Inverse kinetic theory for quantum hydrodynamic equations

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A remarkable feature of standard quantum mechanics is its analogy with classical fluid dynamics. This has motivated in the past efforts to formulate phase-space techniques based on various statistical models of quantum hydrodynamic equations. In this work an inverse kinetic theory for the Schrödinger equation has been constructed in order to formally describe the standard quantum dynamics by means of a classical dynamical system (to be denoted as phase-space Schrödinger dynamical system). It is shown that the inverse kinetic theory can be (non)uniquely determined under suitable mathematical prescriptions. In particular, when the quantum linear momentum is identified with a suitable linear kinetic momentum, it follows that the fluctuations of the position vector and the kinetic linear momentum satisfy identically the Heisenberg theorem.

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I. INTRODUCTION

The goal of this investigation is to develop a new phase-space approach to quantum mechanics. This is based on an *inverse kinetic theory* for the Schrödinger equation, i.e., a kinetic theory which is equivalent, in a suitable sense (to be recalled below), to the latter equation. Based on recent work by Ellero and Tessarotto [1,2], we intend to show that the complete set of hydrodynamic equations can be generated by means of a kinetic theory of this type which holds for arbitrary initial and boundary conditions for the quantum state.

Starting point is the quantum hydrodynamics formulation of standard quantum mechanics (SQM). In fact, it is well known that the Schrödinger equation [3] is equivalent to a complete set of partial differential equations for suitable real-valued functions of position and time (denoted as *quantum fluid fields*), which are known as *quantum hydrodynamic equations* (QHE) [4]. The quantum hydrodynamic description obtained in this way, which has been studied by several authors [4–13], affords a straightforward physical interpretation in terms of a classical fluid. This is obtained by identifying the classical fluid fields (number density and fluid velocity), respectively, with the quantum probability density in configuration space and the quantum probability current (or quantum fluid velocity). In particular, the quantum hydrodynamic equations can be viewed as the equations of a classical compressible and nonviscous fluid, endowed with potential velocity and quantized velocity circulation.

The analogy (with classical fluid dynamics) has motivated in the past efforts to formulate phase-space techniques based on various statistical models of quantum hydrodynamic equations. These works, although based on different approaches, share the common view that the quantum state corresponds to an underlying statistical description of some sort (for a review of the phase-space route to the quantum hydrodynamic equations see, for example, Ref. [14]).

Following the pioneering work of Wigner [15,16], phase-space techniques typically require that the quantum fluid fields or the wave function itself be represented in terms of, or associated with, appropriate phase-space functions. These are usually identified with quasiprobabilities [17] (for a review see Ref. [18], Chap. 4), although formulations based on pure probability densities are also available (see Ref. [19], Sec. IV.3). Several examples of approaches of this type are known, which include in particular the Wigner representation [15] and the *P*-representation [20,21]. The procedure of representing quantum states by quasiprobabilities in phase space is closely related to the phase space formulation of SQM mechanics based on the noncommutative product known as Moyal product [22,23] However, it is known that quasiprobabilities such as the Wigner distribution, may become singular in the so-called "full quantum regime" [24], i.e., when the potential becomes nonlinear. A related type of approaches are based on moment-expansion techniques [25–27] which seek to reconstruct the density operator or the corresponding phase-space distributions [28–32]. The latter are usually obtained by constructing a set of moments in terms of the Wigner distribution. However, the corresponding moment equations (*quantum hydrodynamic moment equations*), except for particular initial conditions [33] or specialized (see Refs. [34,35]) and asymptotic models (see for example Ref. [36]), in general do not satisfy a closure condition, i.e., the moment equations form an infinite hierarchy.

These facts have motivated in the past the search of alternative phase-space representations of the quantum state. Among such approaches, we recall, first, the phase space representation of SQM due to Torres-Vega and Frederick [37,38], in which the wave function is extended to phase space and is assumed to obey an appropriate "Schrödinger equation in phase space." Another class of statistical approaches is represented by the attempt to interpret SQM in the framework of an underlying statistical process. An example is provided by stochastic models (see, for example, Refs. [39–43] and the review paper [44]), in which the underlying particle dynamics is governed by stochastic differential equations, such as those describing the nondissipative quantum Brownian motion, which traditionally is described

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by Fokker-Planck or diffusion equations. Such equations, generally, lead again to quasiprobability distributions which permit to "reconstruct" the Schrödinger equation only approximately (namely in an asymptotic sense) and under "ad hoc" initial conditions, since quasiprobability functions may become, in general, invalid for nonMarkovian processes with arbitrary noise correlation. Although extensions of the classical theory of Brownian to quantum domain have been proposed which permit the formulation in terms of a well-behaved true probabilistic description [45], the problem of these approaches remains that of explaining the origin of such stochasticity [46,47], which is precisely their weakness.

A second type of statistical approach is provided by kinetic models in which the underlying particle dynamics is purely classical, i.e., the Schrödinger equation is assumed to be based on classical kinetic theory. An example of this type is provided by the approach due to Kaniadakis [48,49], in which each quantum particle is assumed to be composed by $N \gg 1$ identical "subquantum" interacting classical particles (monads), to be described by means of a classical kinetic equation. Also in this case the Schrödinger equation is—at best—recovered only in an approximate sense. Several aspects of this formulation, however, remain unclear, which include—among others—the problem of the closure of the moment equations, the specification of the initial and boundary conditions for the kinetic distribution function and the conditions of convergence to the Schrödinger equation.

In this paper we intend to show that certain difficulties of previous theories (in particular the issue of closure conditions of quantum hydrodynamic moment equations and the possible singularity of the quasiprobability density) can be overcome. For this purpose an *inverse kinetic theory* is adopted for the Schrödinger equation, based on the introduction of a suitable *inverse kinetic equation* (IKE). By definition IKE must be able to yield identically, via suitable moment equations, the complete system of equations forming QHE. In particular, we intend to show that it can be constructed in such a way to satisfy the following requirements.

(1) *Completeness of IKE*. All fluid fields are expressed as moments of the kinetic distribution function and all hydrodynamic equations can be identified with suitable moment equations of IKE.

(2) *Closure condition of moment equations of IKE*. There must exist a subset of moments of IKE which form a complete system of equations, to be identified with the prescribed set of quantum hydrodynamic equations.

(3) *Smoothness for the wave function*. The system wave function is assumed suitably smooth so that the solution of the kinetic distribution function exists everywhere in a suitable extended phase space.

(4) *Arbitrary initial and boundary conditions for the system wave function*. The initial conditions for the Schrödinger equations are set arbitrarily while Dirichlet boundary conditions are considered for the system wave function.

(5) *Self-consistency of IKE*. The kinetic theory must hold for arbitrary (and suitably smooth) initial conditions for the kinetic distribution function. In other words, the initial kinetic distribution function must remain arbitrary even if a suitable set of its moments are prescribed at the initial time.

(6) *Nonasymptotic IKE*. That is, the correct hydrodynamic equations must be recovered by the inverse kinetic theory independently of any physical parameter characterizing the quantum hydrodynamic equations.

The formulation of a theory of this type involves also the identification of an underlying classical dynamical system, in terms of which all relevant observables and related expectation values are advanced in time. This feature is potentially important for numerical simulations both in computational fluid dynamics and quantum mechanics, since the corresponding phase-space trajectories, which determine uniquely the evolution of the fluid fields, can thus be evaluated numerically. This permits the development of Lagrangian particle simulation methods in fluid dynamics which exhibit a low computational complexity [50].

From the mathematical viewpoint inverse kinetic theories can be obtained, in principle, for arbitrary fluid equations, an example being provided by the inverse kinetic theory recently developed for the incompressible Navier-Stokes equation by Ellero and Tessarotto (see Refs. [1,2]). A basic prerequisite for the formulation of an inverse kinetic theory of this type is, however, the proper definition of the relevant *quantum fluid fields* and their identification with suitable momenta (to be denoted as *kinetic fluid fields*), which include the *kinetic temperature* as well as the related definition of *directional temperatures* (see below).

However, the case of Schrödinger equation is peculiar because, as is well known, its related fluid equations apparently depend only on two quantum fluid fields, respectively, to be identified with the observables quantum probability density and the quantum fluid velocity, while the notions of quantum temperature and directional temperatures (to be identified with the corresponding kinetic moments) remain in principle arbitrary.

The problem is not merely of interest for theoretical and mathematical research, but has potential relevance also for the understanding of the fluid description of quantum mechanics and of the underlying statistical models. Our motivation is to exploit the analogy between classical and QM hydrodynamics descriptions in order to prove that the quantum observables and the fluid fields can formally be represented by means of a purely classical statistical model.

Although the mathematical equivalence should not too hastily be regarded as implying physical equivalence of the two formulations, this suggests that some relevant classical reasonings can be transferred to SQM for the construction of the inverse kinetic theory. This concerns, in particular, the adoption of the so-called principle of entropy maximization (PEM) [19,51,52] for the determination of the initial condition for the kinetic distribution function. As a consequence, one finds that a particular solution for the initial kinetic distribution function corresponds to a generalized Maxwellian kinetic distribution function, carrying prescribed number density, flow velocity and directional temperatures. Nevertheless, also non-Maxwellian kinetic distribution functions can be considered as admissible initial conditions.

Another interesting consequence of the kinetic formulation is the formal description of SQM by means of a classical dynamical system (to be denoted as *phase-space*

Schrödinger dynamical system). This can be interpreted as a system of fictitious particles interacting with each other only by means of an appropriate mean-field interaction which depends on appropriate quantum fluid fields and moments of the kinetic distribution function. Such a classical description is realized by means of an appropriate form of the correspondence principle (denoted *kinetic*), whereby the physical observables, quantum fluid fields and quantum hydrodynamic equations are, respectively, identified with ordinary phase-space functions, kinetic moments of the kinetic distribution function and moment equations obtained from IKE.

Here we intend to show that in principle infinite solutions also to this problem exist due, in particular, to the nonuniqueness of the definition of the kinetic temperature. As a consequence, also the inverse kinetic theory results intrinsically nonunique. Such a feature is not surprising since these kinetic models may be viewed simply as examples of the infinite admissible, and physically equivalent, mathematical descriptions of physical reality. Nevertheless, despite such a nonuniqueness feature, we intend to prove that, by suitable prescriptions, the functional form of the kinetic equation and the mean-field force that defines the streaming operator can both be uniquely defined.

The paper is organized as follows.

The mathematical setting of the hydrodynamic description of SQM is recalled in Secs. II–IV. In particular, the quantum hydrodynamic equations for the quantum fluid fields $\{f,\mathbf{V}\}$ are posed in Secs. II and III, while the definition of the remaining quantum fluid fields, provided by the quantum directional temperatures ($T_{\mathrm{QM},i}$, for $i=1,2,3$), is given in Sec. IV, together with their relationship with the Heisenberg inequalities. The construction of the inverse kinetic theory is treated in Secs. V and VI. In particular, the general form of the IKE is laid in V, while in Sec. VI the mean-field force is determined explicitly. The main results of theory are summarized in three theorems which determine the explicit form of the IKE and its basic properties.

II. HYDRODYNAMIC DESCRIPTION OF NRQM

In this section we intend to recall the well-known fluid description of nonrelativistic quantum mechanics (NRQM), based on the property of the Schrödinger equation to be equivalent to a complete set of fluid equations. For the sake of clarity let us introduce the basic definitions and the mathematical formulation of the problem.

In this paper we shall consider, in particular, the case of a system of spinless scalar particles (bosons) described by a single scalar wave function $\psi(\mathbf{r},t)$, with associated probability density

$$f=|\psi(\mathbf{r},t)|^2, \tag{1}$$

requiring that both are defined and continuous in $\bar{\Omega}\times I$. In addition we impose that f is strictly positive in Ω, where $\bar{\Omega}$ denotes the closure of Ω, while f and ψ are, respectively, single valued and possibly multivalued in $\Omega\times I$, with ψ at least of class $C^{(2+k,1+h)}(\Omega\times I)[\equiv C^{(2+k)}(\Omega)\times C^{(1+h)}(I)]$ with $h,k\geqslant 0$. Hence, by assumption, f can only vanish on the boundary $\delta\Omega$ [i.e., in the nodes $\mathbf{r}_n\in\delta\Omega$ where $f(\mathbf{r}_n,t)=0$] and must satisfy the normalization

$$\int_\Omega d\mathbf{r} f(\mathbf{r},t)=1. \tag{2}$$

For definiteness, we shall also assume, without loss of generality, that Ω is a connected subset of $\mathbb{R}^{3N}$ and $\psi(\mathbf{r},t)$ belongs to the functional space $\{\psi\}$, to be identified with the Hilbert space of complex-valued functions which are square integrable in Ω. The N-body wave function $\psi(\mathbf{r},t)$ is required to satisfy in the open set $\Omega\times I$ the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi=H\psi, \tag{3}$$

where $H=H_o+U$ is the N-body Hamiltonian operator. Here, denoting $\boldsymbol{\nabla}_{(j)}\equiv\frac{\partial}{\partial\mathbf{r}_j}$, $H_o=-\Sigma_{j=1,N}\frac{\hbar^2}{2m}\nabla_j^2$ and U are, respectively, the free-particle Hamiltonian (kinetic energy) and the interaction potential, to be identified with a real function defined and suitably smooth in $\Omega\times I$. For well-posedness, appropriate initial and boundary conditions must be imposed on $\psi(\mathbf{r},t)$. The initial conditions are obtained by imposing for all $\mathbf{r}\in\bar{\Omega}$,

$$\psi(\mathbf{r},t_o)=\psi_o(\mathbf{r}), \tag{4}$$

where ψ_o is a suitably smooth complex-valued function. To specify the boundary conditions, we first notice the boundary set $\delta\Omega$ can always be considered prescribed. The boundary conditions can be specified by imposing Dirichlet boundary conditions on $\delta\Omega$. This requires $\forall\ \mathbf{r}_\delta\in\delta\Omega$,

$$\psi(\mathbf{r}_\delta,t)=\psi_w(\mathbf{r}_\delta,t), \tag{5}$$

$$\lim_{\mathbf{r}\to\mathbf{r}_\delta}\mathbf{V}(\mathbf{r},t)=\mathbf{V}_w(\mathbf{r}_\delta,t), \tag{6}$$

where $V(\mathbf{r},t)$ is the quantum velocity field

$$\mathbf{V}(\mathbf{r},t)=\frac{\hbar}{2mi|\psi(\mathbf{r},t)|^2}\{\psi^*\boldsymbol{\nabla}\psi-\psi\boldsymbol{\nabla}\psi^*\}. \tag{7}$$

Here the complex function $\psi_w(\mathbf{r}_\delta,t)$ and the real vector function $\mathbf{V}_w(\mathbf{r}_\delta,t)$ are prescribed, suitably smooth functions. To specify the value of $f(\mathbf{r},t)$ on $\delta\Omega$, let us require that there results additionally

$$\int_\Omega d\mathbf{r}\boldsymbol{\nabla}f(\mathbf{r},t)=\mathbf{0}. \tag{8}$$

In all such cases Eq. (8) implies that there must be $\forall\ \mathbf{r}_\delta\in\delta\Omega$

$$f(\mathbf{r}_\delta,t)=|\psi_w(\mathbf{r}_\delta,t)|^2\equiv f_o\geqslant 0, \tag{9}$$

where f_o is either a constant, whose value may still depend on the specific subset, or at most is a function $f_o(t)$ to be assumed suitably smooth $\forall\ t\in I$. Hence, the points of $\delta\Omega$ are not necessarily nodes. However, if $\mathbf{r}_\delta$ is an improper point of $\mathbb{R}^{3N}$ (hence, Ω is assumed to be an unbounded sub-

set of $\mathbb{R}^{3N}$), since it must be $\lim_{|\mathbf{r}|\to\infty} f(\mathbf{r},t)=0, \mathbf{r}_\delta$ is necessarily a node, i.e.,

$$f_o = 0. \tag{10}$$

This implies for consistency also

$$\lim_{|\mathbf{r}|\to\infty} \psi_w(\mathbf{r},t) = 0. \tag{11}$$

The set of equations (3)–(6), together with (9)–(11), defines the initial-boundary value problem for the Schrödinger equation (*SE problem*). The solution of the SE problem, ψ, must be determined in an appropriate functional space, to be suitably defined (see, for example, Ref. [53]).

The set of hydrodynamic equations corresponding to the Schrödinger equation are well known [4–6,10] and follow immediately from the exponential representation (known as *Madelung transformation* [4])

$$\psi = \sqrt{f} e^{i(S/\hbar)}, \tag{12}$$

where $\{f,S\}$, denoted as *quantum fluid fields,* are, respectively, the *quantum probability density* and the *quantum phase-function* (also denoted as Hamilton-Madelung principal function). Equation (12) is manifestly defined only in the set in which results $f>0$ (i.e., in the configuration space Ω). We stress that in principle $S(\mathbf{r},t)$ remains "*a priori*" unspecified on the subset the boundary $\delta\Omega$ where $f=0$ (subset of the nodes $\mathbf{r}_n$). This indeterminacy, however, is eliminated by requiring that everywhere in $\delta\Omega$, $S(\mathbf{r},t)$ can be prolonged on the same set by imposing $\forall\ \mathbf{r}_n \in \delta\Omega$,

$$S(\mathbf{r}_n,t) \equiv \lim_{\mathbf{r}\to\mathbf{r}_n} S(\mathbf{r},t). \tag{13}$$

Hence, the real functions $\{f,S\}$ can both be assumed continuous in $\bar{\Omega}\times I$ and at least $C^{(2,1)}(\Omega\times I)$. Obviously, $S(\mathbf{r},t)$ is defined up to an additive constant $2\pi k$, being $k\in\mathbb{Z}$, while S itself is generally not single valued. In addition, if ψ is single valued, it is obvious that S must satisfy a well-defined condition of multivaluedness. In fact, in this case on any regular closed curve C of Ω, S it must result

$$\int_C d\mathbf{l}\cdot\nabla S(\mathbf{r},t) = 2\pi n\hbar, \tag{14}$$

where n is an appropriate relative number [54]. Introducing the single-valued potential velocity field, defined in $\Omega\times I$,

$$\mathbf{V}(\mathbf{r},t) = \frac{1}{m}\nabla S(\mathbf{r},t), \tag{15}$$

this yields the well-known condition of quantization of the velocity circulation

$$\kappa \equiv \int_C d\mathbf{l}\cdot\mathbf{V}(\mathbf{r},t) = \frac{2\pi n\hbar}{m}. \tag{16}$$

Hence, by denoting $\frac{D}{Dt}=\frac{\partial}{\partial t}+\mathbf{V}\cdot\nabla$ (convective derivative), it follows that in the open domain $\Omega\times I$ (where by definition $f>0$) the fluid fields $\{f,S\}$ obey the complete set of hydrodynamic equations represented, respectively, by

$$\frac{Df}{Dt} + f\nabla\cdot\mathbf{V} = 0, \tag{17}$$

$$\frac{\partial S}{\partial t} + \frac{1}{2m}|\nabla S|^2 = -U_{\mathrm{QM}}. \tag{18}$$

These are denoted as *quantum hydrodynamic equations*. The first one is manifestly the continuity equation for the quantum probability density $f(\mathbf{r},t)$. Instead, the second one is the Hamilton-Jacobi equation for the quantum phase function S. Moreover, U_{QM} is the so-called quantum potential [6] related to the interaction potential U by means of the equation $U_{\mathrm{QM}}=-\frac{\hbar^2}{2}\left(\frac{1}{2}\nabla^2\ln f+\frac{1}{4}|\nabla\ln f|^2\right)+U$. Since by assumption U is single valued in Ω, it follows that Eq. (17) and (18) must also be single valued. Nevertheless, both $\frac{\partial S}{\partial t}$ and U_{QM} are not unique since they are determined up to an arbitrary real smooth function $z(t)$ since they are invariant with respect to the gauge transformation

$$S(\mathbf{r},t) \to S'(\mathbf{r},t) = S(\mathbf{r},t) + \frac{1}{\hbar}\int dt' z(t'),$$

$$U(\mathbf{r},t) \to U'(\mathbf{r},t) = U(\mathbf{r},t) + z(t),$$

$$f(\mathbf{r},t) \to f'(\mathbf{r},t) = f(\mathbf{r},t). \tag{19}$$

The initial conditions to be satisfied by the quantum fluid fields $\{f,S\}$, stem from Eq. (4) and read

$$f(\mathbf{r},t_o) = f_o(\mathbf{r}), \tag{20}$$

$$S(\mathbf{r},t_o) = S_o(\mathbf{r})\mathrm{mod}(2\pi). \tag{21}$$

Instead, the boundary conditions implied by Eqs. (3)–(6), together with (9)–(11), read, respectively, $\forall\ \mathbf{r}_\delta \in \delta\Omega$,

$$f(\mathbf{r}_\delta,t) = f_w(\mathbf{r}_\delta,t), \tag{22}$$

$$S(\mathbf{r}_\delta,t) = S_w(\mathbf{r}_\delta,t)\mathrm{mod}(2\pi), \tag{23}$$

$$\lim_{\mathbf{r}\to\mathbf{r}_\delta} \mathbf{V}(\mathbf{r},t) = \mathbf{V}_w(\mathbf{r}_\delta,t), \tag{24}$$

where $S_w(\mathbf{r}_\delta,t)$ and $\mathbf{V}_w(\mathbf{r}_\delta,t)$ are suitably smooth real functions and $f_w(\mathbf{r}_\delta,t)$ is specified either by Eq. (9) and (10), depending on the definition of the domain Ω.

Equations (17) and (18), together with the initial conditions (20) and (21) and the boundary conditions (22)–(24), define the quantum hydrodynamic initial-boundary problem (*QHE problem*).

III. GAUGE-INVARIANT FORM OF THE HYDRODYNAMIC EQUATIONS

The gauge function $z(t)$ can be eliminated by taking the gradient of Eq. (18) term by term. The resulting gauge-independent equations for the quantum fluid fields $\{f,\mathbf{V}\}$, again valid in the open domain $\Omega\times I$, are provided by the *gauge-invariant quantum hydrodynamic equations,* which are defined by the continuity equation (17) and by

$$\frac{D}{Dt}\mathbf{V}(\mathbf{r},t) = \frac{1}{m}\mathbf{F} \equiv -\frac{1}{m}\boldsymbol{\nabla} U_{\mathrm{QM}}. \tag{25}$$

As a consequence, Eqs. (17) and (25) can be viewed as the *hydrodynamic equations of a compressible fluid*. On the other hand, Eq. (25) implies

$$\frac{\partial}{\partial t}\boldsymbol{\nabla} \times \mathbf{V}(\mathbf{r},t) + \boldsymbol{\nabla} \times (\mathbf{V}\cdot\boldsymbol{\nabla}\mathbf{V}(\mathbf{r},t)) = 0, \tag{26}$$

where $\mathbf{V}\cdot\nabla\mathbf{V} = -\mathbf{V}\times(\nabla\times\mathbf{V}) - \nabla V^2$ and

$$\boldsymbol{\nabla} \times (\mathbf{V}\cdot\boldsymbol{\nabla}\mathbf{V}(\mathbf{r},t)) = -\boldsymbol{\nabla}\times[\mathbf{V}\times\boldsymbol{\xi}] = -\boldsymbol{\xi}\cdot\boldsymbol{\nabla}\mathbf{V} + \mathbf{V}\cdot\boldsymbol{\nabla}\boldsymbol{\xi}, \tag{27}$$

where $\boldsymbol{\xi}=\nabla\times\mathbf{V}$ is the vorticity vector. Therefore, if we impose in the whole domain Ω the initial condition $\xi(\mathbf{r},t_o)=\mathbf{0}$ it results

$$\xi(\mathbf{r},t) = \mathbf{0} \tag{28}$$

for all $t\in I$. Notice that Eq. (28) is not in contradiction with the condition of quantization for the velocity circulation κ [see Eq. (16)] since the phase function $S(\mathbf{r},t)$ results generally nonsingle valued. As a consequence, the vector field $\mathbf{V}(\mathbf{r},t)$ is necessarily of the form (15). Hence, the fluid described by the fluid fields $\{f,\mathbf{V}=\frac{1}{m}\nabla S(\mathbf{r},t)\}$ is necessarily *vorticity free,* while at the same time its velocity circulation is nonvanishing [see Eq. (16)]. This equation is known as the so-called *quantum Newton equation* [6](or *quantum Navier-Stokes equation* [9]). The initial-boundary conditions for these equations are defined again by (20)–(24), which imply in particular for $\mathbf{V}(\mathbf{r},t_o)$ the initial condition

$$\mathbf{V}(\mathbf{r},t_o) = \mathbf{V}_o(\mathbf{r}) \equiv \frac{1}{m}\boldsymbol{\nabla} S_o(\mathbf{r},t_o). \tag{29}$$

Equations (17) and (25), together with the initial conditions (20) and (21) and the boundary conditions (22)–(24), define the gauge-invariant quantum hydrodynamic initial-boundary problem (*GI-QHE problem*).

In summary, by construction it follows that

(a) the QHE problem is equivalent to the SE problem, namely $\{f,S\}$ is a solution of the first problem if and only if $\psi(\mathbf{r},t)$ is a solution of the second one; as a consequence the solution $\{f,S \bmod(2\pi)\}$ of the QHE problem is unique;

(b) if $\{f,S \bmod(2\pi)\}$ is a solution of the QHE problem then $\{f,\mathbf{V}=\frac{1}{m}\nabla S(\mathbf{r},t)\}$ is necessarily a solution of the GI-QHE problem;

(c) vice versa, a solution $\{f,\mathbf{V}\}$ of the GI-QHE problem, determines uniquely $\{f,S\}$ up to an arbitrary gauge transformation of the form (19).

Finally, it is worthwhile to mention that, in principle, it is also possible to introduce sets of "reduced" hydrodynamic equations, defined in appropriate subspaces of the N-body configuration space, in particular the one-particle subspaces Ω_i (for $i=1,N$). The latter can be obtained adopting for the N-body quantum system the one-particle reduced representation described in Appendix A [see Eq. (A1)]. Manifestly, these reduced descriptions are not equivalent to the full N-body description. For example, the N-body system can be considered as formed by N one-body subsystem, one for each particle $(j=1,N)$. For each one-body subsystem it is possible to introduce a set of reduced quantum fluid fields $\{f_j,\mathbf{V}_j=\frac{1}{m}\nabla_j S_j(\mathbf{r}_j,t)\}$, both defined in the set $\Omega_j\times I$ and uniquely associated to the one-particle wave function $\psi_j(\mathbf{r}_j,t)$ by means of Eqs. (1) and (15). It is immediate to prove that the fluid fields $\{f_j,\mathbf{V}_j\}$ for $j=1,N$ obey a set of fluid equations formally analogous to Eqs. (17) and (23), to be denoted as *reduced hydrodynamic equations*, which can be viewed as describing the dynamics of an *immiscible fluid mixture*.

IV. HEISENBERG THEOREM AND THE CONCEPT OF QUANTUM TEMPERATURE

The set fluid equations Eqs. (17) and (23) for the quantum fluid fields $\{f,\mathbf{V}\}$ provide a complete description of quantum systems. This means, in particular, that *no other* independent observable or fluid field is required to describe the quantum state. However, for the subsequent analysis it is useful to introduce the concepts of quantum directional temperatures and quantum temperature, which can be defined by analogy with classical statistical mechanics and interpreted as additional quantum fluid fields. The definition of these observables follows from Heisenberg theorem. We recall, for this purpose, that the latter is realized by means of the (Heisenberg) inequalities (holding for $i=1,2,3$)

$$\langle(\Delta r_i)^2\rangle\langle(\Delta p_i)^2\rangle \geqslant \frac{\hbar^2}{4}, \tag{30}$$

or

$$\bar{\Delta} r_i \bar{\Delta} p_i \geqslant \frac{\hbar}{2}. \tag{31}$$

Here the notation is standard. Thus, $\bar{\Delta} r_i = \langle(\Delta r_i)^2\rangle^{1/2}$, $\bar{\Delta} p_i = \langle(\Delta p_i)^2\rangle^{1/2}$ (for $i=1,2,3$) are the *quantum standard deviations* for position and (quantum) linear momentum, $\langle(\Delta r_i)^2\rangle$, $\langle(\Delta p_i)^2\rangle$ are the corresponding *average quadratic quantum fluctuations*, while Δr_i, Δp_i denote, respectively, the *quantum position and momentum fluctuations* $\Delta r_i = r_i - \langle r_i\rangle$, $\Delta p_i = p_i - \langle p_i\rangle$. Finally, $\langle Q\rangle \equiv \langle\psi|Q\psi\rangle = \int_\Omega d\mathbf{r} f(\mathbf{r},t) Q(\mathbf{r},t)$ is the expectation value of a generic dynamical variable Q. As usual, we identify the quantum linear momentum $\mathbf{p}$ with the linear differential operator

$$\mathbf{p} = -i\hbar\boldsymbol{\nabla} \tag{32}$$

which acts on the functional space $\{\psi\}$. It follows $\langle\mathbf{p}\rangle \equiv \langle\psi|\mathbf{p}\psi\rangle = m\int_\Omega d\mathbf{r} f\mathbf{V} \equiv \langle\mathbf{P}\rangle$, where

$$\mathbf{P} = m\mathbf{V} \tag{33}$$

is the *fluid (linear) momentum*, while the expectation value of $(\Delta p_i)^2$, upon integration on the set Ω, reads

$$\langle(\Delta p_j)^2\rangle = \frac{\hbar^2}{4}\int_\Omega d\mathbf{r} f(\partial_j \ln f)^2 + \langle(\partial_j S)^2\rangle - \langle\partial_j S\rangle^2. \tag{34}$$

As is well known, Heisenberg theorem follows by invoking the identity

$$\int_\Omega d\mathbf{r} f(\mathbf{r},t) = \int_\Omega d\mathbf{r}(r_i - \langle r_i\rangle)\frac{\partial}{\partial r_i} f(\mathbf{r},t) = 1, \tag{35}$$

which implies

$$\int_\Omega d\mathbf{r}\sqrt{f(r_i - \langle r_i\rangle)^2}\sqrt{f\left(\frac{\partial}{\partial r_i}\ln f(\mathbf{r},\mathbf{v},t)\right)^2} \geqslant 1. \tag{36}$$

Hence, Schwartz inequality delivers

$$\langle(\Delta r_i)^2\rangle\int_\Omega d\mathbf{r} f\left(\frac{\partial}{\partial r_i}\ln f(\mathbf{r},\mathbf{v},t)\right)^2 \geqslant 1, \tag{37}$$

where by definition $\langle(\Delta r_i)^2\rangle \equiv \int_\Omega d\mathbf{r} f(r_i - \langle r_i\rangle)^2$.

A peculiar aspect of the Heisenberg inequality (30) is that it can also be written in terms of the relative fluctuations $\Delta^{(1)}p_i = p_i - P_i$, which are *defined with respect to the components of fluid momentum* $P_i = mV_i$ (for $i=1,2,3$) *instead of the corresponding expectation values* $\langle P_i\rangle$. This property is useful to establish a relationship with the concept of kinetic temperature [as well as, the related one of directional kinetic temperatures; see Eq. (48) in the next section], which is defined in terms of fluctuations with respect to the local fluid velocity $\mathbf{V}(\mathbf{r},t)$, instead its expectation value $\langle\mathbf{V}(\mathbf{r},t)\rangle$. Indeed, it is immediate to prove that, by definition of the quantum linear momentum (32), the following identity holds (for $i=1,2,3$):

$$\langle(\Delta p_i)^2\rangle = \langle(\Delta^{(1)}p_i)^2\rangle + \langle(\Delta^{(2)}p_i)^2\rangle, \tag{38}$$

where $\langle(\Delta^{(1)}p_i)^2\rangle$ and $\langle(\Delta^{(2)}p_i)^2\rangle$ read, respectively,

$$\langle(\Delta^{(1)}p_i)^2\rangle = \frac{\hbar^2}{4}\int_\Omega d\mathbf{r} f(\partial_j \ln f)^2, \tag{39}$$

$$\langle(\Delta^{(2)}p_i)^2\rangle \equiv \langle(\partial_j S)^2\rangle - \langle\partial_j S\rangle^2, \tag{40}$$

and hence can be interpreted as the average quadratic momentum fluctuations carried, respectively, by the quantum probability density f and the phase function S. By analogy with classical statistical mechanics, the notions of *quantum directional temperature* $T_{\mathrm{QM},i}(t)$ and *quantum temperature* $T_{\mathrm{QM}}(t)$ can be introduced, which are defined, respectively,

$$mT_{\mathrm{QM},i}(t) \equiv \langle(\Delta^{(1)}p_i)^2\rangle, \tag{41}$$

$$T_{\mathrm{QM}}(t) = \frac{1}{3}\sum_{i=1,2,3} T_{\mathrm{QM},i}(t) \tag{42}$$

(*constitutive equations for* $T_{\mathrm{QM},i}$ *and* T_{QM}). We notice that if $\Omega \equiv \mathbb{R}^{3N}$ and $\psi(\mathbf{r},t)$ is dynamically consistent [53], necessarily it must result $T_{\mathrm{QM}}(t) > T_{\mathrm{QM},i}(t) > 0$ in $\bar{\Omega}$. In the remainder we shall assume, however, that it results $T_{\mathrm{QM}}(t) > 0$ for all $\in I$ also in the case in which Ω is a bounded set. As a consequence the following *modified Heisenberg inequality* holds:

$$\langle(\Delta r_i)^2\rangle[mT_{\mathrm{QM},i}(t) + \langle(\Delta^{(2)}p_i)^2\rangle] \geqslant \frac{\hbar^2}{4}. \tag{43}$$

A particular case is the one in which the *condition of (quantum temperature) isotropy*

$$T_{\mathrm{QM},i}(t) = T_{\mathrm{QM}}(t) \tag{44}$$

holds identically for $i=1,2,3$. In the following sections for greater generality we shall require, however,

$$T_{\mathrm{QM},i}(t) \neq T_{\mathrm{QM},j}(t), \tag{45}$$

for $i \neq j$ (with $i,j=1,2,3$). In fact, generally for arbitrary quantum systems, Eq. (44) cannot be assumed to hold.

V. PROBLEM: THE SEARCH OF AN INVERSE KINETIC THEORY FOR NRQM

In this section we intend to develop two key aspects of the theory. The first one deals with the basic assumptions of the inverse kinetic theory, while the second is concerned with the construction of a classical dynamical system which provides the dynamical evolution of the quantum system.

A. Basic assumptions: construction of the inverse kinetic theory

Let us now set the problem of searching an inverse kinetic theory for the Schrödinger equation, i.e., a kinetic theory yielding exactly, by means of suitable moment equations, the quantum hydrodynamic equations. The theory must hold for arbitrary (and suitably smooth) initial and boundary conditions both for the wave function and the kinetic probability density.

The form of the quantum fluid equations (17) and (25) suggests that they can be obtained as moment equations of a continuous inverse kinetic theory, analogous to that developed recently for the incompressible Navier-Stokes equation (see Ref. [1,2]).

In the sequel we consider, without loss of generality, the case of one-body quantum systems; the theory here developed is applicable, in fact, with minor changes also for systems with $N>1$ particles. For definiteness, let us assume that the quantum fluid fields $\{f(\mathbf{r},t), \mathbf{V}, T_{\mathrm{QM},i}$, for $i=1,2,3,\}$ are, respectively, solutions of the GI-QHE problem [i.e., Eqs. (17), (25), and (20)–(24)] and imposing also the constitutive equation (41). To restrict the class of possible kinetic models, following the approach of ET, let us introduce a probability density $g(\mathbf{x},t)$, with $\mathbf{x}=(\mathbf{r},\mathbf{v})$, defined in the phase space $\bar{\Gamma} = \bar{\Omega}\times U$ (where $U \equiv \mathbb{R}^{3N}$) and assume that it belongs to the functional class $\{g(\mathbf{x},t)\}$ of real functions which satisfy the following properties (1)–(4) (denoted together as *Assumption No. 1*). More precisely, it is assumed that

(1) $g(\mathbf{x},t)$ is non-negative and continuous in $\bar{\Gamma}\times I$, in particular, is strictly positive and of class $C^{(2+k,1+h)}(\Gamma\times I)$, with $h,k \geqslant 1$;

(2) $\forall(\mathbf{r},t) \in \bar{\Omega}\times I, g(\mathbf{x},t)$ admits the kinetic moments $M_X[g] \equiv \int_U d\mathbf{v}\mathbf{X}g$, with $\mathbf{X}(\mathbf{r},\mathbf{v},t) = 1, \mathbf{v}, u_i^2$ (for $i=1,2,3$), $\mathbf{uu}$, $\mathbf{u}u^2$, $\ln g$, where $\mathbf{v},\mathbf{u}=\mathbf{v}-\mathbf{V}$ are, respectively, the kinetic and the relative kinetic velocities and $u_i = v_i - V_i$ (for $i=1,2,3$) are the orthogonal Cartesian components of $\mathbf{u}$ defined with

respect to an arbitrary inertial reference frame;

(3) $g(\mathbf{x},t)$ admits the kinetic moments $\mathbf{X}(\mathbf{r},\mathbf{v},t)=1,\mathbf{v},u_i^2$ (for $i=1,2,3$). The latter are prescribed by imposing a suitable set of constraint equations, to be denoted as *kinetic correspondence principle*, which relate the quantum fluid fields and the corresponding kinetic moments. For this purpose the following equations are assumed to hold identically, respectively, in $\bar{\Omega}\times I$:

$$f = M_1[g] \equiv \int_U d\mathbf{v} g(\mathbf{r},\mathbf{v},t), \tag{46}$$

$$M_2[g] \equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v}\mathbf{v} g(\mathbf{r},\mathbf{v},t) = \mathbf{V}(\mathbf{r},t), \tag{47}$$

and in I for $i=1,2,3$

$$T_i(t) \equiv M_{3i}[g] \equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v} m u_i^2 g(\mathbf{r},\mathbf{v},t) = T_{\mathrm{QM},i}(t) > 0. \tag{48}$$

Consistently with (45), we shall generally consider $T_i \neq T_j$ for $i \neq j$ (with $i,j=1,2,3$). Here the moments $T_i \equiv M_{3i}[g]$ (for $i=1,2,3$) and $T=(T_1+T_2+T_3)/3$ are denoted, respectively, the *(quantum) kinetic directional temperatures* and the *(quantum) kinetic temperature*.

(4) Finally, we impose an appropriate regularity condition for the fluid fields and the quantum force $\mathbf{F}(\mathbf{r},t)$. In particular, besides imposing that the fluid fields $\{f, \mathbf{V}, T_{\mathrm{QM},i}$, for $i=1,2,3,\}$ are solutions of the GI-QHE problem, let us require the stronger requirement that they belong to the functional settings:

$$f,\mathbf{V},T_i(\mathbf{r},t) \in C^{(2+k,1+h)}(\Omega\times I), \tag{49}$$

$$T_i(\mathbf{r},t), f(\mathbf{r},t) > 0,$$

$$f,\mathbf{V},T_i(\mathbf{r},t) \in C^{(0)}(\bar{\Omega}\times\bar{I}),$$

$$\mathbf{F}(\mathbf{r},t) \in C^{(2+k,1+h)}(\Omega\times I),$$

with $h,k\geqslant 1$.

The constraint provided by Eq. (48) implies that the kinetic directional temperatures T_i (for $i=1,2,3$) are assumed position-independent. This assumption, although consistent with the definition of the quantum directional temperatures given above [see Eq. (41)], may in principle be avoided (see related discussion in Appendix B and at the end of Sec. VI).

Furthermore, let us require that in the open set $\Gamma=\Omega\times U$ the probability density $g(\mathbf{r},\mathbf{v},t)$ satisfies a Vlasov-type kinetic equation of the form (*Assumption No. 2*)

$$Lg(\mathbf{x},t) = 0 \tag{50}$$

(*inverse kinetic equation*), where L is the Vlasov streaming operator

$$L = \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}}\cdot(\mathbf{X}) \equiv \frac{d}{dt} + \frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{\mathbf{K}}{m}\right), \tag{51}$$

where $\mathbf{X}$ now indicates the vector field

$$\mathbf{X} = \left\{\mathbf{v}, \frac{1}{m}\mathbf{K}\right\}, \tag{52}$$

$\mathbf{x}=(\mathbf{r},\mathbf{v})$ and $\mathbf{K}(\mathbf{x},t)$, to be denoted as *mean field force*, is a suitably smooth real vector field.

Since the correspondence principle defined by Eqs. (46)–(48) must hold identically in the open set $\bar{\Omega}\times I$ it follows that the moment equations for $M_1[g]$, $M_2[g]$, and $M_{3i}[g]$, for $i=1,2,3$, must necessarily coincide identically, respectively, with the quantum hydrodynamic equations (17) and (25) and the constitutive equation for the directional temperature (41). In addition, it is obvious these moment equations must hold also for arbitrary quantum fluid fields satisfying assumptions (49). Such implications will be discussed in detail below (see Theorems 1 and 2).

B. The phase-space Schrödinger dynamical system

Let us remark that the kinetic equation (50) determines uniquely the time evolution of the kinetic distribution function $g(\mathbf{x},t)$ in the whole extended phase-space $\bar{\Gamma}\times I$ and consequently prescribes uniquely also the quantum fluid fields in the set $\bar{\Omega}\times I$. In fact, it can also be cast, respectively, in the equivalent Lagrangian and integral forms

$$\frac{d}{dt}g(\mathbf{x}(t),t) = -g(\mathbf{x}(t),t)\frac{\partial}{\partial \mathbf{v}(t)}\cdot\frac{\mathbf{K}(\mathbf{x}(t),t)}{m}, \tag{53}$$

$$J(\mathbf{x}(t),t)g(\mathbf{x}(t),t) = g(\mathbf{x}_o,t_o), \tag{54}$$

where $g(\mathbf{x}_o,t_o)$ is the initial kinetic distribution function and the curves $\{\mathbf{x}(t), t\in I\}$ define suitable phase-space Lagrangian trajectories. Moreover, the map

$$\gamma_{(x_o,t_o)}:\mathbf{x}_o \to \mathbf{x}(t) = \chi(\mathbf{x}_o,t_o,t) \tag{55}$$

is the flow generated by the initial-value problem

$$\frac{d}{dt}\mathbf{x} = \mathbf{X}(\mathbf{x},t), \tag{56}$$

$$\mathbf{x}(t_o) = \mathbf{x}_o, \tag{57}$$

and

$$J(\mathbf{x}(t),t) = \exp\left\{\int_{t_0}^{t} dt' \frac{\partial}{\partial \mathbf{v}(t')}\cdot\frac{\mathbf{K}(\mathbf{x}(t'),t')}{m}\right\} \tag{58}$$

is its Jacobian. Here we shall prove that, due to continuity of the kinetic distribution function and of the Schrödinger dynamical system, this equation holds identically in the closure $\bar{\Gamma}\times I$, except possibly in the nodes $\mathbf{r}_n \in \delta\Omega$, where $f(\mathbf{r}_n,t)=0$. However, by construction, the limit

$$\lim_{\mathbf{r}(t)\to\mathbf{r}_\delta} J(\mathbf{x}(t),t)g(\mathbf{x}(t),t) = g(\mathbf{x}_o,t_o) \tag{59}$$

exists for all $\mathbf{r}_\delta \in \delta\Omega$, including all nodes. Instead, one can prove that the limit $\lim_{\mathbf{r}(t)\to\mathbf{r}_\delta} J(\mathbf{x}(t),t)$ does not exist if $\mathbf{r}_\delta$ is a node. In particular, by suitable definition of the vector field $\mathbf{K}(\mathbf{x},t)$, we shall prove that $\chi(\mathbf{x}_o,t_o,t)$ results suitably regular so that the set of maps (55) generates a (generally nonconservative) classical dynamical system $\{\gamma_{(\mathbf{x}_o,t_o)}\}$, to be denoted as *phase-space Schrödinger dynamical system*.

These include in particular—besides Assumptions Nos. 1 and 2—the hypothesis that the kinetic distribution function $g(\mathbf{x}_o,t_o)$ and its initial condition $g(\mathbf{x}_o,t_o)$ are suitably smooth in the whole set $\Gamma\times I$. For example, we let us require that the vector field (52) $\mathbf{X}(\mathbf{x},t) \in C^{(2+k,1+h)}(\Gamma\times I)$ and $g(\mathbf{x}_o,t_o) \in C^{(2+k,1+h)}(\Gamma\times I)$, with $h,k\geqslant 1$. Then it follows that $\chi(\mathbf{x}_o,t_o,t)$ is a diffeomorphism. of class $C^{(2+k,2+k,1+h)}(\Gamma\times I\times I)$ and $g(\mathbf{x}(t),t) \in C^{(2+k,1+h)}(\Gamma\times I)$, with $h,k\geqslant 1$, so that the moments $\{f,\mathbf{V},T_i,i=1,2,3\}$ are necessarily of class $C^{(2+k,1+h)}(\Omega\times I)$ (*Assumption No. 3*).

Manifestly the Schrödinger dynamical system, if it exists, provides a deterministic description of quantum mechanics since it advances in time both the kinetic probability density and the quantum fluid fields $\{f(\mathbf{r},t),\mathbf{V}\}$. Thus, a fundamental issue is the question of the existence of a vector field $\mathbf{K}(\mathbf{r},\mathbf{v},t)$ which satisfies the minimal assumptions indicated above. To be more specific, however, it is convenient to further specify the mathematical model imposing an appropriate set of assumptions (denoted together as *Assumption No. 4*), which include the following ones [1,2]:

(1) *the kinetic equation admits local Maxwellian kinetic equilibria for arbitrary kinetic moments and quantum fluid fields which satisfy the kinetic correspondence principle (46)–(48) and the regularity requirements (49)*;

(2) *the vector field* $\mathbf{X}(x,t)$ *is prescribed in such a way that it depends, besides on* $\mathbf{x}$, *only on the fluid fields and suitable differential operators acting on them*;

(3) *the kinetic distribution function satisfies appropriate boundary conditions*;

(4) *the Heisenberg theorem is satisfied identically*.

To complete the specification of the inverse kinetic equation, however, it must be supplemented with suitable initial and boundary conditions. In particular since the kinetic correspondence principle must hold both on the boundary $\delta\Omega$ and at the initial time t_o, this means that on the boundary $\delta\Gamma$ (which includes $\delta\Omega$) bounce-back boundary conditions are imposed on the kinetic distribution function [1].

C. Bounce-back boundary conditions

We intend to define boundary conditions for the kinetic distribution function $g(\mathbf{x},t)$ which are consistent with the Dirichlet boundary condition defined on the boundary $\delta\Omega$ for the quantum fluid fields. Denoting $\mathbf{V}_w(\mathbf{r}_\delta(t),t)=\frac{d}{dt}\mathbf{r}_\delta(t)$ the velocity of the point of the boundary determined by the vector $\mathbf{r}_\delta(t) \in \delta\Omega$ and assuming $|\mathbf{v}-\mathbf{V}_\mathbf{w}| \neq 0$, let us introduce the unit vector

$$\mathbf{b} = \sigma\frac{\mathbf{v}-\mathbf{V}_w}{|\mathbf{v}-\mathbf{V}_\mathbf{w}|} \tag{60}$$

and the variable

$$\xi \equiv [\mathbf{v}-\mathbf{V}_\mathbf{w}]\cdot\mathbf{b}. \tag{61}$$

Here $\sigma=\pm 1$ and its sign is defined so that when $\mathbf{b}$ is a vector applied at the position $\mathbf{r}_\delta$ it is always oriented inward with respect to the domain Ω. For sake of definiteness, we shall assume that $\delta\Omega$ is a piecewise regular surface and that the vector $\mathbf{b}$ belongs to the open tangent cone to $\delta\Omega$ in $\mathbf{r}_n$ which is oriented inward with respect to Ω. Then, at an arbitrary position $\mathbf{r}_\delta \in \delta\Omega$, the sign of the variable ξ determines *incoming and outgoing velocity subdomains,* defined, respectively, as the subdomains of velocity space U for which $\xi<0$ and $\xi>0$. Therefore $g(\mathbf{r}_\delta,\mathbf{v},t)|_{\xi<0}$ and $g(\mathbf{r}_\delta,\mathbf{v},t)|_{\xi>0}$ denote the incoming and outgoing kinetic distribution functions at position $\mathbf{r}_\delta$. These notations permit us to define properly the boundary conditions for the kinetic distribution function on $\delta\Omega$.

For any boundary $\delta\Omega$, position $\mathbf{r}_n \in \delta\Omega_i$ and for all nonvanishing vectors $\mathbf{v}-\mathbf{V}_\mathbf{w}$ taking at $\mathbf{r}_\delta$ the directions specified above, we impose, respectively, for $\xi>0$ and $\xi<0$ the boundary conditions for $g(\mathbf{r},\mathbf{v},t)$ (*Assumption No. 5*),

$$g(\mathbf{r}_\delta,\mathbf{v},t)|_{\xi>0} = g(\mathbf{r}_\delta,2\mathbf{V}_\mathbf{w}-\mathbf{v},t)|_{\xi<0}, \tag{62}$$

$$g(\mathbf{r}_\delta,\mathbf{v},t)|_{\xi<0} = g(\mathbf{r}_\delta,2\mathbf{V}_\mathbf{w}-\mathbf{v},t)|_{\xi>0}, \tag{63}$$

to be denoted as *bounce-back boundary conditions for* $g(\mathbf{x},t)$. It is immediate to prove that they are consistent with Dirichlet boundary conditions defined by Eq. (24). In fact, they results are

$$\begin{aligned} f\mathbf{V}(\mathbf{r}_\delta,t) &= \int_U d\mathbf{v}\mathbf{v}g(\mathbf{r}_\delta,\mathbf{v},t) \\ &= \int_U^{\xi<0} d\mathbf{v}\mathbf{v}g(\mathbf{r}_\delta,\mathbf{v},t) + \int_U^{\xi>0} d\mathbf{v}\mathbf{v}g(\mathbf{r}_\delta,\mathbf{v},t) \\ &= \frac{1}{2}\int_U^{\xi<0} d\mathbf{v}\mathbf{v}\{g(\mathbf{r}_\delta,\mathbf{v},t)+g(\mathbf{r}_\delta,2\mathbf{V}_\mathbf{w}-\mathbf{v},t)\} \\ &\quad + \frac{1}{2}\int_U^{\xi>0} d\mathbf{v}\mathbf{v}\{g(\mathbf{r}_\delta,\mathbf{v},t)+g(\mathbf{r}_\delta,2\mathbf{V}_\mathbf{w}-\mathbf{v},t)\}. \end{aligned} \tag{64}$$

Thanks to the identities

$$\frac{1}{2}\int_U d\mathbf{v}\mathbf{v}g(\mathbf{r}_\delta,2\mathbf{V}_\mathbf{w}-\mathbf{v},t) = \left(\mathbf{V}_\mathbf{w}-\frac{1}{2}\mathbf{V}(\mathbf{r}_\delta,t)\right)f, \tag{65}$$

$$\int_U d\mathbf{v}\mathbf{v}g(\mathbf{r}_\delta,\mathbf{v},t) = \mathbf{V}(\mathbf{r}_\delta,t)f, \tag{66}$$

it follows that

$$\mathbf{V}_w(\mathbf{r}_n,t) = \frac{1}{f}\int_U d\mathbf{v}\mathbf{v}g(\mathbf{r}_n,\mathbf{v},t) = \mathbf{V}(\mathbf{r}_n,t). \tag{67}$$

We impose, furthermore, the Dirichlet boundary condition (*Assumption No. 6*)

$$\int_U d\mathbf{v} g(\mathbf{r}_\delta, \mathbf{v}, t) = f_w(\mathbf{r}_\delta, t), \tag{68}$$

where $f_w(\mathbf{r}_\delta, t)$ is the prescribed probability density on the boundary $\delta\Omega$ defined by (22).

VI. CONSTRUCTION OF THE MEAN-FIELD FORCE K

A. The assumption of PEM

In order to construct explicitly the mean-field force let us now invoke the principle of entropy maximization (PEM) [19,51,52] to determine uniquely the initial distribution function at a prescribed initial time $t_o \in I$. For this purpose it is necessary to define the functional class $\{g(\mathbf{x}, t_o)\}$.

First, let us assume that the sole information on the initial condition $g(\mathbf{x}, t_o)$ is provided by the knowledge of the initial fluid fields. In this case the kinetic correspondence principle requires that at the initial time $t_o \in I$ the kinetic moments of $g(\mathbf{x}, t_o)$ [i.e., $M_X[g] \equiv \int_U d\mathbf{v} \mathbf{X} g$, with $\mathbf{X}(\mathbf{r}, \mathbf{v}, t_o) = 1, \mathbf{v}, u_i^2$ (for $i=1,2,3$)] must coincide with the quantum fluid fields $\{ f(\mathbf{r}, t_o)$, $\mathbf{V}(\mathbf{r}, t_o)$, $T_{\mathrm{QM},i}(t_o)$, for $i=1,2,3,\}$. In such a case it is immediate to prove that PEM yields necessarily for $t=t_o$ the distribution function

$$g(\mathbf{x}, t) = g_M(\mathbf{r}, \mathbf{v}, t) \equiv f(\mathbf{r}, t) \frac{1}{\pi^{3/2} v_{th1} v_{th2} v_{th3}} \exp(-x_i x_i), \tag{69}$$

to be denoted as *generalized Maxwellian distribution*. Here in the exponential the sum is understood on repeated indexes $(i=1,2,3)$, while the notation is analogous to Refs. [1,2], thus for $i=1,2,3$, $v_{thi} = \sqrt{2T_i(\mathbf{r}, t)/m}$ and $x_i = u_i / v_{thi}$. Due to the arbitrariness of $t_o \in I$ it is natural to assume that Eq. (69) holds identically for IKE.

It is obvious, however, that other definitions of the functional class $\{g(\mathbf{x}, t_o)\}$ are possible, and hence more general (nonMaxwellian) initial conditions are in principle allowed. This occurs, for example, if the fluid fields are stochastic and the information on the initial fluid fields is provided only by means of suitable stochastic averages. However, the treatment of non-Maxwellian kinetic distributions is potentially relevant, also for direct numerical simulations, in which the kinetic distribution function is simulated numerically by means of test particles. In such a case, in fact, small numerical errors may imply that locally the kinetic distribution function is actually nonMaxwellian. Thus, for greater generality we can consider the case in which $\{g(\mathbf{x}, t_o)\}$ is determined by imposing for all $\mathbf{r} \in \bar{\Omega}$ just that

$$g(\mathbf{x}, t_o) = g_o(\mathbf{x}). \tag{70}$$

Here, by definition, $g_o(\mathbf{x})$ is an arbitrary, non-Maxwellian, distribution function whose moments coincide identically with $\{f, \mathbf{V}, T_{\mathrm{QM},i}$, for $i=1,2,3,\}$ at $t=t_o$. It is manifest that in this case PEM is identically satisfied by $g_o(\mathbf{x})$.

B. Case of the generalized Maxwellian distribution

Due to the arbitrariness of the initial time t_o, it is natural to assume that, if the initial condition Eq. (69) is satisfied, $g_M(\mathbf{r}, \mathbf{v}, t)$ results identically $\forall (\mathbf{x}, t) \in \Gamma \times I$ a particular solution of the inverse kinetic equation (50). In such a case, invoking Assumptions Nos. 1–6 (and in particular the hypothesis that the kinetic directional temperatures can only depend on time), the mean-field force $\mathbf{K}(g_M)$ results necessarily *(Assumption No. 7)*

$$\mathbf{K}(g_M) = \mathbf{K}_0(g_M) + \mathbf{K}_1(g_M), \tag{71}$$

with

$$\mathbf{K}_0(g_M) = \mathbf{F}(\mathbf{r}, t) + \frac{1}{f} \frac{m}{2} v_{thi}^2 \hat{\mathbf{e}}_i \hat{\mathbf{e}}_i \cdot \nabla f = \mathbf{F}(\mathbf{r}, t) + \frac{1}{f} \nabla p, \tag{72}$$

$$\mathbf{K}_1(g_M) = m\mathbf{u} \cdot \nabla \mathbf{V} + \frac{m}{2} u_i \hat{\mathbf{e}}_i \frac{\partial}{\partial t} \ln T_i, \tag{73}$$

where the sum is understood on repeated indexes and $p = fT$ denotes the kinetic scalar pressure. Here, $\mathbf{K}_0(g_M)$ and $\mathbf{K}_1(g_M)$ have been distinguished for being, respectively, constant and velocity dependent. In particular, $\mathbf{K}_0(g_M)$ contains, besides the quantum force $\mathbf{F}(\mathbf{r}, t)$, a corrective term ("pressure term") which depends explicitly only the logarithmic gradient of f; instead $\mathbf{K}_1(g_M)$ contains a "convective term," proportional to $\nabla \mathbf{V}$ and a contribution proportional to the logarithmic time derivatives of the directional temperatures. For the sake of reference, the more general case in which the kinetic directional temperature are taken as spatially nonuniform is reported in Appendix B.

Let us now examine the main implications which stem, in the particular case $g = g_M$, from positions (71)–(73) and Assumptions Nos. 1–7. We first notice that the Schrödinger dynamical system generated by $\mathbf{K}(g_M)$, defined as the solution of the initial value problem (56) and (57), exists and is unique in the whole extended phase space $\Gamma \times I$. This property is manifestly assured by assumption, thanks to to previous definition of $\mathbf{K}(g_M)$ and the regularity properties of the quantum fluid fields (Assumption No. 1). In the same set the kinetic distribution function $g_M(\mathbf{r}, \mathbf{v}, t)$ is, by construction, a particular solution, i.e., exists, is unique and results strictly positive. In fact, this property holds if and only if the quantum fluid fields are solutions of the GI-QHE problem and—in validity of Eqs. (71)–(73)—if the kinetic directional temperatures are assumed to be only functions of time, i.e., $T_i(t)$ $(i=1,2,3)$. In addition, by continuity, the kinetic distribution function $g_M(\mathbf{r}, \mathbf{v}, t)$ (and its moments) are uniquely defined also on the boundary set $\delta\Omega$ and hence, in particular, in the nodes. Finally, it is immediate to prove that Eq. (50) is also an inverse kinetic equation for the quantum hydrodynamic equations. Indeed its moment equations, evaluated with respect to the weight functions $G(\mathbf{x}, t) = 1, \mathbf{v}$, coincide identically (in $\Omega \times I$) with the Eqs. (17) and (25). As a consequence, the following theorem holds for Maxwellian kinetic distributions of the type (69):

Theorem 1. Generalized Maxwellian solution of the inverse kinetic equation.

Besides the validity of Assumptions Nos. 1–7, let us assume that

(1) the kinetic distribution function fulfills Eq. (69) at least at the initial time $t_o \in I$;

(2) the mean-field force $\mathbf{K}$ can only depend functionally on g_M; moreover $\mathbf{K}$ can only depend on the quantum fluid fields $\{f(\mathbf{r},t)$, $\mathbf{V}$, T_i, *for* $i=1,2,3\}$.

Then it follows that

(a) $\forall(\mathbf{x},t) \in \bar{\Gamma}\times I$ the generalized Maxwellian distribution (69) is a particular solution of the inverse kinetic equation (50) if and only if the mean field force $\mathbf{K}$ has the form defined by Eqs. (71)–(73).

(b) The Schrödinger dynamical system exists, is unique and is continuous in $\bar{\Gamma}\times I$, except in the nodes, i.e., when $\mathbf{r}(t)=\mathbf{r}_n$, with $f(\mathbf{r}(t),t)=0$. Moreover, it is $C^{(2+k,1+h)}(\Gamma \times I)$ with $h,k \geqslant 1$. This result holds for arbitrary quantum dynamical systems and both for isotropic and nonisotropic quantum directional temperatures.

(c) The Jacobian of the phase-flow $\mathbf{x}_o \to \mathbf{x} \equiv \mathbf{x}(t) = \chi(\mathbf{x}_o,t_o,t)$, generated by the initial value problem (56) and (57), is defined $\forall(\mathbf{x},t) \in \bar{\Gamma}\times I$, except in the nodes. There results in such cases

$$K_1(\mathbf{r}_o,t_o)f(\mathbf{r}(t),t)\exp\{-x_i(t)x_i(t)\} \neq 0 \tag{74}$$

so that $J(\mathbf{x}(t),t)$ reads

$$J(\mathbf{x}(t),t) = \frac{K_1(t)f((\mathbf{r}_o,t_o))\exp(-x_{io}x_{io})}{K_1(t_o)f(\mathbf{r}(t),t)\exp[-x_i(t)x_i(t)]}, \tag{75}$$

where $K_1=(T_1T_2T_3)^{1/2}$, $x_{oi}=u_{oi}/v_{th,i}(t_o)$, $\mathbf{u}_o=\mathbf{v}_o-\mathbf{V}(\mathbf{r}_n,t_o)$, $x_i(t)=u_i(t)/v_{th,i}(t_o)$, and $\mathbf{u}(t)=\mathbf{v}(t)-\mathbf{V}(\mathbf{r}(t),t)$.

(d) The limit

$$\lim_{\mathbf{r}(t)\to\mathbf{r}_n} J(\mathbf{x}(t),t)g_M(\mathbf{x}(t),t) \tag{76}$$

exists and is unique.

(e) $\forall(\mathbf{x},t) \in \Gamma\times I$, the velocity-moment equations of the inverse kinetic equation (50) evaluated for the weight functions $G(\mathbf{x},t)=1,\mathbf{v}$ and for $g=g_M$ coincide with the fluid equations (17) and (25).

(f) $\forall(\mathbf{x},t) \in \Gamma\times I$, the moment equations for the directional kinetic temperatures are satisfied identically.

Proof.

(a) If the mean-field force $\mathbf{K}$ is assumed of the form (71)–(73) the proof of (a) follows by straightforward algebra as a consequence of Eq. (50) [or in an equivalent way of the integral equation (54)].

(b) Due to Assumption No. 3 the quantum fluid fields $\{f,\mathbf{V},T_i,i=1,2,3\}$ the quantum force $\mathbf{F}(r,t)$ belong to the functional setting (49). Hence, the vector field $\mathbf{X}=\{\mathbf{v},\frac{1}{m}\mathbf{K}\}$ is necessarily $C^{(2+k,1+h)}(\bar{\Gamma}\times I)$ with $h,k \geqslant 1$. The proof of (b) is therefore a consequence of the fundamental (existence and uniqueness) theorem for ordinary differential equations. In particular, it is obvious that the solution of the Schrödinger dynamical system is not defined in the nodes since the mean-field force $\mathbf{K}$ is not defined for $f=0$.

(c) The proof of Eq. (75) is implied by (b) and follows invoking Liouville theorem (58).

(d) The only possible singular behavior of $J(\mathbf{x}(t),t)$ can occur either in the nodes $\mathbf{r}_n \in \delta\Omega$, i.e., if at some time $t_1 \in I$ there results $f(\mathbf{r}_n,t_1)=0$, or if least one of the directional temperatures T_i vanishes. The second possibility is excluded by assumption. Hence $J(\mathbf{x}(t),t)$ is not defined at $(\mathbf{x}(t),t)$ only if $\mathbf{r}(t)=\mathbf{r}_n$ is a node. Nevertheless, it is obvious that the limit (76) exists.

(e) and (f) Finally it is immediate to determine the moment equations satisfied by the inverse kinetic equation for $g=g_M(\mathbf{r},\mathbf{v},t)$, which is manifestly defined everywhere in $\bar{\Omega}\times I$. Indeed, the first two moments $G=1,\mathbf{v}$ coincide, respectively, with the quantum hydrodynamic equations (17) and (25), while for $G=u_i^2$ $(i=1,2,3)$ one obtains the moment equations for the directional temperature which are satisfied identically.

C. Case of the non-Maxwellian distributions

As in Ref. [1] the inverse kinetic theory can be formulated for non-Maxwellian kinetic distribution functions too. It suffices for this purpose to assume that the initial kinetic distribution function $g(\mathbf{r},v,t_o)=g_o(\mathbf{r},\mathbf{v})$ results suitably smooth, strictly positive and summable in $\bar{\Gamma}$. A unique definition of $\mathbf{K}(g)$ which yields the correct fluid equations and satisfies also the constitutive equations can readily be obtained also in this case, which reads (*Assumption No. 7b*)

$$\mathbf{K}(g) = \mathbf{K}_0(g) + \mathbf{K}_1(g), \tag{77}$$

$$\mathbf{K}_0(g) = \mathbf{F}(\mathbf{r},t) + \frac{1}{f}\nabla\cdot\underline{\underline{\Pi}}, \tag{78}$$

$$\mathbf{K}_1(g) = m\mathbf{u}\cdot\nabla\mathbf{V} + \frac{m}{2}u_i\hat{\mathbf{e}}_i\left(\frac{\partial}{\partial t}\ln T_i + \frac{3}{fT_i}\nabla\cdot\mathbf{Q}_i\right), \tag{79}$$

where again the sum is understood on repeated indexes. Equations (77) and (79) hold if the kinetic directional temperatures are assumed to be only functions of time $[T_i(t)$, for $i=1,2,3]$. In this case the corrective term in the mean-field force $\mathbf{K}_0(g)$ depends on the tensor pressure $\underline{\underline{\Pi}}$, instead of the scalar pressure p, while $\mathbf{K}_1(g)$ contains an additional term depending on the relative heat fluxes $\mathbf{Q}_i$ $(i=1,2,3)$. The kinetic moments $\underline{\underline{\Pi}}$ and $\mathbf{Q}_i$ (for $i=1,2,3$), assumed to exist, are, respectively,

$$\underline{\underline{\Pi}} = \int d\mathbf{v}\mathbf{u}\mathbf{u}g, \tag{80}$$

$$\mathbf{Q}_i = \int d\mathbf{v}\frac{1}{3}\mathbf{u}u_i^2 g. \tag{81}$$

The mean-field force defined by Eqs. (77)–(79) is manifestly consistent with the previous definition when $g=g_M$, since in

such a case there results $\underline{\underline{\mathbf{\Pi}}}=fT\underline{\underline{\mathbf{1}}}=p\underline{\underline{\mathbf{1}}}$ and $\mathbf{Q}_i=\mathbf{0}$ $(i=1,2,3)$.

It is immediate to prove that also in this case the Schrödinger dynamical system generated by $\mathbf{K}(g)$ exists and is unique in the whole extended phase-space $\Gamma\times I$. In the same set the kinetic distribution function $g(\mathbf{r},\mathbf{v},t)$ exists, is unique, results strictly positive and by continuity is uniquely defined also on the boundary set $\delta\Omega$. Finally, by construction the moments of the inverse kinetic equation (50), evaluated with respect to the weight functions $G(\mathbf{x},t)=1,\mathbf{v}$, coincide identically (in $\Omega\times I$) with the quantum hydrodynamic equation Eqs. (17) and (25). As a consequence, in the case of non-Maxwellian kinetic distributions the following theorem holds.

Theorem 2. Non-Maxwellian solutions of the inverse kinetic equation. Besides the validity of Assumptions Nos. 1#7, with No. 7b replacing No. 7, let us require that

(1) the kinetic distribution function is a smooth function of class $C^{(2+k,1+h)}(\Gamma\times I)$, with $h,\ k\geqslant 1$, which is suitably summable in Γ;

(2) the mean-field force $\mathbf{K}$ can depend functionally but not explicitly on g; moreover $K_0(g)$ and $K_1(g)$ depend, besides $\{f(\mathbf{r},t),\mathbf{V},T_i$, for $i=1,2,3\}$, on the minimal number of moments, which include $\underline{\underline{\mathbf{\Pi}}}$ and $\mathbf{Q}_i$ $(i=1,2,3)$.

Then it follows that

(a) if at a prescribed time $t\in I$ and $\forall\mathbf{x}\in\bar{\Gamma}$ the kinetic distribution function $g(\mathbf{x},t)$ is of the form (69) then it results $g(\mathbf{x},t)=g_M(\mathbf{x},t)$, $\forall(\mathbf{x},t)\in\bar{\Gamma}\times I$;

(b) $\forall(\mathbf{x},t)\in\Gamma\times I$ and for arbitrary smooth $g(\mathbf{x},t)$ the velocity-moment equations of the inverse kinetic equation (50) evaluated for the weight functions $G(\mathbf{x},t)=1,\mathbf{v}$ coincide with the fluid equations Eqs. (17) and (25);

(c) $\forall(\mathbf{x},t)\in\Gamma\times I$, the moment equations for the directional kinetic temperatures are satisfied identically;

(d) the Jacobian of the phase-flow $\mathbf{x}_o\rightarrow\mathbf{x}\equiv\mathbf{x}(t)=\chi(\mathbf{x}_o,t_o,t)$, generated by the initial value problem (56) and (57), is defined $\forall(\mathbf{x},t)\in\bar{\Gamma}\times I$ reads in this case

$$J(\mathbf{x}(t),t)=\frac{K_1(\mathbf{r}(t),t)f(\mathbf{r}_o,t_o)}{K_1(\mathbf{r}_o,t_o)f(\mathbf{r}(t),t)}\exp\left\{\int_{t_o}^{t}dt'G(\mathbf{x}(t'),t')\right\},\tag{82}$$

where $K_1=(T_1T_2T_3)^{1/2}$ and

$$G(\mathbf{x}(t),t)=\frac{1}{f}\mathbf{u}\cdot\boldsymbol{\nabla}f+\frac{1}{2}\frac{1}{fT_i}\boldsymbol{\nabla}\cdot\mathbf{Q}_i.\tag{83}$$

(e) If $g(\mathbf{x},t_o)$ is strictly positive $\forall(\mathbf{x})\in\bar{\Gamma}$, then for all $\forall(\mathbf{x},t)\in\bar{\Gamma}\times I$, $g(\mathbf{x},t)$ is also strictly positive;

(f) the Schrödinger dynamical system exists and is unique and is continuous in $\bar{\Gamma}\times I$, except in the nodes, i.e., when $\mathbf{r}(t)=\mathbf{r}_n$, with $f(\mathbf{r}(t),t)=0$. Moreover it is $C^{(2+k,1+h)}(\Gamma\times I)$ with $h,k\geqslant 1$. This result holds for arbitrary quantum dynamical systems and both for isotropic and nonisotropic quantum directional temperatures.

Proof.

(a) is manifestly a consequence of Theorem 1, while the proof of (b) follows by direct inspection. Regarding (c), we notice that the directional temperatures T_i $(i=1,2,3)$ remain in principle completely arbitrary. Hence they can be uniquely determined according to Eq. (48). Also see Eq. (82). (d) again follows from Liouville theorem (58). In particular, once again it follows that $J(\mathbf{x}(t),t)$ is not defined if $\mathbf{r}(t)$ (or $\mathbf{r}_n$) coincide with a node $r_w\in\delta\Omega$ where $f(\mathbf{r}_n,t)=0$. As a consequence $\forall(\mathbf{x},t)\in\boldsymbol{\Gamma}\times I$, $J(\mathbf{x}(t),t)>0$. This proves also propositions (e) and (f).

Finally, to reach the proof of uniqueness of the mean-field force $\mathbf{K}(g)$ it is sufficient to prescribe, besides the assumption that its does not depend explicitly on g, also an appropriate dependence in terms of higher-order kinetic moments (see Assumption No. 2 of Theorem 2). An important consequence is the uniqueness of the mean-field force $\mathbf{K}(g)$ and hence of the inverse kinetic equation.

Theorem 3. Uniqueness theorem for $\mathbf{K}(g)$.

In validity of Theorem 1 and 2 the mean-field force, for which (a)–(e) hold, $\mathbf{K}(g)$ is unique. For $g=g_M$ it has the form defined by Eqs. (71)–(73); for $g\neq g_M$ the mean-field force has the form defined by Eqs. (77)–(79).

Proof.

For example, let us prove that in validity of Assumption No. 3 of Theorem 1 the mean-field force $\mathbf{K}(g_M)$ is unique. Let us assume that there is a nonvanishing vector field $\Delta\mathbf{K}$ such that $\mathbf{K}'=\mathbf{K}+\Delta\mathbf{K}$ is also an admissible mean-field force. Hence it must be

$$\frac{\partial}{\partial\mathbf{v}}\cdot(\Delta\mathbf{K}g_M)=0.\tag{84}$$

This means that $\Delta\mathbf{K}g_M$ has necessarily the form

$$\Delta\mathbf{K}g_M=\frac{\partial A}{\partial\mathbf{v}}\times\frac{\partial B}{\partial\mathbf{v}},\tag{85}$$

where A and B are suitably smooth real scalar fields. If both A and B are independent of g_M then it must be $\Delta\mathbf{K}\equiv 0$. Instead, for example, let us assume that only A depends on g_M. Letting

$$\frac{1}{g_M}\frac{\partial A(g_M,\mathbf{r},\mathbf{v},t)}{\partial\mathbf{v}}=\hat{\mathbf{A}},\tag{86}$$

if follows that $\hat{\mathbf{A}}$ must depend on g_M too. Hence, in order that $\Delta\mathbf{K}$ results independent of g_M it must vanish identically. This proves that it must be $\Delta\mathbf{K}\equiv\mathbf{0}$ and hence $\mathbf{K}$ is unique.

Let us briefly comment on these results.

First, we stress that Schrödinger dynamical system [defined by the initial-value problem (56) and (57)] uniquely generates the time evolution of the kinetic distribution function g and hence of its moments. The result holds not only for generalized Maxwellian distributions (69) but also for arbitrary, but otherwise suitably smooth, kinetic probability densities (Theorem 2). An interesting aspect concerns, in particular, the behavior of the kinetic distribution function and of the Schrödinger dynamical system in the nodes, i.e., the

points of the boundary $\delta\Omega$ in which the probability density $f(\mathbf{r},t)$ vanishes. Their occurrence is usually associated to the possible singular behavior of the wavefunction, i.e., its nonuniqueness (for a review see Ref. [13]). Therefore, the question arises whether the existence of these roots is reflected in any way in the inverse kinetic approach (and therefore on the quantum system). It is manifest that in these points the dynamical system is not defined and hence the Jacobian of the Schrödinger dynamical system [given by (75) or more generally by Eq. (82)] vanishes or is not defined. However, in these points the kinetic probability density can still be uniquely defined, thanks to continuity. Consequently, the kinetic distribution function g and its moments, and in particular those corresponding to the relevant quantum fluid fields, are defined without exceptions in the whole domain $\bar{\Omega}\times I$. As a consequence, it follows that no singularity appears, i.e., the quantum fluid fields (and hence the quantum wave function) are unique in $\bar{\Omega}\times I$.

D. The kinetic representation of Heisenberg inequalities

It is interesting to examine the role of the kinetic directional temperatures T_i $(i=1,2,3)$ in the framework of the inverse kinetic approach and the consequent interpretation of the Heisenberg theorem. For this purpose, let us analyze the implications due to the kinetic correspondence principle. It is immediate to prove that the Heisenberg inequalities (31) can be represented, in terms of the *kinetic standard deviations* for position and *kinetic linear momentum* $\bar{\Delta}r_i^{\mathrm{kin}}$, $\bar{\Delta}p_i^{\mathrm{kin}}$, in the form:

$$\bar{\Delta}r_i^{\mathrm{kin}}\bar{\Delta}p_i^{\mathrm{kin}} \geqslant \frac{\hbar}{2}. \tag{87}$$

Here $\bar{\Delta}r_i^{\mathrm{kin}}$ and $\bar{\Delta}p_i^{\mathrm{kin}}$ are defined in terms of appropriate phase-space averages which are defined as $\langle\langle A\rangle\rangle = \int_\Gamma d\mathbf{x} g(\mathbf{r},\mathbf{v},t)A(\mathbf{r},\mathbf{v},t)$, where $A(\mathbf{r},\mathbf{v},t)$ is an arbitrary summable phase-space function. In particular, we pose, respectively, $\bar{\Delta}r_i^{\mathrm{kin}}=\langle\langle(\Delta r_i)^2\rangle\rangle^{1/2}$, $\bar{\Delta}p_i^{\mathrm{kin}}=\langle\langle(\Delta\bar{p}_i^{\mathrm{kin}})^2\rangle\rangle^{1/2}$ (for $i=1,2,3$), where $\langle\langle(\Delta r_i)^2\rangle\rangle$ and $\bar{\Delta}p_i^{\mathrm{kin}}=\langle\langle(\Delta\bar{p}_i^{\mathrm{kin}})^2\rangle\rangle$ are denoted as *average quadratic kinetic fluctuations*. Here $\Delta\mathbf{r}=\mathbf{r}-\langle\mathbf{r}\rangle$ is the position fluctuation, while $\Delta\bar{\mathbf{p}}^{\mathrm{kin}}=\mathbf{p}^{\mathrm{kin}}-m\langle\mathbf{V}\rangle$ and $\mathbf{p}^{\mathrm{kin}}=m\mathbf{v}$ are, respectively, the *kinetic momentum fluctuation*, and the *kinetic momentum*. It is immediate to prove that (87) are equivalent to (31). In fact, in analogy with Eq. (38), one finds that the average quadratic momentum fluctuation $\langle\langle(\Delta\bar{p}_i^{\mathrm{kin}})^2\rangle\rangle$ can be written in the form

$$\langle\langle(\Delta\bar{p}_i^{\mathrm{kin}})^2\rangle\rangle = \langle\langle(\Delta p_i^{\mathrm{kin}})^2\rangle\rangle + \langle(\Delta^{(2)}p_i)^2\rangle \tag{88}$$

$(i=1,2,3)$, where $\Delta\mathbf{p}^{\mathrm{kin}}$ denotes $\Delta\mathbf{p}^{\mathrm{kin}}=\mathbf{p}^{\mathrm{kin}}-m\mathbf{V}(\mathbf{r},t)$ and $\langle(\Delta^{(2)}p_i)^2\rangle$ is given by Eq. (40). Moreover, by definition, it follows that the momentum fluctuation $\langle\langle(\Delta p_i^{\mathrm{kin}})^2\rangle\rangle$ reads

$$\langle\langle(\Delta p_i^{\mathrm{kin}})^2\rangle\rangle = mT_i(t), \tag{89}$$

where and $T_i(t)$ (for $i=1,2,3$) are the directional kinetic temperatures. As a consequence, the constraint $T_i(t)=T_{\mathrm{QM},i}(t)$, set (for $i=1,2,3$) by Eq. (48) of the correspondence principle, implies

$$\langle(\Delta^{(1)}p_i)^2\rangle = \langle\langle(\Delta p_i^{\mathrm{kin}})^2\rangle\rangle. \tag{90}$$

It follows that the Heisenberg inequalities can be interpreted in terms of kinetic fluctuations, i.e., as constraints between $\langle\langle(\Delta r_i)^2\rangle\rangle$ and $\bar{\Delta}p_i^{\mathrm{kin}}=\langle\langle(\Delta\bar{p}_i^{\mathrm{kin}})^2\rangle\rangle$, whereby the quantum observable $\mathbf{p}=-i\hbar\nabla$ and its average quadratic quantum fluctuation are replaced by the kinetic momentum $\mathbf{p}^{\mathrm{kin}}=m\mathbf{v}$ and the corresponding average quadratic kinetic fluctuation. This result is a direct consequence of the assumption set by Eq. (48) for the directional kinetic temperatures T_i $(i=1,2,3)$.

E. Generalizations: nonuniqueness

It is obvious that the present results can be generalized in several ways. In particular, the definition of the kinetic directional temperatures remains in principle arbitrary since they do not enter explicitly the quantum hydrodynamic equations. Thus, for example, it is possible to require that the functions T_i $(i=1,2,3)$ are also position dependent (see Appendix B).

Due to the arbitrariness of the kinetic temperatures, it follows that there exist infinite equivalent realizations of the Schrödinger dynamical system and of the associated Lagrangian trajectories $\{\mathbf{x}(t),t\in I\}$ which yield the same quantum hydrodynamic equations. Therefore, the unique inverse kinetic theory here presented, which corresponds to a well-defined set of prescriptions and in particular the assumption of spatially constant directional temperatures, is simply one of the infinite possible mathematical realizations.

A side aspect concerns the so-called uniqueness problem of the deterministic viewpoint of SQM [6,12,13], i.e., the Bohmian program, of reproducing the predictions of SQM within the framework of suitable deterministic Lagrangian trajectories. In fact, the Schrödinger dynamical system determined by the initial-value problem (56) and (57) yields in terms of the associated Lagrangian trajectories $\{\mathbf{x}(t),t\in I\}$ a deterministic description of SQM. Hence, it can also be viewed a phase-space generalization of Bohmian mechanics [6–8]. An implication of the present theory is that such a program has by no means a unique solution. In fact, there are infinite equivalent Lagrangian trajectories determined as solutions of the initial-value problem (56) and (57), which differ only by the choice of the spatial-dependency assumed for the directional temperatures (see Appendix B).

VII. CONCLUSIONS

Motivated by the analogy between hydrodynamic description of SQM and classical fluid dynamics an inverse kinetic theory has been developed for the quantum hydrodynamic equations. We have shown that, although in principle infinite solutions to this problem exist (in particular due to the indeterminacy in the kinetic directional temperatures), the inverse kinetic theory can be uniquely determined, provided appropriate hypotheses are introduced. The results presented are relevant for the fluid description of quantum mechanics and a deeper understanding of the underlying statistical (in particular, kinetic) descriptions.

For this purpose the full set of gauge-invariant quantum hydrodynamic equations, including the Heisenberg inequali-

ties, have been related to the appropriate quantum fluid fields. As a result the notions of quantum temperature and quantum directional temperatures have been introduced. The present approach has the following main features:

(1) the inverse kinetic equation (50) has been assumed to be a Vlasov-type kinetic equation;
(2) its solution, i.e., the kinetic distribution function has been required, in particular, to admit kinetic directional temperatures T_i $(i=1,2,3)$ which, consistent with the correspondence principle [defined by Eqs. (46)–(48)], depend only on time;
(3) the inverse kinetic theory is complete, namely all fluid fields are expressed as moments of the kinetic distribution function and all hydrodynamic equations can be identified with suitable moment equations.
(4) the theory holds for arbitrary quantum fluid fields, i.e., arbitrary initial and boundary conditions for the system wave function;
(5) IKE is nonasymptotic, i.e., the quantum hydrodynamic equations are satisfied exactly and self-consistent. i.e., it holds for arbitrary (and suitably smooth) initial conditions for the kinetic distribution function;
(6) the moment equations form a complete system of equations (closure condition for the moment equations of IKE);
(7) under suitable assumption, the inverse kinetic theory and the mean-field force which defines the streaming operator are unique.

An interesting result of the theory, relevant for the mathematical investigation of the Schrödinger equation, concerns the discovery of the underlying dynamical system, i.e., the phase-space Schrödinger dynamical system. We have found that this can be identified with the nonconservative dynamical system advancing in time the kinetic distribution function and generated by the kinetic equation itself. The evolution of the fluid fields is proven to be determined uniquely by this dynamical system. Formally the Schrödinger dynamical system can be interpreted as describing the dynamics of system of classical fictitious particles which interact with each other only by means of the mean-field force **K** and are characterized by a dynamics which fulfills a suitable set of regularity assumptions.

To conclude, a further interesting feature of the present treatment is its adoption of the mean-field force kinetic model. This permits, in principle, numerical implementations by means of appropriate algorithms based on the inverse kinetic theory (see related discussion in Refs. [1,2]).

A side aspect concerns also the uniqueness and regularity of the quantum fluid fields and of the related quantum wave function. We have shown, in fact, that the kinetic distribution function is smooth in the whole extended phase space $\Gamma \times I$, while it is uniquely defined also in the nodes, i.e., in the "singular" points of configuration space $\bar{\Omega}$ where the quantum probability density $f(\mathbf{r},t)$ vanishes. As a consequence, the quantum fluid fields are necessarily unique in $\bar{\Omega} \times I$ too.

Finally, have pointed out that the Heisenberg inequalities afford a simple statistical interpretation, which permits the representation of the quantum statistical fluctuations of the components of the linear momentum in terms of the kinetic directional temperatures.

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APPENDIX A: REDUCED ONE-PARTICLE DESCRIPTION OF QUANTUM SYSTEMS

In SQM the state of a system of N interacting particles is, by assumption, represented by its N- body wave function $\psi(\mathbf{r},t)$, with $\mathbf{r}=(\mathbf{r}_1,\ldots,\mathbf{r}_N) \in \bar{\Omega}$, $\mathbf{r}_j \in \bar{\Omega}_j$ (for $j=1,N$) and $t \in I$. This is defined in the set $\bar{\Omega} \times I$, where Ω is the configuration space $\Omega \equiv \Pi_{j=1,N}\Omega_j$, $\Omega_i \subseteq \mathbb{R}^3$ (for $j=1,N$) and I is an open subset of $\mathbb{R}$. However, since the number of particles forming a quantum dynamical system is "*a priori*" arbitrary, also "reduced" quantum descriptions of an N-body system are permitted. These descriptions, however, are not equivalent to the full N-body description based on the N-body wave function. Thus, it is in principle possible to obtain a *reduced description* based, for example, on one-particle wave functions, whereby the N-body system is represented by the *reduced vector state*

$$\psi_R(\mathbf{r},t) \equiv (\psi_1(\mathbf{r}_1,t),\ldots,\psi_N(\mathbf{r}_N,t)), \tag{A1}$$

instead of the single scalar N-particle wave function $\psi(\mathbf{r},t)$. The one-particle wave function $\psi_j(\mathbf{r}_j,t)$—which prescribes the state of the jth one-particle subsystem—is defined by means of the integral

$$c_{(j)}(t)\psi_j(\mathbf{r}_j,t) = L_j\psi^{(N)}(\mathbf{r},t) \equiv \hat{\psi}_j(\mathbf{r}_j,t), \tag{A2}$$

where L_j is the integral operator

$$L_j = \int_{\Pi_{k=1,N;k\neq j}\Omega_k} \frac{d\mathbf{r}_1 \cdots d\mathbf{r}_N}{d\mathbf{r}_j}. \tag{A3}$$

Here $c_j(t)$ (for $j=1,N$) are a real functions defined so that there results identically

$$\int_{\Omega_j} d\mathbf{r}_j |\psi_j(\mathbf{r}_j,t)|^2 = \frac{1}{c_j^2(t)} \int_{\Omega_j} d\mathbf{r}_j |\hat{\psi}_j(\mathbf{r}_j,t)|^2 = 1 \tag{A4}$$

and $f_j=|\psi_j(\mathbf{r}_j,t)|^2$ are the associated one-particle probability densities. The Schrödinger equation for $\psi_j(\mathbf{r}_j,t)$ follows immediately from the N-body Schrödinger equation (3). Let us assume for definiteness that the N-body Hamiltonian takes the form

$$H = \sum_{k=1,N} H_{ok} + \sum_{k,m=1,N;k<m} U_{km}(\mathbf{r}_k,\mathbf{r}_m,t) \tag{A5}$$

$$+\sum_{k=1,N} U_{0k}(\mathbf{r}_k,t), \tag{A6}$$

where $U_{km}(\mathbf{r}_k,\mathbf{r}_m,t)$ and $U_{0k}(\mathbf{r}_k,t)$ are, respectively, binary and unary interaction potentials. Introducing the position

$$L_j \sum_{k,m=1,N;k<m} U_{km}(\mathbf{r}_k,\mathbf{r}_m,t)\psi^{(N)}(\mathbf{r},t) \tag{A7}$$

$$=c_{(j)}(t)U_1(\mathbf{r}_j,t)\psi_j(\mathbf{r}_j,t), \tag{A8}$$

it follows

$$L_j H\psi = c_{(j)}(t)\{H_{o(j)} + U_1(\mathbf{r}_j,t) + U_{0j}\}\psi_j(\mathbf{r}_j,t). \tag{A9}$$

Hence, $\psi_j(\mathbf{r}_j,t)$ obeys necessarily the one-particle Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi_j = H_{(j)}\psi_j, \tag{A10}$$

where the index j (for $j=1,N$) identifies the particle subsystem (or *species* index) and

$$H_j = H_{oj} + U_{0j} - i\hbar\frac{\partial}{\partial t}\ln c_{(j)} \tag{A11}$$

is the jth particle Hamiltonian. The reduced one-particle description of a N-body quantum system is, therefore, obtained by means of the vector wavefunction $\psi(\mathbf{r},t)\equiv(\psi_1,\ldots,\psi_N)$, $\psi_j(\mathbf{r}_j,t)$, for $j=1,N$, being the one-particle wave functions which obey Eq. (A10).

APPENDIX B: CASE OF POSITION-DEPENDENT DIRECTIONAL TEMPERATURES

We notice that the correspondence principle (48) can be modified by assuming instead $T_i=T_i(\mathbf{r},t)$ $(i=1,2,3)$ and imposing, in place of Eq. (48), the constraint equation

$$\langle T_i(\mathbf{r},t)\rangle = T_{\mathrm{QM},i}(t), \tag{B1}$$

with general solution of the form

$$T_i(\mathbf{r},t) = k_{(i)}(\mathbf{r},t)\langle T_i(\mathbf{r},t)\rangle, \tag{B2}$$

$$\langle k_{(i)}(\mathbf{r},t)\rangle = 1. \tag{B3}$$

The functions $k_{(i)}(\mathbf{r},t)$ $(i=1,2,3)$ which satisfy Eq. (B3) are manifestly nonunique. In this case it is immediate to prove that for the generalized Maxwellian solution (59) the mean-field $\mathbf{K}(g_M)$ is obtained by imposing (71) and (72) with

$$\mathbf{K}_1(g_M) = m\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{V} + \frac{m}{2}u_i\hat{\mathbf{e}}_i\frac{D}{Dt}\ln T_i - \frac{m}{2}\hat{\mathbf{e}}_i\hat{\mathbf{e}}_i v_{th,i}^2\cdot\sum_{j=1,2,3}\boldsymbol{\nabla}\ln T_j\left(x_j^2-\frac{1}{2}\right) - \frac{m}{2}\hat{\mathbf{e}}_i\hat{\mathbf{e}}_i v_{th,i}^2\cdot\boldsymbol{\nabla}\ln T_i \tag{B4}$$

replacing Eq. (73). Here, the sum is understood on repeated indexes. The general case in which $g\neq g_M$ can be obtained immediately from Eqs. (B4), (78), and (79).

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