), and \( r \geq 2 \) (the higher-order
fluxes). Hence, we do have
\[ h(\mathbf{r}, t) = \int d^3 p \, \frac{p^2}{2m} \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{20} \]
\[ n(\mathbf{r}, t) = \int d^3 p \, \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{21} \]
\[ \mathcal{I}_h(\mathbf{r}, t) = \int d^3 p \, \frac{p^2}{2m} \, u \, \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{22} \]
\[ \mathcal{I}_n(\mathbf{r}, t) = \int d^3 p \, u \, \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{23} \]
\[ \hat{I}_h^{[r]}(\mathbf{r}, t) = \int d^3 p \, \frac{p^2}{2m} \, u^{[r]} \, \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{24} \]
\[ \hat{I}_n^{[r]}(\mathbf{r}, t) = \int d^3 p \, u^{[r]} \, \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle, \tag{25} \]
where
\[ \langle \hat{n}_1(\mathbf{r}, \mathbf{p}) | t \rangle = \int d\Gamma \, \hat{n}_1(\mathbf{r}, \mathbf{p}) \, \mathcal{R}_\epsilon(t). \tag{26} \]
Similarly for the contributions associated to the two-particle dynamical operator we do have the corresponding thermodynamic variables

\[ \mathcal{C}^{[r+r']}(r, r', t) = \int d\Gamma \hat{\mathcal{C}}^{[r+r']}(r, r') \mathcal{R}_\epsilon(t), \]  

(27)

with \( \mathcal{C} \) given by Eq.(18).

The complete set of thermo-hydrodynamic variables are presented in Table I organized, as one is going up in both columns, in increasing order of tensorial rank.

| Generalized Grand-Canonical Description |
|----------------------------------------|
| Single-Particle                        |
| ···                                     |
| \( I_{h1}^{[r]}(r, t) ; I_{n1}^{[r]}(r, t) \) |
| ···                                     |
| \( I_{h2}^{[2]}(r, t) ; I_{n2}^{[2]}(r, t) \) |
| \( \mathcal{C}_{pp'}^{[r+1]}(r, r', t) ; \mathcal{C}_{pp'}^{[2+0]}(r, r', t) \) |
| \( \mathcal{C}_{pp'}^{[1+0]}(r, r', t) ; \mathcal{C}_{pp'}^{[0+1]}(r, r', t) \) |
| \( h(r, t) ; n(r, t) \) |
| \( \hat{n}_1(r, p) \) |
| Two-Particle                           |
| ···                                     |
| \( \mathcal{C}_{pp'}^{[r+1]}(r, r', t) ; \mathcal{C}_{pp'}^{[2+0]}(r, r', t) \) |
| \( \mathcal{C}_{pp'}^{[1+0]}(r, r', t) ; \mathcal{C}_{pp'}^{[0+1]}(r, r', t) \) |
| \( \hat{n}_2(r, p', r', p') \) |

TABLE I: The basic set of macrovariables one- and two-particle dynamical operators description and the generalized grand-canonical description.

We call the attention to the fact that the generalized nonequilibrium grand-canonical statistical operator is the one of Eq.(4) once in it is introduced the auxiliary operator of Eq.(7); explicitly

\[ \mathcal{R}_\epsilon(t) = \rho_e(t) \times \rho_R, \]  

(28)

with

\[ \rho_e(t) = \exp \left\{ -\hat{\mathcal{S}}(t, 0) + \int_{-\infty}^{t} dt' e^{\epsilon(t'-t)} \frac{d}{dt'} \hat{\mathcal{S}}(t, t' - t) \right\}. \]  

(29)

Furthermore, we recall that it can be introduced the separation of \( \rho_e \) into two parts [coming from each contribution in the exponent of Eq.(20)], namely

\[ \rho_e(t) = \bar{\rho}(t, 0) + \rho_e'(t), \]  

(30)
with $\bar{\rho}$ of Eq.(6), and that for the basic variables (in this case those of Table I) and only the basic variables, it follows that

$$I^{[r]}_p(r, t) = \int d\Gamma \hat{I}^{[r]}_p(r) \rho_c(t) = \int d\Gamma \hat{I}^{[r]}_p(r) \bar{\rho}(t, 0),$$

(31)

$$C^{[r+r']}_{pp'}(r, r'; t) = \int d\Gamma \hat{C}^{[r+r']}_{pp'}(r, r') \rho_c(t) = \int d\Gamma \hat{C}^{[r+r']}_{pp'}(r, r') \bar{\rho}(t, 0),$$

(32)

i.e., $\rho'_c$ does not contribute for the average value of, we stress, the basic variables only. Finally, it can be noticed that the quantities of Eq.(32) can be related to fluctuations of the densities and their fluxes. In fact we can write

$$\sigma^{[r+r']}_{pp'}(r, r', t) = \int d\Gamma \left( \hat{I}^{[r]}_p(r) - I^{[r]}_p(r, t) \right) \left( I^{[r']}_{p'}(r', t) - \hat{I}^{[r']}_{p'}(r', t) \right) \rho_c(t)$$

$$= C^{[r+r']}_{pp'}(r, r'; t) - I^{[r]}_p(r, t) I^{[r']}_{p'}(r', t),$$

(33)

which are instantaneous at time $t$ but containing space correlations.

Let us next proceed to derive the equations of evolution of the basic variables, that is, the generalized hydrodynamic equations.

### III. NONLINEAR HIGHER-ORDER THERMO-HYDRODYNAMICS (NLHOTH)

We begin considering a NLHOTH for a system of independent particles, say, an ideal fluid or, more generally, a system of particles with the interaction between them treated in an average-field approximation (a quite interesting case is the fluid of mobile electrons in crystals). Hence, the set of basic variables consists of the one on the left side of Table I, and Eq.(19), that is the one composed of

$$\{ h(r, t), n(r, t), I_h(r, t), I_n(r, t), \left\{ I^{[r]}_h(r, t) \right\}, \left\{ I^{[r]}_n(r, t) \right\} \}. \tag{34}$$

The hydrodynamical motion of this fluid of single particles is described by the set of coupled highly-nonlinear integro-differential equations consisting of the kinetic equations provided by the formalism (see Appendix E), which are the generalized hydrodynamic equations given by

$$\frac{\partial}{\partial t} h(r, t) + \nabla \cdot I_h(r, t) = J_h(r, t),$$

(35)
\[
\frac{\partial}{\partial t} n(r, t) + \nabla \cdot I_n(r, t) = J_n(r, t), \quad (36)
\]
\[
\frac{\partial}{\partial t} I_h(r, t) + \nabla \cdot I_h^{[2]}(r, t) = J_h(r, t), \quad (37)
\]
\[
\frac{\partial}{\partial t} I_n(r, t) + \nabla \cdot I_n^{[2]}(r, t) = J_n(r, t), \quad (38)
\]
\[
\frac{\partial}{\partial t} I_h^{[r]}(r, t) + \nabla \cdot I_h^{[r+1]}(r, t) = J_h^{[r]}(r, t),\quad (39)
\]
\[
\frac{\partial}{\partial t} I_n^{[r]}(r, t) + \nabla \cdot I_n^{[r+1]}(r, t) = J_n^{[r]}(r, t), \quad (40)
\]

with \( r \geq 2 \), \( \nabla \cdot \) is the tensorial divergence operator, and where, on the right, are present the collision operators
\[
J_p^{[r]}(r, t) = \int_0^t dt' e^{\chi(t'-t)} \int d\Gamma \left\{ \left\{ \tilde{I}_p^{[r]}, \tilde{H}'(t' - t)_0 \right\}, \tilde{H}' \right\} \rho_e(t) \times \rho_R, \quad (41)
\]

for \( r = 0, 1, 2, \ldots, p = h \) or \( n \), \{ \ldots \} is Poisson parentheses (see Appendix E), and subindex nought stands for evolution in the interaction representation. We recall that \( \tilde{H}' \) contains the internal interactions plus the one with the reservoir, and, eventually, with external sources of perturbation. Moreover, if the collision operators are neglected we do have the conservation equation for each quantity. As a matter of practicality, one needs - depending on the problem in hands - to resort to a truncation in the chain of generalized hydrodynamic equations, Eqs.(35) to (40), say for \( r = n \): the point is discussed in Ref.[26], and further considerations are presented in Refs.[11,27]. Hence, once the equation for the \( n \)-th flux contains a term with the divergence of the \((n+1)\)-th flux, to close the system of hydrodynamic variables one needs to express the latter in terms of all the other basic variables (the densities and the fluxes up to order \( n \)), and this involves a nonlinear expression. Thus we do face nonlinearities at this point, but also, and more importantly, in the collision integrals \( J \). They are - see Eq.(41) - depending on a highly nonlinear way on the nonequilibrium thermodynamic variables \( F \)'s [cf. Eqs.(8) and (9)], and therefore the system of hydrodynamic equations needs be coupled with the set of nonequilibrium equations of states, namely, Eqs.(20) to (25) and (27) (let us noticed that such dependence comes from the statistical operator in the calculation of averages). Consequently, the collision operators depend on a highly nonlinear way on the
nonequilibrium thermodynamic variables, which, in turn depend on a highly nonlinear way on the basic hydrodynamic variables. All this is illustrated in the follow up article in a simple model and a first-order hydrodynamics \((n = 1)\).

Summarizing, Eqs.(35) to (40) provide the thermo-hydrodynamics of the nonequilibrium many-body system, which describe the evolution of an infinite set of coupled highly-nonlinear integro-differential equations. Moreover, as noticed, practical usage requires us to introduce a truncation procedure, meaning the analog of the one in the Hilbert-Chapmann-Enskog approach to the Boltzmann equation, or, more precisely, one which is closely related to Grad’s moments method \([32]\); This is discussed in Ref.[33], and a particular case - a phoinjected plasma in semiconductors - is considered in Refs.[34] and [35]; we return to this important question in a future article on NLHOTH.

It can also be noticed that, alternatively, Eqs.(35) to (40) can be closed writing on the right-hand side the basic variables in terms of the intensive ones, but for building this NLHOTH it is more satisfactory the first choice of description (i.e. in term of the variables of Eq.(34)).

We also call the attention to the fact that if we introduce a nonequilibrium generalized grand-canonical-like partition function as

\[
\phi(t) = \ln \overline{Z}(t),
\]

with \(\phi(t)\) of Eq.(3) but for \(F_2 = 0\) once we are working in a single-particle representation, it follows that

\[
I_{p}^{(r)}(r, t) = -\delta \ln \overline{Z}(t)/\delta F_{p}^{(r)}(r, t),
\]

an alternative of Eq.(23) and where \(\delta\) stands for functional derivative \([36]\). Moreover, defining the nonequilibrium-informational entropy \([37]\)

\[
\overline{S}(t) = \int d\Gamma \, \hat{S}(t, 0),
\]

it is verified that

\[
F_{p}^{(r)}(r, t) = \delta \overline{S}(t)/\delta I_{p}^{(r)}(r, t).
\]

It can be noticed that Eq.(45) and Eq.(43) - the latter an alternative form of the Eqs.(20) to (25) - relate the basic variables (the densities and their fluxes) \(I_{p}^{(r)}(r, t)\), to the nonequilibrium thermodynamic variables, \(F_{p}^{(r)}(r, t)\), which, as noticed, can be labelled, in analogy
to the case of systems in equilibrium, *nonequilibrium equations of state*. As also commented above, they are fundamental for closing the generalized hydrodynamic equations, Eqs.(35) to (40), that is, the set of equations of evolution is coupled to the set of nonequilibrium equations of state.

On the other hand, if the physical situation we are considering requires to further introduce as basic variables the pair-correlation-like contributions of Eq.(27), use must be made of the statistical operator of Eq.(4) where the auxiliary statistical operator of Eqs.(6) to (9) must be introduced. The set of Eqs.(35) to (40) - in which it must be understand that the average values are calculated using the above said statistical operator -, is now extended to incorporate the equations of evolution of the added variables, namely

\[
\frac{\partial}{\partial t} C_{pp'}^{[r+r']}(r, r'; t) = \int d\Gamma \left\{ \hat{C}_{pp'}^{[r+r']}(r, r'), \hat{H}_0 \right\} \bar{\rho}(t, 0) \\
+ \int d\Gamma \int d\Gamma_R \left\{ \hat{C}_{pp'}^{[r+r']}(r, r'), \hat{H}' \right\} \rho_\epsilon(t) \times \rho_R,  \tag{46}
\]

or

\[
\frac{\partial}{\partial t} C_{pp'}^{[r+r']}(r, r'; t) + \int d\Gamma \left[ \nabla \cdot \hat{I}_{p'}^{[r^*+1]}(r) \hat{I}_{p'}^{[r']}(r') + \hat{I}_{p'}^{[r]}(r) \nabla' \cdot \hat{I}_{p'}^{[r^*+1]}(r') \right] \bar{\rho}(t, 0) \\
= \frac{\partial}{\partial t} C_{pp'}^{[r+r']}(r, r'; t) + \nabla' \cdot \int d\Gamma C_{pp'}^{([r^*+1]+r']}(r, r'; t) + \nabla' \cdot \int d\Gamma C_{pp'}^{[r+(r^*+1)]}(r, r'; t) \\
= \mathcal{J}_{pp'}^{[r+r']}(r, r'; t),  \tag{47}
\]

The set of equations of evolution needs, as noticed, be coupled to the equations of state, that is, those of Eqs.(43) or (45), and now with the ones associated to the two-particle contributions, namely

\[
C_{pp'}^{[r+r']}(r, r'; t) = \delta \ln \bar{Z}(t)/\delta F_{pp'}^{[r+r']}(r, r'; t), \tag{48}
\]

or

\[
\delta F_{pp'}^{[r+r']}(r, r'; t) = -\delta S(t)/\delta C_{pp'}^{[r+r']}(r, r'; t). \tag{49}
\]

We restate that both cases, the one involving only single-particle operators and the other with single- and two-particle operators, the *nonlinearity* is present in the scattering operators $\mathcal{J}$’s, which are in general depending on a highly nonlinear variables $F$’s, and then, through the nonequilibrium equations of state, depend on a highly nonlinear way on the basic variables. This is illustrated in the follow-up article.
IV. CONCLUDING REMARKS

Briefly summarizing the results, it has been shown how a statistical nonequilibrium ensemble formalism (applicable to the study of systems even in conditions far from equilibrium) provides - via the use of a quite general nonequilibrium grand-canonical ensemble - a microscopic foundation for a Nonlinear Higher-Order and Fluctuations-dependent Hydrodynamics. Its description is based on the set of macrovariables consisting of the densities of energy and matter (particles), their fluxes of all order, and the direct and cross correlations between all of them: In that way higher-order descriptions and fluctuations, respectively, are included in the theory, (cf. Table I).

All these macrovariables are the average value over the nonequilibrium ensemble of the corresponding microscopic mechanical operators. Once the complete set of macrovariables is given we can obtain the nonlinear hydrodynamic equations, which are the average value over the nonequilibrium ensemble of Hamilton equations of motion (in the classical level or Heisenberg equations at the quantum level) of the basic microvariables (mechanical observables): cf. Eqs.(35) to (40) and (46) to (47).

These generalized hydrodynamic equations present on the left side the conserving part of the corresponding quantity, and on the right-hand side are present the collision integrals which include the action of external sources and the contributions of scattering processes responsible for dissipative effects. As noticed before, these collision integrals depend on a highly nonlinear way on the nonequilibrium thermodynamic variables (the Lagrange multipliers that the variational method introduces, namely, $F_p^{[r]}$ and $F_{pp}^{[r+r']}$ in Eqs.(7) to (9)). Hence, this set of hydrodynamic equations is closed after it is coupled with the set of nonequilibrium equations of state, that is, Eqs.(43) and (48), or Eqs.(45) and (49) or simply Eqs.(19) and (27).

In that way we do have a quite generalized hydrodynamics under any arbitrary condition of excitation, which, as noticed, can be referred to as Nonlinear Higher-Order and correlation-dependent Hydrodynamics. In the follow up article we present an illustration of its application, consisting of a simple model of two ideal fluids in mutual interaction - one of them acting as a reservoir - and in a truncated NLHOH of order 1.
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APPENDIX A: DYNAMICAL DENSITY OPERATORS (REDUCED DISTRIBUTION FUNCTIONS)

For the sake of completeness, we notice that in classical mechanics the one-particle and two-particle operators $\hat{n}_1$ and $\hat{n}_2$ are given, respectively, by

$$
\hat{n}_1(\mathbf{r}, \mathbf{p}) = \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j), \quad (A1)
$$

$$
\hat{n}_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}') = \sum_{j=1}^{N} \sum_{k=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j) \delta(\mathbf{r}' - \mathbf{r}_k) \delta(\mathbf{p}' - \mathbf{p}_k), \quad (A2)
$$

for each one of the different $S$ types of particles that can be present [cf. Eq.(2)], and where, as usual, $\mathbf{r}_j$ and $\mathbf{p}_j$ are the coordinate and momentum of the $j$-th particle, and $\mathbf{r}$ and $\mathbf{p}$ the so-called coordinate and momentum field variables.

In quantum mechanics the one- and two-particle density operators are ($\sigma$ is the spin index)

$$
\hat{n}_1(\mathbf{r}, \sigma, \mathbf{r}', \sigma') = \Psi_{\sigma}^\dagger(\mathbf{r}) \Psi_{\sigma}^\dagger(\mathbf{r}), \quad (A3)
$$

$$
\hat{n}_2(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2, \mathbf{r}'_2, \sigma'_2, \mathbf{r}'_1, \sigma'_1) = \Psi_{\sigma_1}^\dagger(\mathbf{r}_1) \Psi_{\sigma_2}^\dagger(\mathbf{r}_2) \Psi_{\sigma'_2}(\mathbf{r}'_2) \Psi_{\sigma'_1}(\mathbf{r}'_1), \quad (A4)
$$

where $\Psi(\Psi^\dagger)$ are single-particle field operators in second quantization (an excellent didactical description of them is available in the article by B. Robertson of Ref.[38]). These operators can be expressed in terms of annihilation and creation operators in single-particle states with, say, wavefunction $\varphi_{k\sigma}$ and energy levels $\varepsilon_{k\sigma}$, in the form

$$
\Psi_{\sigma}(\mathbf{r}) = \sum_{k} \varphi_{k\sigma} c_{k\sigma}, \quad (A5)
$$

$$
\Psi_{\sigma}^\dagger(\mathbf{r}) = \sum_{k} \varphi_{k\sigma}^* c_{k\sigma}^\dagger, \quad (A6)
$$
This is quite convenient since it introduces a description in the reciprocal k-space, with practical advantages in calculations and physical interpretations. In this way we can introduce instead of \( \hat{n}_1 \) and \( \hat{n}_2 \) of Eqs. (A3) and (A4), matrices composed with the quantities

\[
\left\{ \left\{ c_{k\sigma}^{\dagger} c_{k'\sigma'} \right\}, \left\{ c_{k\sigma}^{\dagger} c_{k'\sigma'}^{\dagger} c_k c_k' \right\} \right\}, \tag{A7}
\]

Hence, any one-particle mechanical observable can be expressed in terms of the quantities

\[
\left\{ \hat{n}_{k\sigma\sigma'} = c_{k\sigma}^{\dagger} c_{k'\sigma'}, \hat{n}_{kQ\sigma\sigma'} = c_{k+\frac{1}{2}Q\sigma}^{\dagger} c_{k-\frac{1}{2}Q\sigma} \right\}, \tag{A8}
\]

with \( Q \neq 0 \), where we have separated out diagonal terms and non-diagonal ones: the first are so-called populations and the others coherences [39] (while the former appear in the description of whole properties - or uniform states -, the latter describe local properties - or inhomogeneous states). Any one-particle mechanical observable is then written in second quantization in the known form

\[
\hat{A} = \sum_{k\sigma, k'\sigma'} \langle k\sigma | \hat{A} | k'\sigma' \rangle c_{k\sigma}^{\dagger} c_{k'\sigma'}, \tag{A9}
\]

for any pair \( k\sigma \) and \( k'\sigma' \), and where is present the matrix element of \( \hat{A} \) between one-particle states \( \langle k\sigma | \) and \( | k'\sigma' \rangle \).

For two-particle mechanical observables, using in Eq. (A7) the change of indexes \( k + \frac{1}{2}Q \) for \( k, k' - \frac{1}{2}Q' \) for \( k' \), \( k - \frac{1}{2}Q \) for \( k_1, k' + \frac{1}{2}Q' \) for \( k_2 \), we have

\[
\hat{n}_{k\sigma_1, k'\sigma'_1, k\sigma_2, k'\sigma'_2} = c_{k\sigma_1}^{\dagger} c_{k'\sigma'_1}^{\dagger} c_k c_k', \tag{A10}
\]

for \( Q, Q' \neq 0 \). A two-particle observable takes the form [40, 41]

\[
\hat{B} = \sum_{k,k',Q,Q',\sigma_1\sigma'_1\sigma_2\sigma'_2} \left( \langle k + \frac{1}{2}Q\sigma_1, k' - \frac{1}{2}Q'\sigma_2 | \hat{B} | k' + \frac{1}{2}Q'\sigma_2, k - \frac{1}{2}Q\sigma_1 \rangle \times \right.
\]

\[
\times \left[ \hat{n}_{kQ\sigma_1, k'Q'\sigma_2}^{\dagger} \hat{n}_{k'Q'\sigma_2, kQ\sigma_1} + \delta_{kQ\sigma_1, k'Q'\sigma_2} c_{k+\frac{1}{2}Q\sigma_1}^{\dagger} c_{k'+\frac{1}{2}Q'\sigma_1} \right], \tag{A11}
\]

where we have rearranged the order in the product of four operators in Eq. (A11), to obtain a contribution as a product of two \( \hat{n}_1 \)-type operators and another involving \( \hat{n}_1 \) already present in Eq. (A8); upper sign minus stands for the case of fermions and lower plus for bosons.

For example, Coulomb interaction between pairs of electrons is given by

\[
\hat{H}_C = \sum_{Q \neq 0} V(Q) \left[ \hat{n}_Q \hat{n}_Q^{\dagger} - N \right], \tag{A12}
\]

17
where, once a complete set of plane-wave states has been taken as one-particle quantum states, $\mathcal{V}(Q) = 4\pi e^2/VQ^2$ ($V$ is the sample volume),

$$\hat{n}_Q = \sum_{k\sigma\sigma'} \delta_{\sigma\sigma'} \hat{n}_{kQ\sigma\sigma'}, \quad (A13)$$

is the $Q$-wave-number Fourier transform of the operator density of charge of the electrons (in units of the electron charge), and $\hat{N} = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}$ is the operator number of particles.

We call attention to the fact that if the particles are bosons, then coherent states are possible to be present and then, besides the one- and two-particle density operators, we must also add the individuals amplitudes $c_{k\sigma}$ (and $c_{k\sigma}^\dagger$) for the description of the boson system (for example coherent photons in a laser, coherent phonons in semiconductors, etc).

**APPENDIX B: THE QUANTUM MECHANICAL NONEQUILIBRIUM STATISTICAL OPERATOR**

In the quantum case the auxiliary statistical operator of Eq.(2) is

$$\bar{\rho}(t, 0) = \exp \left\{ -\phi(t) - \sum_{k} F_k(t) \hat{n}_k - \sum_{kQ, k'Q'} F_{kQ,k'Q'}(t) \hat{n}_{kQ} \hat{n}^\dagger_{k'Q'} \right\}, \quad (B1)$$

which is written in terms of the quantities of Eqs.(A8) and (A11), with spin indexes omitted. The quantum nonequilibrium statistical operator is given by Eq.(4), where now enters $\bar{\rho}$ of Eq.(6), and

$$\bar{\rho}(t, t' - t) = \exp \left\{ -\frac{1}{\hbar} (t' - t) \hat{H} \right\} \bar{\rho}(t, 0) \exp \left\{ \frac{1}{\hbar} (t' - t) \hat{H} \right\}. \quad (B2)$$

The three $F$‘s in Eq(B1) are the corresponding Lagrange multipliers in the variational approach (intensive nonequilibrium thermodynamic variables conjugated to the dynamical operators). Moreover, the macrovariables for describing the nonequilibrium thermodynamic state of the system are the average value of the same quantities over the nonequilibrium ensemble, namely

$$n_k(t) = Tr \{ \hat{n}_k \mathcal{R}_e(t) \}, \quad (B3)$$

$$n_{kQ}(t) = Tr \{ \hat{n}_{kQ} \mathcal{R}_e(t) \}, \quad (B4)$$
with \( Q \neq 0 \), and

\[
n_{kQ,k'Q'}(t) = Tr \left\{ \hat{n}_{kQ} \hat{n}^\dagger_{k'Q'} R_c(t) \right\},
\]

(B5)

with no restriction on \( Q \) and \( Q' \).

APPENDIX C: CLASSICAL NONEQUILIBRIUM GRAND-CANONICAL STATISTICAL OPERATOR

Consider thermodynamic intensive variable \( F_1(r,p; t) \) in the auxiliary statistical operator of Eq.(2), and let us perform a Taylor series expansion in \( p \), i.e.

\[
F_1(r,p; t) = \Phi(r,t) + \Phi(r,t) \cdot p + \Phi^{[2]}(r,t) \otimes [pp] \\
+ \sum_{r \geq 3} \Phi^{[r]}(r,t) \otimes [p \ldots r-times \ldots p], \tag{C1}
\]

where \( \Phi = F_1(r,p; t)|_{p=0}, \Phi^{[r]} = \frac{1}{r!}[\nabla_p \ldots r-times \ldots \nabla_p F_1(r,p; t)]_{p=0}, \) for \( r = 1, 2, 3, \ldots \) indicating the tensorial rank, \([\ldots]\) stands for tensorial product of vectors, dot as usual as scalar product, and \( \otimes \) for fully contracted product of tensors. Next, we redefine quantities \( \Phi \) in the following way

\[
\Phi(r,t) \equiv A_n(r,t), \tag{C2}
\]

\[
\Phi(r,t) \equiv V_n(r,t), \tag{C3}
\]

\[
\Phi^{[r]}(r,t) \equiv \frac{F^{[r]}_n(r,t)}{m^r} \left[ \left( \Phi^{[r]}(r,t) \otimes 1^{[2]} \right) 1^{[2]} \right], \tag{C4}
\]

further introducing

\[
\frac{F^{[r-2]}_n(r,t)}{2m^{r-1}} \equiv \frac{1}{3} \Phi^{[r]}(r,t) \otimes 1^{[2]}, \tag{C5}
\]

where \( 1^{[2]} \) is the unit tensor of rank two, it can be noticed that it is satisfied the rule

\[
F^{[r]}_n(r,t) \otimes 1^{[2]} = 0, \tag{C6}
\]

and that

\[
Ph^{[r]}_n(r,t) \otimes [p \ldots r-times \ldots p] = F^{[r]}_n(r,t) \otimes u^{[r]}(p) + F^{[r-2]}_h(r,t) \otimes \frac{p^2}{2m} u^{[r-2]}, \tag{C7}
\]
where

\[ u^{[r]} = [u \ldots r-times \ldots u], \]  
\[ (C8) \]

is the \( r \)-rank tensor resulting from the inner tensorial product of \( r \) characteristics velocities

\[ u = p/m. \]  
\[ (C9) \]

Finally, defining the generalized fluxes operators

\[ \hat{J}^{[r]}_n(r) = \int d^3p \, u^{[r]} \hat{n}_1(r, p), \]  
\[ (C10) \]

\[ \hat{J}^{[r]}_h(r) = \int d^3p \, \frac{p^2}{2m} u^{[r]} \hat{n}_1(r, p), \]  
\[ (C11) \]

and taking into account that

\[ \hat{n}_2(r, p, r', p') = \hat{n}_1(r, p) \hat{n}_1(r', p'), \]  
\[ (C12) \]

we can write the auxiliary statistical operator of Eq.(6).

\[ \textbf{APPENDIX D: THERMO-HYDRODYNAMIC VARIABLES FOR SYSTEM WITH ARBITRARY ENERGY-DISPERSION RELATION} \]

As shown elsewhere at a quantum-mechanical description the fluxes of energy (index \( h \)) and of matter (index \( n \)) are in reciprocal space (of wavevectors \( Q \)) given by

\[ I^{[r]}_n(Q, t) = \sum_k \frac{1}{2} \left( \varepsilon_{k+\frac{1}{2}Q} + \varepsilon_{k-\frac{1}{2}Q} \right) u^{[r]}(k, Q) n_{kQ}(t), \]  
\[ (D1) \]

\[ I^{[r]}_h(Q, t) = \sum_k u^{[r]}(k, Q) n_{kQ}(t), \]  
\[ (D2) \]

where

\[ u^{[r]}(k, Q) = [u(k, Q) \ldots r-times \ldots u(k, Q)], \]  
\[ (D3) \]

is a rank-\( r \) tensor composed by the tensorial product of \( r \)-times the generating velocity

\[ u(k, Q) = \frac{1}{\hbar} \nabla_k \varepsilon_k + \sum_{l=1}^{\infty} \frac{1}{(2l + 1)!} \left( \frac{1}{2} Q \cdot \nabla_k \right)^{2l} \frac{1}{\hbar} \nabla_k \varepsilon_k. \]  
\[ (D4) \]
We recall that $\varepsilon_k$ is the energy dispersion relation of the single particles, and

$$n_{kQ}(t) = Tr \left\{ c_{k+\frac{1}{2}Q} c_{k-\frac{1}{2}Q} \hat{\rho}(t,0) \right\}, \quad (D5)$$

is the average over the nonequilibrium ensemble of Dirac-Landau-Wiegner single-particle dynamical operator. It can be noticed in Eq.(D4) that the generating velocity is composed of a first contribution consisting of the group velocity of the wavepacket of a single particle in state $|k\rangle$, and the following terms - depending on $Q$ - can be considered as contributions indicating the change from point to point of the group velocity, once in direct space we can write

$$u(k, r) = \left\{ \frac{1}{\hbar} \nabla_k \varepsilon_k + \frac{1}{24} (\nabla \cdot \nabla_k)^2 \frac{1}{\hbar} \nabla_k \varepsilon_k + \ldots \right\} \delta(r), \quad (D6)$$

where $\nabla$ is the gradient in $r$-space, and we can see that this expression contains a series of even powers of such gradient. These expressions in a classical mechanical levels retain the form except that we must introduce the linear momentum $\mathbf{p}$ in place of $\hbar \mathbf{k}$.

**APPENDIX E: THE KINETIC THEORY**

The kinetic theory that can be derived out of the nonequilibrium ensemble formalism can be considered a far-reaching generalization of Mori’s approach, involving nonlinearity, all order of particle collisions, and covering arbitrarily far-from-equilibrium situations. The presentation unavoidably involves a lengthy and somehow cumbersome mathematical handling, but we call the attention to the simplest form (the Markovian approximation) which is usually the one to be used, once in most problems are verified the restrictions that, say, validate it $[26, 42, 43]$.

We begin recalling the separation of the total Hamiltonian as given by

$$\hat{H} = \hat{H}_0 + \hat{H}', \quad (E1)$$

where $\hat{H}' = \hat{H}_1 + \hat{W}$, with $\hat{H}_1$ containing the internal interactions and $\hat{W}$ those with the reservoir and eventual external sources of perturbation, while $\hat{H}_0$ is the kinetic energy operator. Moreover, let us call in a generic way as $\left\{ \hat{P}_j \right\}$, $j = 1, 2, \ldots$ the set of basic variables, which for the case we are considering on the main text are those of Eq.(26), for which stands the selection rule

$$\left\{ \hat{P}_j, \hat{H}_0 \right\} = \sum_m \alpha_{jm} \hat{P}_m, \quad (E2)$$
where $\alpha_{jm}$ are $c$-numbers or differential operators depending on the representation being used, and in the case of the variables of Eq.(26) we have that

$$\left\{ \hat{I}^{[r]}_p(r), \hat{H}_0 \right\} = -\nabla \cdot \hat{I}^{[r+1]}_p(r), \quad \text{(E3)}$$

with $p = h$ or $n$ and $r = 0, 1, 2, \ldots$. We also recall that for the nonequilibrium statistical operator of the system holds the separation into two parts, as given by Eq.(22) namely

$$\rho_\epsilon(t) = \bar{\rho}(t, 0) + \rho'_\epsilon(t), \quad \text{(E4)}$$

consisting of the "instantaneously frozen" $\bar{\rho}$, and the part $\rho'_\epsilon$ responsible for the irreversible evolution of the macrostate of the system.

The equations of evolution for the basic variables are the average over the nonequilibrium ensemble of Hamilton equation of motion for the basic dynamical variables, namely

$$\frac{d}{dt} Q_j(t) = \frac{d}{dt} Tr \left\{ \hat{P}_j \rho_\epsilon(t) \times \rho_R \right\} = Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H} \right] \rho_\epsilon(t) \times \rho_R \right\}, \quad \text{(E5)}$$

where $Tr$ is to be understood as integration over the composite phase space of system and reservoir. Using Eqs.(D1) to (D4) we can alternatively write that

$$\frac{d}{dt} Q_j(t) = Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H}_0 \right] \bar{\rho}(t, 0) \times \rho_R \right\} + Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H} \right] \rho'_\epsilon(t) \times \rho_R \right\} + Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H}' \right] \rho_\epsilon(t) \times \rho_R \right\} + Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H} \right] \rho'_\epsilon(t) \times \rho_R \right\}, \quad \text{(E6)}$$

But the second term on the right-hand side of this Eq.(D6) is null; in fact

$$Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j, \hat{H}_0 \right] \rho'_\epsilon(t) \times \rho_R \right\} = \sum_{jm} \alpha_{jm} Tr \left\{ \hat{P}_m \rho'_\epsilon(t) \times \rho_R \right\} = 0, \quad \text{(E7)}$$

once we take into account that

$$Tr \left\{ \hat{P}_m \rho_\epsilon(t) \times \rho_R \right\} = Tr \left\{ \hat{P}_m \bar{\rho}(t, 0) \times \rho_R \right\}, \quad \text{(E8)}$$

[cf. Eq.(23)]. The remaining term can be handled through an elaborate algebra to obtain that the kinetic equations acquire the form of a far-reaching generalization of Mori’s equations, namely

$$\frac{d}{dt} Q_j(t) = J_j^{(0)} + J_j^{(1)} + \sum_{m=2}^{\infty} \Omega_j^{(m)}(t), \quad \text{(E9)}$$
where $J^{(0)}$ is the first contribution on the right of Eq. (D6), $J^{(1)}$ the third followed by a series of partial collision operators involving increasing orders in the interaction strengths ($m = 1, 2, \ldots$), and containing memory effects, space correlations, and are highly nonlinear in the basic variables (the collision operators on the right-hand side of Eq. (E9) are dependent on the intensive nonequilibrium thermodynamic variables, $F’s$ in Eq. (2), which are dependent on the basic variables through the constitutive equations, cf. Eq. (19) or Eqs. (43) and (45)).

In the extremely complicated set of coupled equations (E9), we can single out the simplified form consisting of the Markovian approximation. The Markovian limit of the kinetic theory is of particular relevance as a result that, for a large class of problems, the interactions involved in $\hat{H}'$ are weak and the use of lowest order in the equations of motion constitutes an excellent approximation of good practical value. In chapter 6 in Ref. [26] are described several examples of its application for which there follows an excellent agreement between the calculation and the experimental data. By means of a different approach, E. B. Davies [44] has shown that in fact the Markovian approach can be validated in the weak coupling (in the interaction) limit (retaining only the quadratic contribution).

Making it explicit, the Markovian equations in the kinetic theory are

$$
\frac{d}{dt}Q_j(r, t) = J^{(0)}_j(r, t) + J^{(1)}_j(r, t) + J^{(2)}_j(r, t),
$$

(E10)

where we have introduced explicitly the eventual dependence on position $r$. The three terms on the right-hand side of Eq. (D10) are

$$
J^{(0)}_j(r, t) = Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j(r), \hat{H}_0 \right] \rho(t, 0) \times \rho_R \right\},
$$

(E11)

$$
J^{(1)}_j(r, t) = Tr \left\{ \frac{1}{i\hbar} \left[ \hat{P}_j(r), \hat{H}' \right] \rho(t, 0) \times \rho_R \right\},
$$

(E12)

$$
J^{(2)}_j(r, t) = \left( \frac{1}{i\hbar} \right)^2 \int_{-\infty}^{t} dt' \ e^{i(t'-t)} \times Tr \left\{ \left[ \hat{H}'(t' - t)_0, \left[ \hat{H}', \hat{P}_j(r) \right] \right] \rho(t, 0) \times \rho_R \right\},
$$

(E13)

$$
J^{(2)}_j(r, t) = \left( \frac{1}{i\hbar} \right)^2 \sum_k \int_{-\infty}^{t} dt' \ e^{i(t'-t)} \times Tr \left\{ \left[ \hat{H}'(t' - t)_0, \hat{P}_k(r) \right] \rho(t, 0) \times \rho_R \right\} \frac{\delta J^{(1)}_j(r, t)}{\delta Q_k(r, t)},
$$

(E14)

and we recall that $J^{(0)}_j$ and $J^{(1)}_j$, which in Mori’s terminology [45] are called precession terms, are related to the non-dissipative part of the motion, while dissipative effects are accounted
for \(J^{(2)}\). In many cases, as a result of particular symmetries in \(\hat{H}'\) and \(\hat{\rho}\), there follows that \(J^{(1)}_{\rho} = 0\).

Finally, we notice that in Eqs.(35) to (40), we do have in the right-hand side that the collision operator is

\[
J^{[r]}_p(r, t) = J^{[r(1)]}_p(r, t) + \sum_{m \geq 2} \Omega^{[r(m)]}_p(r, t),
\]  

(E15)
in the general case, or

\[
J^{[r]}_p(r, t) \simeq J^{[r(1)]}_p(r, t) + J^{[r(2)]}_p(r, t),
\]  

(E16)
in the Markovian regime [26, 42, 43].

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