IKT approach for quantum hydrodynamic equations

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(Dated: June 30, 2008)

Abstract

A striking feature of standard quantum mechanics is its analogy with classical fluid dynamics. In particular it is well known the Schrödinger equation can be viewed as describing a classical compressible and non-viscous fluid, described by two (quantum) fluid fields \{\rho, \mathbf{V}\}, to be identified with the quantum probability density and velocity field. This feature has suggested the construction of a phase-space hidden-variable description based on a suitable inverse kinetic theory (IKT; Tessarotto et al., 2007). The discovery of this approach has potentially important consequences since it permits to identify the classical dynamical system which advances in time the quantum fluid fields. This type of approach, however requires the identification of additional fluid fields. These can be generally identified with suitable directional fluid temperatures \(T_{QM,i}\) (for \(i = 1, 2, 3\)), to be related to the expectation values of momentum fluctuations appearing in the Heisenberg inequalities. Nevertheless the definition given previously for them (Tessarotto et al., 2007) is non-unique. In this paper we intend to propose a criterion, based on the validity of a constant H-theorem, which provides an unique definition for the quantum temperatures.

PACS numbers: 03.65.-w, 05.20.Dd, 05.20.-y
I. INTRODUCTION

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. Following the pioneering work of Wigner [1, 2], 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 quasi-probabilities [3] (for a review see Ref. [4], Chapter 4). This fact has motivated in the past the search of alternative phase-space representations of the quantum state. These works, although based on different treatments, 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 [5]). A type of statistical approach is provided by statistical models based on kinetic theory. Examples are provided by the kinetic models due to Kaniadakis [6, 7] and Goldstein and Pesci [8, 9, 10], which are based on the adoption of the Boltzmann kinetic equation to map quantum hydrodynamic equations. However, also in this cases the relevant wave equations are - at best - recovered only in an approximate sense.

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) can be overcome. For this purpose an inverse kinetic theory is adopted for the Schrödinger equation, based on the introduction a suitable inverse kinetic theory (IKT) (Ref. A [11]). By definition an IKT [12, 13] must be able to yield identically, via suitable moment equations, the complete system of fluid equations. In particular, this can shown to satisfy the following requirements:

1. completeness: 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: 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**: 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. **non-asymptotic IKT**: i.e., 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 [14].

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 [12, 13]. 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) for the Shannon information entropy [15, 16] 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 kinetic correspondence principle, 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. In principle infinite solutions to this problem exist due to the non-uniqueness of the definition of the kinetic directional temperatures. Nevertheless, here we intend to show that the adoption of the principle of constant Shannon entropy for isolated quantum systems permits to determine them uniquely.
II. HYDRODYNAMIC DESCRIPTION OF NRQM

The fluid description of non-relativistic quantum mechanics (NRQM) is well-known [17]. It is based on the property of the Schrödinger equation to be equivalent to a complete set of fluid equations, i.e., respectively the continuity and Euler equations

\[
\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{V} = 0, \tag{1}
\]

\[
\frac{D}{Dt} \mathbf{V}(\mathbf{r}, t) = \frac{1}{m} \mathbf{F} \equiv -\frac{1}{m} \nabla U_{QM}, \tag{2}
\]

which are assumed to hold in a domain \( \Omega \subseteq \mathbb{R}^3 \). These are known as quantum hydrodynamic equations (QHE). For the sake of clarity, let us recall the basic definitions and the mathematical formulation of the problem. Let us consider, for definiteness the equation for one spinless scalar particle (boson) described by a single scalar wavefunction \( \psi(\mathbf{r}, t) = \sqrt{\rho e^{iS/\hbar}} \), where \( \rho = |\psi(\mathbf{r}, t)|^2 \) and \( S(\mathbf{r}, t) \) are two smooth real function denoting respectively the quantum probability density and the quantum phase-function (also denoted as Hamilton-Madelung principal function). Furthermore,

\[
\mathbf{V}(\mathbf{r}, t) = \frac{1}{m} \nabla S(\mathbf{r}, t), \tag{3}
\]

is the quantum velocity field, while \( U_{QM} \) is the so-called quantum potential

\[
U_{QM} = -\frac{\hbar^2}{2} \left( \frac{1}{2} \nabla^2 \ln f + \frac{1}{4} |\nabla \ln f|^2 \right) + U, \tag{4}
\]

with \( U \) a suitably smooth real function denoting an appropriate interaction potential. For well-posedness, appropriate initial and boundary conditions must be imposed on the fluid fields \( \{\rho(\mathbf{r}, t), \mathbf{V}(\mathbf{r}, t)\} \). In particular, \( \{\rho(\mathbf{r}, t), \mathbf{V}(\mathbf{r}, t)\} \) are both assumed continuous in \( \Omega \times I \) and at least \( C^{(2,1)}(\Omega \times I) \). The set fluid equations 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 dynamical variable) is required to describe the quantum state. However, it is useful to introduce the concept of quantum directional temperatures. The definitions can be obtained invoking the Heisenberg theorem, which requires (for \( i = 1, 2, 3 \))

\[
\langle (\Delta r_i)^2 \rangle \langle (\Delta p_i)^2 \rangle \geq \frac{\hbar^2}{4},
\]

where \( \overline{\Delta r_i} = \langle (\Delta r_i)^2 \rangle^{1/2}, \overline{\Delta p_i} = \langle (\Delta p_i)^2 \rangle^{1/2} \) (for \( i = 1, 2, 3 \)) are the quantum standard deviations for position and (quantum) linear momentum and \( \langle (\Delta r_i)^2 \rangle, \langle (\Delta p_i)^2 \rangle \) the corre-
sponding average quadratic quantum fluctuations. It follows that
\[ \langle (\Delta p_j)^2 \rangle = \langle (\Delta^{(1)} p_i)^2 \rangle + \langle (\Delta^{(2)} p_i)^2 \rangle, \tag{5} \]
where
\[ \langle (\Delta^{(1)} p_i)^2 \rangle = \frac{\hbar^2}{4} \int_{\Omega} df (\partial_j \ln f)^2, \tag{6} \]
\[ \langle (\Delta^{(2)} p_i)^2 \rangle \equiv \langle (\partial_j S)^2 \rangle - \langle \partial_j S \rangle^2. \tag{7} \]
Hence the first term [on the r.h.s. of Eq.()] is by definition strictly positive. By analogy with classical statistical mechanics, it is therefore natural to introduce the notion of quantum directional temperatures \( T_i(t) \) (for \( i = 1, 2, 3 \))
\[ T_i(t) \equiv T_0(t) + T_{QM,i}(t) \tag{8} \]
\[ T_{QM,i}(t) = \frac{1}{m} \langle (\Delta^{(1)} p_i)^2 \rangle \tag{9} \]
to be viewed as a constitutive equation for \( T_i \). By definition each \( T_i \) results strictly positive, while \( T_0(t) \) is a strictly positive smooth real function of time to be suitably defined.

III. IKT FOR QHE

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 wavefunction and the kinetic probability density. The form of the quantum fluid equations 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. 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 arbitrary \( N \)-body systems with \( N > 1 \) particles. For definiteness, let us assume that the quantum fluid fields \( \{ f(r,t), V, T_i \} \), for \( i = 1, 2, 3 \), are respectively solutions of the QHE indicated above and of the constitutive equation [8]. To restrict the class of possible kinetic models, following the approach of Ref. A, let us introduce a probability density \( g(x,t) \), with \( x = (r, v) \), defined in the phase space
Γ = Ω × U (where $U \equiv \mathbb{R}^{3N}$) and assume 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 #2)

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

(10)

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

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

(11)

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

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

(12)

$\mathbf{x} = (\mathbf{r}, \mathbf{v})$ and $\mathbf{K}(\mathbf{x}, t)$, to be denoted as mean field force, is a suitably smooth real vector field. The functional class $\{g(\mathbf{x}, t)\}$ and the vector field $\mathbf{K}(\mathbf{x}, t)$ are determined in such a way that:

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

2. $\forall (\mathbf{r}, t) \in \Gamma \times I$, $g(\mathbf{x}, t)$ 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 $i = 1, 2, 3$), $\mathbf{uu}, uu^2, \ln g$, 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. The kinetic moments $\mathbf{X}(\mathbf{r}, \mathbf{v}, t) = 1, \mathbf{v}, u_i^2$ (for $i = 1, 2, 3$) satisfy a suitable set of constraint equations, to be denoted as kinetic correspondence principle, namely the following equations are assumed to hold identically for $i = 1, 2, 3$

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

(13)

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

(14)

$$= \mathbf{V}(\mathbf{r}, t),$$

$$M_{3i} [g] \equiv$$

$$\frac{1}{f(\mathbf{r}, t)} \int_U d\mathbf{v} u_i^2 g(\mathbf{r}, \mathbf{v}, t) = T_i(t) > 0.$$
4. the kinetic equation admits local Maxwellian kinetic equilibria for arbitrary kinetic
moments and quantum fluid fields which satisfy the kinetic correspondence principle
(13), (14), (15);

5. The vector field $\mathbf{X}(\mathbf{x},t)$ 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.

In Ref. A it was proven that, provided the directional quantum temperatures $T_i(t)$ are
considered as prescribed, the vector field $K(r, \mathbf{v}, t)$ which satisfies the assumptions indicated
above can be uniquely constructed and reads \[11\]

$$K(g) = m\mathbf{u} \cdot \frac{\partial}{\partial r} \mathbf{V} +$$

$$+ \frac{m}{2} u_i e_i \left[ \frac{\partial}{\partial t} \ln T_i + \frac{1}{\rho T_i} \nabla \cdot \mathbf{Q} \right] +$$

$$+ \mathbf{F}(r,t) + \frac{m}{\rho} \nabla \cdot \Pi,$$

where $\mathbf{Q} = \int d\mathbf{v} \frac{1}{3} u_i^2 g$ and $\Pi = \int d\mathbf{v} \mathbf{uu} g$.

Nevertheless, the complete specification of the IKT requires the unique definition of the
observables $T_i(t)$. In fact, the definition of the kinetic directional temperatures remains
in principle arbitrary since they do not enter explicitly the quantum hydrodynamic equa-
tions. This means that there actually exist infinite equivalent realizations of the IKT for the
Schrödinger equation. This poses, therefore, the issue whether uniqueness can be established
based on first principles.

IV. CONSTANT H-THEOREM FOR THE SHANNON KINETIC ENTROPY

Let us now introduce the Shannon entropy for the kinetic probability density $g(x, t)$

$$S(g) = - \int_{\mathcal{R}} d\mathbf{x} g \ln g,$$

(Shannon kinetic entropy). We intend to prove that provided the function $T_0(t)$ is suitably
prescribed $S(g)$ can be imposed to be constant in time. For this purpose let us evaluate
the entropy production:

$$\frac{\partial}{\partial t} S(g) = \int_{\mathcal{R}} d\mathbf{x} g \frac{\partial}{\partial \mathbf{v}} \cdot \frac{1}{m} \mathbf{K}(f).$$
Then the following result holds:

**Theorem - Constant H-theorem**

Let us assume that the quantum system fulfills the following assumptions: (1) the initial-boundary-value problem associated to the Schrödinger equation admits a suitably smooth global solution (i.e., which exists and is unique for all \( t \in \mathbb{R} \)); (2) the following integrals exist all \( t \in \mathbb{R} \):

\[
I_1 = \int_{\Omega} d\mathbf{r} \mathbf{g} \cdot \mathbf{V}
\]

\[
I_2 = \frac{1}{2} \int_{\Omega} d\mathbf{r} \cdot \mathbf{Q} \sum_{i=1,2,3} \frac{1}{T_i}
\]

(3) that the directional quantum temperatures, are defined by equations (8) for all \( t \in I \); (4) we impose the initial condition \( T_0(t_0) = T_0 \), where \( T_0 > 0 \) is an appropriate constant.

It follows that \( T_0(t) \), is uniquely determined for all \( t \in I \) and for \( t \geq t_0 \) by imposing that there results identically:

\[
\frac{\partial}{\partial t} S(g) = 0.
\]  

**PROOF**

The proof follows by explicit evaluation of the entropy production rate, which delivers

\[
\frac{\partial}{\partial t} S(g) = \int_{\Omega} d\mathbf{r} \mathbf{g} \cdot \mathbf{V} +
\]

\[
+ \frac{1}{2} \left[ \sum_{i=1,2,3} \frac{1}{T_i} \frac{\partial T_{QM,i}}{\partial t} + \int_{\Omega} d\mathbf{r} \cdot \mathbf{Q} \sum_{i=1,2,3} \frac{1}{T_i} \right] +
\]

\[
+ \frac{\partial T_0}{\partial t} \frac{1}{2} \sum_{i=1,2,3} \frac{1}{T_i} \equiv 0.
\]

This is an ode for \( T_0(t) \) which under suitable smoothness assumptions admits an unique solution.

**V. 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. This includes the validity of a constant H-theorem for the Shannon kinetic entropy. This requirement, on the other hand, is consistent with the formulation of an IKT, both for classical and quantum fluids. The conclusion here presented is potentially relevant for the fluid description of quantum mechanics and a deeper understanding of the underlying statistical description. In particular, we stress that the concept of Shannon kinetic entropy, here adopted, which is completely analogous to the one adopted for classical systems, is potentially relevant also for the investigation of irreversible phenomena in non-isolated quantum systems.

Acknowledgments

Work developed (M.T.) in the framework of the MIUR (Italian Ministry of University and Research) PRIN Research Program “Modelli della teoria cinetica matematica nello studio dei sistemi complessi nelle scienze applicate” and the European COST action P17 (M.T). The partial of the GNFM (National Group of Mathematical Physics) of INDAM (National Institute of Advanced Mathematics, Italy) (M.T. and P.N.) and of the Deutsche Forschungsgemeinschaft via the project EL503/1-1 (M.E.) is acknowledged.

Notice

§ contributed paper at RGD26 (Kyoto, Japan, July 2008).
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