Hamiltonian inverse kinetic theory for the Schrödinger equation

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In this paper we intend to show that a particular realization of the IKT for the Schrödinger equation can be achieved in terms of a classical Hamiltonian dynamical system.

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IMPORTANT REMARKS (to be added):

1) **Comparison between IKT and the method of configuration-space characteristics:**

A) the phase-space (Schrödinger) dynamical system advances in time the kinetic PDF and therefore, through it, determines uniquely also the time-evolution of the complete set of quantum fluid fields;

B) instead the method of characteristics (based on the definition of a configuration-space Lagrangian dynamical system) determines only a parametrization for the QHE's.

Recently, the quantum trajectory method (QTM) has been utilized in solving several quantum mechanical wave packet scattering problems including barrier transmission and electronic nonadiabatic dynamics. By propagating the real-valued action and amplitude functions in the Lagrangian frame, only a fraction of the grid points needed for Eulerian fixed-grid methods are used while still obtaining accurate solutions. Difficulties arise, however, near wave function nodes and in regions of sharp oscillatory features, and because of this many quantum mechanical problems have not yet been amenable to solution with the QTM.

2) restrictions on IKT:

- *single and multiple-temperature cases;*
- *the definition of quantum temperature.*
- *related non-Hamiltonian features;*

3) **further implications of IKT:**

- *constant weak H-theorem;*
- *Heisenberg inequalities;*
- *role of thermal fluctuations and temperature effects.*

I. INTRODUCTION

In the stardard approach to quantum mechanics (SQM), systems of classical point particles, defining classical Hamiltonian systems, are described by corresponding *quantum Hamiltonian systems,* obeying the Schrödinger equation. This means that while the canonical state and Hamiltonian function, which define classical Hamiltonian systems, $\{\mathbf{x} =(\mathbf{q},\mathbf{p}), H(\mathbf{x},t)\}$, are represented by ordinary functions defined in a suitable *extended phase-space* $\Gamma \equiv V_{\mathbf{q}} \times V_{\mathbf{p}} \times I$ [with $V_{\mathbf{q}}, V_{\mathbf{p}}$ and I, respectively, suitable subspaces of $\mathbb{R}^n$ and $\mathbb{R}$], in SQM they are replaced - via an euristic correspondence principle denoted as *quantization* - by well-known (quantum) operators, $\mathbf{p}$ and $H(\mathbf{x},t)$, acting on the quantum wave-function $\psi(\mathbf{q},t)$, the latter being complex functions defined [only] on the *extended configuration domain* $V \equiv V_{\mathbf{q}} \times I$.

In a recent paper Tessarotto *et al.* [1] have shown, however, that the time evolution of the quantum wave-function is actually uniquely determined by means of a suitable class of phase-space classical dynamical systems, which can be realized in the framework of the so-called inverse kinetic theory (IKT). The question arises, however, whether there exists - in particular - among them a subset of *abstract classical Hamiltonian systems*, which determine uniquely the time evolution of $\psi(\mathbf{q},t)$ in terms of the corresponing Hamiltonian evolution operator $T^{(H)}_{t_o,t}$. In this paper we intend to show that a particular realization of IKT developed for the Schrödinger equation (Tessarotto *et al.* [1]) can be realized to satisfy precisely this requirement. This means that also SQM admits, in some abstract sense, an Hamiltonian description, and hence - just like classical mechanics - quantum dynamics can be uniquely described in terms of the extremal curve of an appropriate Hamiltonian action.

II. HYDRODYNAMIC DESCRIPTION OF NRQM

In this section we intend to recall the well-known fluid description of non-relativistic 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 wavefunction $\psi(\mathbf{r},t)$,with associated probability density

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

requiring that both are defined and continuous in $\overline{\Omega} \times I$, where $\overline{\Omega}$ denotes the closure of a suitable open set Ω. In addition we impose that f is strictly positive in Ω, while f and ψ are respectively single-valued and possibly multi-valued in $\overline{\Omega} \times I$, 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 $h,k \geq 0$. 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

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

Here H is the $N-$body Hamiltonian operator. Thus, for a single charged particle (with electric charge q and mass m), subject both to the action both a scalar field U and of the EM field generated by the EM potentials $\{\phi, \mathbf{A}\}$, it follows

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + U + q\phi, \tag{4}$$

where

$$\mathbf{p} = -i\hbar\nabla$$

is the quantum momentum and U is a possible additional potential. 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 $\mathbf{r} \in \overline{\Omega}$

$$\psi(\mathbf{r},t_o) = \psi_o(\mathbf{r}), \tag{5}$$

where ψ_o is a suitably smooth complex-valued function. To specify the boundary conditions, we first notice that 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 $\forall \mathbf{r}_\delta \in \delta\Omega$

$$\psi(\mathbf{r}_\delta,t) = \psi_w(\mathbf{r}_\delta,t), \tag{6}$$

$$\lim_{\mathbf{r}\to\mathbf{r}_\delta} \mathbf{V}(\mathbf{r},t) = \mathbf{V}_w(\mathbf{r}_\delta,t), \tag{7}$$

where $V(\mathbf{r},t)$ is the quantum velocity field (to be defined below), while the complex function $\psi_w(\mathbf{r}_\delta,t)$ and the real vector function $\mathbf{V}_w(\mathbf{r}_\delta,t)$ are prescribed and suitably smooth functions. To specify the value of $f(\mathbf{r},t)$ on $\delta\Omega$, let us require that there results additionally

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

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

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

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 subset 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),(5),(6),(7) together with (9) or (10) and (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 [5, 7, 8, 12] and follow immediately from the exponential representation (known as *Madelung transformation* [5])

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

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).

We stress that while Eq. (12) is defined in the set in which results $f \geq 0$ (i.e., in the closure of the configuration space $\overline{\Omega}$) $S(\mathbf{r}, t)$ remains in principle unspecified on the subset the boundary $\delta\Omega$ where $f(\mathbf{r}_n, t) = 0$, i.e., the subset $\{\mathbf{r}_n\}$ of the so-called *nodes* of ψ.

REMARK:

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 $\overline{\Omega} \times I$ and at least $C^{(2,1)}(\Omega \times I)$. Obviously, $S(\mathbf{r}, t)$ is defined up to an additive constant $2\pi k\hbar$, 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 multi-valuedness. In fact, in this case on any regular closed curve C of Ω, for S it must result

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

where n is an appropriate relative number [52]. 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

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

III - QUANTUM HYDRODYNAMIC EQUATIONS (QHE) - CASE OF THE 1-BODY PROBLEM

Let us derive explicitly the complete set of PDE's, to be fulfilled by a suitable set of fluid fields $\{Z\}$, which correspond to the Schrödinger equation. Invoking the position (12) there follows

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi &= \psi\left[\frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f-\frac{\partial}{\partial t}S\right],\\
\frac{1}{2m}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}\right)^2\psi &= \frac{1}{2m}\left(-i\hbar\nabla-\frac{q}{c}\mathbf{A}\right)\cdot\psi\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S-\frac{q}{c}\mathbf{A}\right]=\\
&= \frac{\psi}{2m}\left[-\frac{\hbar^2}{2}\nabla^2\ln f-i\hbar\nabla^2 S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]+\\
&\quad+\frac{\psi q}{2mc}\left[\frac{i\hbar}{2}\mathbf{A}\cdot\nabla\ln f-\mathbf{A}\cdot\nabla S+\frac{q}{c}\left|\mathbf{A}\right|^2\right]+\\
&\quad+\frac{\psi}{2m}\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S\right].
\end{aligned}$$

Hence the imaginary part of the equation yields

$$\begin{aligned}
\frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f &= \frac{1}{2m}\left[-i\hbar\nabla^2 S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]+\frac{q}{2mc}\frac{i\hbar}{2}\mathbf{A}\cdot\nabla\ln f+\\
&\quad-\frac{1}{2m}\frac{i\hbar}{2}\nabla\ln f\cdot\nabla S-\frac{1}{2m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\frac{i\hbar}{2}\nabla\ln f=\\
&= \frac{1}{2m}\left[-i\hbar\nabla^2 S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]-\frac{i\hbar}{2m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\nabla\ln f
\end{aligned}$$

namely

$$\frac{\partial}{\partial t}\ln f+\frac{1}{m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\nabla\ln f+\frac{1}{m}\nabla^2 S=\frac{q}{mc}\nabla\cdot\mathbf{A}. \tag{17}$$

Imposing the Coulomb gauge $\nabla\cdot\mathbf{A}=0$ and introducing the (quantum) fluid velocity field $\mathbf{V}=\mathbf{V}(\mathbf{r},t)$:

$$\mathbf{V}=\frac{1}{m}\left(\nabla S-\frac{q}{c}\mathbf{A}\right), \tag{18}$$

one obtains the countinuity equation:

$$\frac{\partial}{\partial t}\ln f+\mathbf{V}\cdot\nabla\ln f+\nabla\cdot\mathbf{V}=0. \tag{19}$$

Similarly the real part of the equation delivers the *quantum Hamilton-Jacobi equation*:

$$\frac{\partial}{\partial t}S+H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)=0, \tag{20}$$

where $H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)$ is the Hamiltonian function

$$H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)=\frac{1}{2m}\left(\nabla S-\frac{q}{c}\mathbf{A}\right)^2+U_{QM}+q\phi. \tag{21}$$

Moreover, here U_{QM} denotes the so-called *free-particle quantum potential* [8]

$$U_{QM}=\frac{\hbar^2}{2}\left(\frac{1}{2}\nabla^2\ln f+\frac{1}{4}\left|\nabla\ln f\right|^2\right). \tag{22}$$

Applying the operator $(\frac{1}{m}\nabla)$ to the previous equation and introducing the position (164) there follows

$$\frac{\partial}{\partial t}\mathbf{V}+\frac{1}{2m^2}\nabla\left(\nabla S-\frac{q}{c}\mathbf{A}\right)^2=-\frac{q}{mc}\frac{\partial}{\partial t}\mathbf{A}-\frac{1}{m}\nabla U_{QM}-\frac{1}{m}\nabla q\phi.$$

Now we notice that

$$\frac{1}{2m^2}\nabla\left(\nabla S-\frac{q}{c}\mathbf{A}\right)^2 = \frac{1}{m^2}\left(\nabla S-\frac{q}{c}\mathbf{A}\right)\cdot\nabla\left(\nabla S-\frac{q}{c}\mathbf{A}\right)+\frac{1}{m^2}\left(\nabla S-\frac{q}{c}\mathbf{A}\right)\times\left[\nabla\times\left(\nabla S-\frac{q}{c}\mathbf{A}\right)\right]=$$
$$= \mathbf{V}\cdot\nabla\mathbf{V}-\frac{q}{mc}\mathbf{V}\times[\nabla\times\mathbf{A}]=\mathbf{V}\cdot\nabla\mathbf{V}-\frac{q}{mc}\mathbf{V}\times\mathbf{B}.$$

Hence it follows the *quantum Euler equation*:

$$\frac{\partial}{\partial t}\mathbf{V}+\mathbf{V}\cdot\boldsymbol{\nabla}\mathbf{V}=\frac{1}{m}\mathbf{F}(\mathbf{r},t), \tag{23}$$

where $\mathbf{F}(\mathbf{r},t)$ (*quantum force-field*) is the vector field

$$\mathbf{F}(\mathbf{r},t)\equiv q\left\{\mathbf{E}+\frac{1}{c}\mathbf{V}\times\mathbf{B}\right\}-\nabla U_{QM} \tag{24}$$

and

$$\mathbf{E}=-\nabla\phi-\frac{1}{c}\frac{\partial}{\partial t}\mathbf{A} \tag{25}$$
$$\mathbf{B}=\boldsymbol{\nabla}\times\mathbf{A} \tag{26}$$

are the EM fields.

The PDE's (165) and (169) are denoted *quantum hydrodynamic equations* (QHE) and $\{Z\}\equiv\{f,\mathbf{V}\}$ as corresponding *quantum fliid fields.*

III-b. Lagrangian representation of QHE

A *Lagrangian representation* for QHE can be obtained by introducing a parametrization in terms of a family of smooth curves $\{\mathbf{r}(t)\}$ belonging to the configuration space (Ω) in which the fluid fields $\{Z\}$ are defined. A possibility for the definition [of these curves] is realized by the curves $\mathbf{r}(t)$, to be denoted as *characteristics*, or *Lagrangian paths* (LP) *associated to the fluid velocity field* $\mathbf{V}(\mathbf{r},t)$, which are solutions of the initial-value problem

$$\frac{D}{Dt}\mathbf{r}(t) = \mathbf{V}(\mathbf{r},t), \tag{27}$$
$$\mathbf{r}(t_o) = \mathbf{r}_o,$$

where $\frac{D}{Dt}$ denotes the *fluid Lagrangian derivative, defined with respect to the fluid velocity* $\mathbf{V}(\mathbf{r},t)$,

$$\frac{D}{Dt}\mathbf{V}\equiv\frac{\partial}{\partial t}\mathbf{V}+\mathbf{V}\cdot\boldsymbol{\nabla}\mathbf{V}. \tag{28}$$

Then a *Lagrangian representation of QHE* is then simply provided by the set of *Lagrangian differential equations* represented by Eq.(27) together with

$$\frac{D}{Dt}\ln f(\mathbf{r}(t),t) = -\nabla\cdot\mathbf{V}(\mathbf{r},t)|_{\mathbf{r}=\mathbf{r}(t)}, \tag{29}$$
$$\frac{D}{Dt}\mathbf{V}(\mathbf{r}(t),t) = \frac{1}{m}\mathbf{F}(\mathbf{r}(t),t). \tag{30}$$

We notice that Eqs.(27)-(30) are manifestly coupled. In particular, if $f(\mathbf{r},t)$ is considered prescribed, Eqs.(27) and (30) (must) determine uniquely the set of vector functions $\{\mathbf{r}(t),\mathbf{V}(\mathbf{r}(t),t)\}$. It follows that these equations can also be represented in the equivalent integral form

$$\left\{\begin{array}{c}\mathbf{r}(t)=\mathbf{r}_o+\int_{t_o}^{t}dt'\mathbf{V}(\mathbf{r}(t'),t'),\\ f(\mathbf{r}(t),t)=f(\mathbf{r}_o,t_o)+\exp\left\{-\int_{t_o}^{t}dt'\ \nabla\cdot\mathbf{V}(\mathbf{r},t')|_{\mathbf{r}=\mathbf{r}(t')}\right\},\\ \mathbf{V}(\mathbf{r}(t),t)=\mathbf{V}(\mathbf{r}_o,t_o)+\frac{1}{m}\int_{t_o}^{t}dt'\mathbf{F}(\mathbf{r}(t'),t').\end{array}\right. \tag{31}$$

IV - CASE OF THE N-BODY PROBLEM

Let us now consider the case of the N-body system, represented by an ensemble of (N) charged point particles subject to an external EM field defined by the EM potentials $\{\phi, \mathbf{A}\}$. The Hamiltonian [of the N-body system] is defined as

$$\begin{aligned} H_N &= \sum_{i=1,N} H_i, && (32)\\ H_i &= \frac{1}{2m_i}\left(\mathbf{p}_i - \frac{q_i}{c}\mathbf{A}_i\right)^2 + q_i\phi_i, && (33)\\ \mathbf{A}_i &\equiv \mathbf{A}(\mathbf{r}_i, t), && (34)\\ \phi_i &\equiv \phi_T(\mathbf{r}_i, t), && (35) \end{aligned}$$

$\phi_T(\mathbf{r}_i, t)$ deniting a suitable effective potential (which can include the action of a gravitational field). If binary Coulomb interactions are included the previous Hamiltonian should be replaced by

$$H_N = \sum_{i=1,N} H_i + H_N^{(int)},$$

$H_N^{(int)}$ denoting the interaction Hamiltonian

$$H_N^{(int)} = \sum_{i,j=1,N;j<i} q_i q_j \phi_{ij} \equiv \left[q_i q_j \phi_{ij}\right]' \tag{36}$$

and $q_i q_j \phi_{ij}$ the Coulomb interaction potental.

This corresponds to the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi = H_N\psi. \tag{37}$$

where $\psi = \psi(\mathbf{r},t)$ and $\mathbf{r} \equiv (\mathbf{r}_1, ..., \mathbf{r}_N)$ denote respectively the quantum wave function and the configuration vector of the N-body system. It follows:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi &= \psi\left[\frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f - \frac{\partial}{\partial t}S\right],\\ \frac{1}{2m_j}\left(\mathbf{p}_j - \frac{q_j}{c}\mathbf{A}_j\right)^2 &= \frac{1}{2m_j}\left(-i\hbar\nabla_j - \frac{q_j}{c}\mathbf{A}_j\right)\cdot\psi\left[-\frac{i\hbar}{2}\nabla_j\ln f + \nabla_j S - \frac{q_j}{c}\mathbf{A}_j\right] =\\ &= \frac{\psi}{2m_j}\left[-\frac{\hbar^2}{2}\nabla_j^2\ln f - i\hbar\nabla_j^2 S + \frac{q_j}{c}i\hbar\nabla_j\cdot\mathbf{A}_j\right] +\\ &\quad + \frac{\psi q_j}{2m_j c}\left[\frac{i\hbar}{2}\mathbf{A}_j\cdot\nabla_j\ln f - \mathbf{A}_j\cdot\nabla_j S + \frac{q_j}{c}\left|\mathbf{A}_j\right|^2\right] +\\ &\quad + \frac{\psi}{2m_j}\left[-\frac{i\hbar}{2}\nabla_j\ln f + \nabla_j S - \frac{q_j}{c}\mathbf{A}_j\right]\cdot\left[-\frac{i\hbar}{2}\nabla_j\ln f + \nabla_j S\right]. \end{aligned}$$

Hence, the imaginary part of the Schrödinger equation yields

$$\begin{aligned} \frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f &= \frac{1}{2m}\left[-i\hbar\nabla_j^2 S + \frac{q}{c}i\hbar\nabla_j\cdot\mathbf{A}_j\right] + \frac{q_j}{2m_j c}\frac{i\hbar}{2}\mathbf{A}_j\cdot\nabla_j\ln f +\\ &\quad - \frac{1}{2m_j}\frac{i\hbar}{2}\nabla_j\ln f\cdot\nabla_j S - \frac{1}{2m_j}\left[\nabla_j S - \frac{q_j}{c}\mathbf{A}_j\right]\cdot\frac{i\hbar}{2}\nabla_j\ln f =\\ &= \frac{1}{2m_j}\left[-i\hbar\nabla_j^2 S + \frac{q_j}{c}i\hbar\nabla_j\cdot\mathbf{A}_j\right] - \frac{i\hbar}{2m_j}\left[\nabla_j S - \frac{q_j}{c}\mathbf{A}_j\right]\cdot\nabla_j\ln f \end{aligned} \tag{38}$$

(with summation to be unserstood on repeated indexes), namely

$$\frac{\partial}{\partial t}\ln f+\frac{1}{m}\left[\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right]\cdot\nabla_j\ln f+\frac{1}{m_j}\nabla_j^2 S=\frac{q_j}{m_j c}\nabla_j\cdot\mathbf{A}_j. \tag{39}$$

Imposing the Coulomb gauge $\nabla\cdot\mathbf{A}=0$ and introducing the (quantum) fluid velocity field $\mathbf{V}_j=\mathbf{V}_j(\mathbf{r},t)$ for $j=1,N$:

$$\mathbf{V}_j=\frac{1}{m_{(j)}}\left(\nabla_j S-\frac{q_{(j)}}{c}\mathbf{A}_j\right), \tag{40}$$

one obtains the countinuity equation:

$$\frac{\partial}{\partial t}\ln f+\mathbf{V}_j\cdot\nabla_j\ln f+\nabla_j\cdot\mathbf{V}_j=0. \tag{41}$$

Similarly the real part [of the same equation] delivers the *quantum Hamilton-Jacobi equation*:

$$\frac{\partial}{\partial t}S+H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)=0, \tag{42}$$

where $H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)$ is the Hamiltonian function

$$H_c(\mathbf{r},\nabla S-\frac{q}{c}\mathbf{A},t)=\frac{1}{2m_j}\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)^2+U_{QM}+q_i\phi_i+\left[q_i q_j\phi_{ij}\right]', \tag{43}$$

and U_{QM} denotes the so-called *free-particle quantum potential* [8]

$$U_{QM} = \sum_{j=1,N}U_{QMj}, \tag{44}$$

$$U_{QMj} \equiv \frac{\hbar^2}{2}\left(\frac{1}{2}\nabla_j^2\ln f+\frac{1}{4}\left|\nabla_j\ln f\right|^2\right). \tag{45}$$

Applying the operator $(\frac{1}{m_{(i)}}\nabla_i)$ to the previous equation and introducing the position (164) there follows (for $i=1,N$)

$$\frac{\partial}{\partial t}\mathbf{V}_i+\frac{1}{2m_{(i)}^2}\nabla_{(i)}\left(\nabla_i S-\frac{q_i}{c}\mathbf{A}_i\right)^2=-\frac{q}{mc}\frac{\partial}{\partial t}\mathbf{A}_i-\frac{1}{m}\nabla_i U_{QM}-\frac{1}{m_{(i)}}\nabla_i\left(q_j\phi_j+\left[q_i q_j\phi_{ij}\right]'\right).$$

Now we notice that

$$\begin{aligned}&\frac{1}{2m_j^2}\nabla_i\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)^2=\frac{1}{m_j^2}\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)\cdot\nabla_i\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)+\\&+\frac{1}{m_j^2}\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)\times\left[\nabla_i\times\left(\nabla_j S-\frac{q_j}{c}\mathbf{A}_j\right)\right]=\\&=\mathbf{V}_j\cdot\nabla_i\mathbf{V}_j-\frac{q_j}{m_j c}\mathbf{V}_j\times\left[\nabla_i\times\mathbf{A}_j\right]=\mathbf{V}_j\cdot\nabla_i\mathbf{V}_j-\frac{q_{(i)}}{m_{(i)}c}\mathbf{V}_{(i)}\times\mathbf{B}_i-\left(\frac{q_j}{m_j c}\mathbf{V}_j\times\left[\nabla_i\times\mathbf{A}_j\right]\right)',\end{aligned}$$

where $()'\equiv\sum_{j=1,N;j\neq i}$. Hence it follows the *quantum Euler equation*:

$$\left(\frac{D}{Dt}\right)_i\mathbf{V}_i\equiv\frac{\partial}{\partial t}\mathbf{V}_i+\mathbf{V}_{(i)}\cdot\boldsymbol{\nabla}_{(i)}\mathbf{V}_i=\frac{1}{m_{(i)}}\mathbf{F}_i(\mathbf{r},t). \tag{46}$$

Furthermore $\mathbf{F}_i(\mathbf{r},t)$ (*quantum force-field*) is the vector field

$$\begin{aligned}&\mathbf{F}_i(\mathbf{r},t)\equiv q_{(i)}\left\{\mathbf{E}_i+\frac{1}{c}\mathbf{V}_{(i)}\times\mathbf{B}_i\right\}-\nabla_{(i)}U_{QMi}+\\&\Delta\mathbf{F}_i(\mathbf{r},t),\end{aligned} \tag{47}$$

while

$$\Delta\mathbf{F}_i(\mathbf{r},t) = -m_{(i)}\left(\mathbf{V}_j\cdot\nabla_i\mathbf{V}_j\right)' - m_{(i)}\left(\nabla_i q_j\phi_j\right)' + \left(\frac{q_j}{m_j c}\mathbf{V}_j\times\left[\nabla_i\times\mathbf{A}_j\right]\right)' - \\ -\left(\nabla_i U_{QMj}\right)' \tag{48}$$

and

$$\mathbf{E}_i = -\nabla_i[\phi_{(i)} + \frac{1}{m_{(i)}}\nabla_i\left(q_j\phi_j + \left[q_j\phi_{ij}\right]'\right)] - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A}_i\ , \tag{49}$$

$$\mathbf{B}_i = \boldsymbol{\nabla}_{(i)}\times\mathbf{A}_i \tag{50}$$

are the EM fields acting on the i-th particle. The PDE's (165) and (169) are denoted as *N-body quantum hydrodynamic equations* (*N-body QHE*), $\{Z\}\equiv\{f,\mathbf{V}\}$ being the corresponding *quantum fluid fields*.

IV BIS - REDUCED 1-BODY FLUID DESCRIPTION

For definiteness let us consider in this subsection the case in which the Coulomb interactions are negligible. In this case the reduced 1-body fluid description is obtained integrating QHE on the configuration space of the N-1 remaining particles. Letting

$$0 < V = \int_\Omega d^3r_i < \infty,$$

introducing the operators

$$G_1 = \frac{1}{V^{N-1}}\int_\Omega d^3r_2 ... \int_\Omega d^3r_N, \tag{51}$$

$$G_j = \frac{1}{V^{N-1}}\prod_{i=1,N;i\neq j}\left(\int_\Omega d^3r_i\right) \tag{52}$$

let us denote $f_1 = G_1\{f\}$, $\overline{\mathbf{V}}_1 = G_1\{\mathbf{V}_1\}$, $\widetilde{\mathbf{V}}_1 = \mathbf{V}_1 - \overline{\mathbf{V}}_1$ and moreover

$$\overline{\mathbf{V}}_j = G_j\left\{\mathbf{V}_{(j)}\right\},$$
$$\widetilde{\mathbf{V}}_j = \mathbf{V}_j - \overline{\mathbf{V}}_{j.},$$

This yields respectively:

$$\frac{\partial}{\partial t}f_1 + \nabla_1\cdot G_1\{f\mathbf{V}_1\} = 0, \tag{53}$$

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1 + G_1\{\mathbf{V}_1\cdot\boldsymbol{\nabla}_1\mathbf{V}_1\} = \frac{1}{m_1}G_1\{\mathbf{F}_1(\mathbf{r},t)\}, \tag{54}$$

where

$$G_1\{f\mathbf{V}_1\} = f_1\overline{\mathbf{V}}_1 + G_1\left\{\widetilde{f}\widetilde{\mathbf{V}}_1\right\}, \tag{55}$$

$$G_1\{\mathbf{V}_1\cdot\boldsymbol{\nabla}_1\mathbf{V}_1\} = \overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1 + G_1\left\{\widetilde{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\widetilde{\mathbf{V}}_1\right\}, \tag{56}$$

$$G_1\left\{\mathbf{F}_1(\mathbf{r},t)\right\} = q_1\left\{\mathbf{E}_1+\frac{1}{c}\overline{\mathbf{V}}_1\times\mathbf{B}_1\right\}+ \\ +\Delta G_1\left\{\mathbf{F}_1(\mathbf{r},t)\right\}, \tag{57}$$

and

$$\Delta G_1\left\{\mathbf{F}_1(\mathbf{r},t)\right\} = -G_1 m_i\left(\mathbf{V}_j\cdot\nabla_i\mathbf{V}_j\right)' - m_1\nabla_1 G_1\left\{(q_j\phi_j)'\right\}+G_1\left(m_i\frac{q_j}{m_j c}\mathbf{V}_j\times\left[\nabla_i\times\mathbf{A}_j\right]\right)' - \\ -m_1\nabla_1 G_1\sum_{j=1,N}U_{QMj}. \tag{58}$$

There it follows

$$G_1 m_i\left(\mathbf{V}_j\cdot\nabla_i\mathbf{V}_j\right)' = m_1\nabla_1 G_1\left(\frac{1}{2}\mathbf{V}_j^2\right)', \\ \left(m_i\frac{q_j}{m_j c}\mathbf{V}_j\times\left[\nabla_i\times\mathbf{A}_j\right]\right)' = 0,$$

hence

$$\Delta G_1\left\{\mathbf{F}_1(\mathbf{r},t)\right\} = -m_1\nabla_1 G_1\left[\left(\frac{1}{2}\mathbf{V}_j^2+q_j\phi_j\right)'+\sum_{j=1,N}U_{QMj}\right]. \tag{59}$$

We conclude therefore that Eq.(54) reads:

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1 = -G_1\left\{\widetilde{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\widetilde{\mathbf{V}}_1\right\}+\frac{q_1}{m_1}\left\{\mathbf{E}_1+\frac{1}{c}\overline{\mathbf{V}}_1\times\mathbf{B}_1\right\}+ \\ -\nabla_1 G_1\left[\left(\frac{1}{2}\mathbf{V}_j^2+q_j\phi_j\right)'+\sum_{j=1,N}U_{QMj}\right]. \tag{60}$$

This will be denoted as *the reduced 1-body quantum Euler equation.*

OPEN PROBLEMS

1. *ISSUE #1*: is it possible to identify in terms of Eq.(60) the *quantum enthalpy density* $E_1=\rho_1 T_{QM}+p_{QM}$? By definition here we shall assume that there results

$$E_1=\rho_1 T_{QM}+p_{QM}\geq 0 \tag{61}$$

(*positivity requirement*). Here, ρ, T_{QM} and p are denoted respectively as *mass density, quantum kinetic temperature and quantum scalar pressure.*

2. *ISSUE #2:* does there exist an asymptotic limit, or a particular solution of the quantum hydrodynamic equations, in which [at least for a neutral fluid, namely if $q_i=0$ for all $i=1,N$] Eqs.(53) and (54) reduce to the classical *incompressible Euler equations (IEE)*? In other words, such that there results:

$$f_1 = const. \tag{62}$$
$$\nabla_1\cdot\overline{\mathbf{V}}_1=0, \tag{63}$$

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1=-\frac{1}{f_1 m_1}\nabla p+\frac{1}{\rho_1}\mathbf{f}, \tag{64}$$

or more generally the classical *incompressible Navier-Stokes equations (INSE),* obtained replacing Eq.(64) with

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1=-\frac{1}{f_1m_1}\nabla p+\frac{1}{f_1m_1}\mathbf{f}+\nu\nabla^2\overline{\mathbf{V}}_1. \tag{65}$$

In the case of a heavy and neutral fluid $\mathbf{f}$ is defined as the volume force produced by the gravitational field, i.e.,

$$\frac{1}{\rho_1}\mathbf{f}=\mathbf{g}, \tag{66}$$

$\mathbf{g}$ denoting the gravitational acceleration and $\rho_1=f_1m_1$ the 1-body mass density) and $\nu>0$ a constant dimensionless parameter (kinematic viscosity)?

CLASSICAL LIMIT OF THE QUANTUM EULER EQUATION

Here we intend to point out that:

- the enthalpy density E_1, as well as the quantum temperature and pressure, $T_{QM}(\mathbf{r}_1,t)$ and $p(\mathbf{r}_1,t)$, can be uniquely prescribed in terms of the reduced 1-body quantum Euler equation.(60). In particular, we intend to prove that a possible definition for E_1, $T_{QM}(\mathbf{r},t)$ and $p(\mathbf{r},t)$ is provided by

$$\frac{E_1}{\rho_1}=T_{QM}(\mathbf{r}_1,t)+\frac{1}{\rho_1}p_{QM}(\mathbf{r}_1,t), \tag{67}$$

$$T_{QM}(\mathbf{r}_1,t)=T_o(t)+T_1(\mathbf{r}_1,t), \tag{68}$$

$$T_1(\mathbf{r},t)=m_1G_1\nabla_1\left[\left(\frac{1}{2}\mathbf{V}_j^2-\frac{1}{2}\widetilde{V}_j^2\right)'+\sum_{j=1,N}\frac{\hbar^2}{8}\left|\nabla_j\ln f\right|^2\right], \tag{69}$$

$$\frac{1}{\rho}p_{QM}(\mathbf{r},t)\equiv G_1\left(\frac{\widetilde{V}_1^2}{2}+\frac{1}{2}\widetilde{V}_j^2\right)'. \tag{70}$$

Here the notation is as follows:

1. $T_o(t)$, to be denoted as *pseudo-temperature*, is defined so that there results identically for all $t\in I$:

$$\frac{\partial}{\partial t}S(g_M)=0$$

(*constant H-theorem for the microscopic BS-entropy*) with $S(g_M)$ the BS entropy (to be defined below);

2. $T_{QM}(\mathbf{r}_1,t)$ and $T_1(\mathbf{r}_1,t)$ are denoted respectively as *quantum and relative temperature;*
3. $p_{QM}(\mathbf{r}_1,t)$ is denoted as *quantum scalar pressure.*

- *The quantum Euler equation (59) implies the classical incompressible Euler equation Eq.(64).*

Definition of E_1, T_{QM} and p_{QM}

Let us first point out the following identity:
LEMMA 1
There its results identically:

$$G_1\left\{\widetilde{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\widetilde{\mathbf{V}}_1\right\}=G_1\nabla_1\left(\frac{\widetilde{\mathbf{V}}_1^2}{2}\right). \tag{71}$$

PROOF: in fact by definition

$$
\begin{aligned}
G_1\left\{\mathbf{V}_1\cdot\boldsymbol{\nabla}_1\mathbf{V}_1\right\} &= \nabla_1 G_1\left(\frac{V_1^2}{2}\right)=\nabla_1 G_1\left(\frac{\left[\overline{\mathbf{V}}_1+\widetilde{\mathbf{V}}_1\right]^2}{2}\right)= \\
&= \nabla_1\left(\frac{\overline{\mathbf{V}}_1{}^2}{2}\right)+G_1\nabla_1\left(\frac{\widetilde{\mathbf{V}}_1^2}{2}\right)= \\
&= \overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1+G_1\left[\overline{\mathbf{V}}_1\times\left(\boldsymbol{\nabla}_1\times\widetilde{\mathbf{V}}_1\right)\right]+G_1\nabla_1\left(\frac{\widetilde{\mathbf{V}}_1^2}{2}\right)
\end{aligned}
\tag{72}
$$

Since

$$
G_1\left[\overline{\mathbf{V}}_1\times\left(\boldsymbol{\nabla}_1\times\widetilde{\mathbf{V}}_1\right)\right]=0 \tag{73}
$$

holds identically, while manifestly

$$
G_1\left\{\mathbf{V}_1\cdot\boldsymbol{\nabla}_1\mathbf{V}_1\right\}=\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1+G_1\left\{\widetilde{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\widetilde{\mathbf{V}}_1\right\}, \tag{74}
$$

so that Eq. (71) follows. Q.E.D.

The Lemma implies that Eq.(60) can be written as

$$
\begin{aligned}
\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1 &= \frac{q_1}{m_1}\left\{\mathbf{E}_1+\frac{1}{c}\overline{\mathbf{V}}_1\times\mathbf{B}_1\right\}+\mathbf{g}+ \\
&\quad -\frac{1}{\rho_1}\nabla_1 E_1- \qquad (75)\\
&\quad -\nabla_1 G_1\left[\left(q_j\phi_j\right)'+\sum_{j=1,N}\frac{\hbar^2}{4}\nabla_j^2\ln f\right]+ \\
&\quad +\frac{E_1}{\rho_1}\nabla_1\ln\rho_1. \qquad (76)
\end{aligned}
$$

where we let

$$
\begin{aligned}
&\frac{E_1}{\rho_1}=\frac{1}{m_1}T_{QM}(\mathbf{r}_1,t)+\frac{1}{\rho_1}p_{QM}(\mathbf{r}_1,t), && (77)\\
&T_{QM}(\mathbf{r}_1,t)=T_o(t)+T_1(\mathbf{r}_1,t), && (78)\\
&\frac{1}{m_1}T_1(\mathbf{r}_1,t)=\left(\frac{1}{2}\mathbf{V}_j^2-\frac{1}{2}\widetilde{V}_j^2\right)'+\sum_{j=1,N}\frac{\hbar^2}{8}\left|\nabla_j\ln f\right|^2 && (79)\\
&\frac{1}{\rho_1}p_{QM}(\mathbf{r}_1,t)=\frac{\widetilde{V}_1^2}{2}+\left(\frac{1}{2}\widetilde{V}_j^2\right)'.
\end{aligned}
$$

In the case of a neutral fluid this reduces to

$$
\begin{aligned}
\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1 &= -\frac{1}{\rho_1}\nabla_1 E_1+\mathbf{g}-\nabla_1 G_1\left[\sum_{j=1,N}\frac{\hbar^2}{4}\nabla_j^2\ln f\right]+ \\
&\quad +\frac{E_1}{\rho_1}\nabla_1\ln\rho_1. \qquad (80)
\end{aligned}
$$

In particular, for an isothermal neutral fluid $[T_1(\mathbf{r}_1,t)=const]$ it follows

$$
\begin{aligned}
\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1 &= -\frac{1}{\rho_1}\nabla_1 p+\mathbf{g}-\nabla_1 G_1\left[\sum_{j=1,N}\frac{\hbar^2}{4}\nabla_j^2\ln f\right]+ \qquad (81)\\
&\quad +\frac{E_1}{\rho_1}\nabla_1\ln\rho_1,
\end{aligned}
$$

where

$$G_1\left[\sum_{j=1,N}\frac{\hbar^2}{4}\nabla_j^2\ln f\right]=\frac{\hbar^2}{4}\nabla_1^2 G_1\left[\ln f\right]. \tag{82}$$

Let us now consider the *semi-classical limit*. This is can be defined by letting:

$$\hbar \;\rightarrow\; 0, \tag{83}$$

$$\frac{\hbar^2}{4}\nabla_1^2 G_1\left[\ln f\right] \;\rightarrow\; 0, \tag{84}$$

$$\sum_{j=1,N}\frac{\hbar^2}{8}\left|\nabla_j\ln f\right|^2 \;\rightarrow\; 0, \tag{85}$$

thus yielding:

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1=-\frac{1}{\rho_1}\nabla_1 p+\frac{1}{\rho_1}\mathbf{f} \tag{86}$$

(*semiclassical limit*), with $\mathbf{f}$ now denoting the vector field:

$$\mathbf{f}\equiv\rho_1\mathbf{g}+E_1\nabla_1\ln\rho_1. \tag{87}$$

We remark that :

- Eq.(86) can be viewed as the *Euler equation of a classical fluid subject to the "modified" volume force density (87). We remark that $E_1\nabla_1\ln\rho_1$ represents an additional volume force density, not usually included in the Euler equation of a classical neutral fluid;*
- *Hence, the classical Euler equation should actually be considered an approximation of Eq.(86), holding when the extra volume force density $E_1\nabla_1\ln\rho_1$ can be considered as negligible.* Manifestly this occurs exactly [i.e., Eq.(86) reduces identically to the customary *Euler equation of a classical ideal fluid*] when it results identically $\rho_1=const.$ (*condition of incompressibility*). In this case one obtains:

THM.1 - Classical incompressible Euler equation
In the case of an incompressible quantum fluid Eq.(81) reduces to:

$$\frac{\partial}{\partial t}\overline{\mathbf{V}}_1+\overline{\mathbf{V}}_1\cdot\boldsymbol{\nabla}_1\overline{\mathbf{V}}_1=-\frac{1}{\rho_1}\nabla_1 p+\mathbf{g}, \tag{88}$$

which coincides with the Euler equation of a classical ideal fluid.

In conclusion:
1) the classical limit [of th quantum Euler equation] can be viewed as the equation of a classical fluid subject to a suitably"modified" volume force density;
2) The extra force represents a new effect, not usually included in the Euler equation of a classical neutral fluid;
3) the classical Euler equation should therefore be considered an approximation of our more correct equation, holding when the extra volume force density is negligible. This occurs exactly for an incompressible fluid;
4) quantum corrections to the classical Euler equations can be clearly identified;
5) the notions of enthaply density, temperature and scalar pressure are (uniquely) achieved, based on the quantum description. This is a prerequisite for achieving IKT for the N-body fluid description.

V - INVERSE KINETIC THEORY FOR QHE

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. - The case of 1-body IKT

Let us first determine an inverse kinetic theory (IKT) for the 1-body Schrödinger equation (i.e., a kinetic theory yielding the 1-body quantum hydrodynamic equations defined above). Here we shall consider in particular the case of a *single-temperature IKT* requiring

$$T \equiv M_3\left[g\right] \equiv \tag{89}$$
$$\equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v} m \frac{u^2}{3} g(\mathbf{r},\mathbf{v},t),$$

[where $\mathbf{u} = \mathbf{v} - \mathbf{V}(\mathbf{r},t)$] while imposing also

$$f = M_1\left[g\right] \equiv \int_U d\mathbf{v} g(\mathbf{r},\mathbf{v},t), \tag{90}$$
$$M_2\left[g\right] \equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v}\mathbf{v} g(\mathbf{r},\mathbf{v},t) = \tag{91}$$
$$= \mathbf{V}(\mathbf{r},t),$$

Assuming that the sole information is provided by the knowledge of the initial fluid fields PEM yields necessarily that the only admissible probability distribution function (PDF) is

$$g(\mathbf{x},t) = g_M(\mathbf{r},\mathbf{v},t) \equiv f(\mathbf{r},t)\frac{1}{\pi^{3/2}v_{th}^{3/2}}\exp\left\{-X^2\right\}, \tag{92}$$

to be denoted as *generalized Maxwellian PDF*. Here $v_{th} = \sqrt{2T/m}$,$X^2 = u^2/v_{th}$ and $\mathbf{u} = \mathbf{v} - \mathbf{V}(\mathbf{r},t)$. Requiring that $g_M(\mathbf{r},\mathbf{v},t)$ satisfies identically the Liouville equation, or *inverse kinetic equation (IKE)*

$$\frac{\partial}{\partial t}g_M + \mathbf{v}\cdot\boldsymbol{\nabla} g_M + \frac{\partial}{\partial \mathbf{v}}\cdot\left(g_M\frac{1}{m}\mathbf{K}(g_M)\right) = 0, \tag{93}$$

iff the fluid fields $\{f(\mathbf{r},t),\mathbf{V}(\mathbf{r},t)\}$ satisfy the QHE initial-boundary value problem, it follows that mean-field force $\mathbf{K}(g_M)$ has the form

$$\mathbf{K}(g_M) = \mathbf{F}(g_M) + \mathbf{K}_u(g_M), \tag{94}$$

where $\frac{1}{m}\mathbf{F}(g_M)$ denotes the fluid acceleration, with $\mathbf{F}(g_M)$ defined as

$$\mathbf{F}(g_M) = q\left[\mathbf{E}(\mathbf{r},t) + \frac{1}{c}\mathbf{V}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)\right] - \nabla U_{QM}(\mathbf{r},t), \tag{95}$$

while $\frac{1}{m}\mathbf{K}_u(g_M)$ is the kinetic contribution to the acceleration. The form of the mean-field force term $\mathbf{K}_u(g_M)$ depends of the definition of the temperature fluid field. Assuming a single temperature (T), in particular one can require either: A) $T = T(t)$ or B) $T = T(\mathbf{r},t)$. It follows that

CASE A - letting $T = T(t)$ there results

$$\mathbf{K}_u(g_M) = T(t)\nabla\ln f(\mathbf{r},t) + m\mathbf{u}\cdot\nabla\mathbf{V} + \frac{m}{2}\mathbf{u}\frac{\partial}{\partial t}\ln T(t); \tag{96}$$

CASE B - letting, instead, $T = T(\mathbf{r},t)$ there results

$$\mathbf{K}_u(g_M) = T(\mathbf{r},t)\nabla\ln f + m\mathbf{u}\cdot\nabla\mathbf{V} + \frac{m}{2}\mathbf{u}\frac{D}{Dt}\ln T(\mathbf{r},t) + \tag{97}$$
$$+\nabla T(\mathbf{r},t)(X^2 - \frac{1}{2}).$$

PROOF:

There results, in fact, from Eq.(93):

$$\frac{\partial}{\partial t}\lg n_M + \mathbf{v}\cdot\boldsymbol{\nabla}\ln g_M = \underset{(1)}{\boxed{\frac{D}{Dt}\ln f}} + \underset{(3)}{\boxed{\mathbf{u}\cdot\boldsymbol{\nabla}\ln f}} + \left(\underset{(5)}{\boxed{\frac{D}{Dt}}} + \underset{(6)}{\boxed{\mathbf{u}\cdot\nabla}}\right)\ln T\left(X^2-\frac{3}{2}\right) + \underset{(2)}{\boxed{\frac{D\mathbf{V}}{Dt}\cdot\frac{2\mathbf{u}}{v_{th}^2}}} + \underset{(4)}{\boxed{\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{V}\cdot\frac{2\mathbf{u}}{v_{th}^2}}}$$

$$\frac{1}{g_M}\frac{\partial}{\partial\mathbf{v}}\cdot\left(g_M\frac{1}{m}\mathbf{K}(g_M)\right) = \underset{(2)}{\boxed{-\frac{2\mathbf{u}}{v_{th}^2}\cdot\frac{1}{m}\mathbf{F}(g_M)}} - \frac{2\mathbf{u}}{v_{th}^2}\cdot\left[\underset{(3)}{\boxed{\frac{1}{m}\mathrm{T}\nabla\ln f}} + \underset{(4)}{\boxed{\nabla\mathbf{V}\cdot\mathbf{u}}} + \underset{(5)}{\boxed{\frac{1}{2}\mathbf{u}\frac{D}{Dt}\ln\mathrm{T}}}\underset{(6)}{\boxed{+\frac{1}{m}\nabla\mathrm{T}(\mathrm{X}^2\text{-}\frac{1}{2})}}\right] +$$
$$+\underset{(1)}{\boxed{\nabla\cdot\mathbf{V}}} + \underset{(5)}{\boxed{\frac{3}{2}\frac{D}{Dt}\ln\mathrm{T}}}\underset{(6)}{\boxed{+\mathbf{u}\cdot\nabla\ln\mathrm{T}}}$$

which proves the statement. Q.E.D.

B. - N-body IKT

Let us now construct an inverse kinetic theory (IKT) for the N-body Schrödinger equation. For this purpose we shall introduce for each particle a *single-temperature IKT,* requiring for $i = 1, N$:

$$T_i(\mathbf{r}_i,t) \equiv M_3\left[g\right] \equiv \tag{98}$$
$$\equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v}m_i\frac{u_i^2}{3}g(\mathbf{r},\mathbf{v},t),$$

where

$$\mathbf{u}_i = \mathbf{v}_i - \mathbf{V}_i,$$

while imposing also

$$f = M_1\left[g\right] \equiv \int_U d\mathbf{v}g(\mathbf{r},\mathbf{v},t), \tag{99}$$
$$M_2\left[g\right] \equiv \frac{1}{f(\mathbf{r},t)}\int_U d\mathbf{v}\mathbf{v}_i g(\mathbf{r},\mathbf{v},t) = \tag{100}$$
$$= \mathbf{V}_i(\mathbf{r},t),$$

Assuming that the sole information is provided by the knowledge of the initial fluid fields PEM yields necessarily that the only admissible probability distribution function (PDF) is then

$$g(\mathbf{x},t) = g_M(\mathbf{r},\mathbf{v},t) \equiv f(\mathbf{r},t)\prod_{i=1,N}\frac{1}{\pi^{3/2}v_{th,i}^{3/2}}\exp\left\{-X_i^2\right\}, \tag{101}$$
$$X_i^2 = \frac{u_i^2}{v_{th,i}^2}, \tag{102}$$
$$v_{th,i}^2 = \frac{2T_i}{m_i}. \tag{103}$$

Here $v_{th} = \sqrt{2T/m}$,$x^2 = u^2/v_{th}$ and $\mathbf{u} = \mathbf{v} - \mathbf{V}(\mathbf{r},t)$.
Again imposing for $g_M(\mathbf{r},\mathbf{v},t)$ the *IKE*

$$\frac{\partial}{\partial t}g_M + \mathbf{v}_i\cdot\boldsymbol{\nabla}_i g_M + \frac{\partial}{\partial\mathbf{v}_i}\cdot\left(g_M\frac{1}{m_i}\mathbf{K}_i(g_M)\right) = 0, \tag{104}$$

it follows that mean-field force $\mathbf{K}_i(g_M)$ has necessarily the form

$$\mathbf{K}_i(g_M) = \mathbf{F}_i + \mathbf{K}_{ui}(g_M), \tag{105}$$

where $\frac{1}{m_i}\mathbf{F}_i$ denotes the fluid acceleration, with $\mathbf{F}_i(g_M)$ defined by Eq.(170), while $\frac{1}{m_i}\mathbf{K}_{ui}(g_M)$ denotes again the kinetic contribution to the acceleration and its form depends on the defintion of the temperature fluid fields, namely either: A) $T_i = T_i(t)$ or B) $T_i = T_i(\mathbf{r}_i,t)$. It follows that

CASE A - letting $T_i = T_i(t)$ one finds

$$\mathbf{K}_{ui}(g_M) = T_i\nabla_i \ln f(\mathbf{r},t) + m_{(i)}\mathbf{u}_{(i)}\cdot\nabla_{(i)}\mathbf{V}_i + (m_{(i)}\mathbf{u}_j\cdot\nabla_j\mathbf{V}_i)' + \frac{m_i}{2}\mathbf{u}_i\frac{\partial}{\partial t}\ln T_i; \tag{106}$$

CASE B - letting, instead, $T_i = T_i(\mathbf{r}_i,t)$ there results

$$\begin{aligned}\mathbf{K}_{ui}(g_M) &= T_i\nabla_i \ln f + m_{(i)}\mathbf{u}_{(i)}\cdot\nabla_{(i)}\mathbf{V}_i + (m_{(i)}\mathbf{u}_j\cdot\nabla_j\mathbf{V}_i)' + \\ &+\frac{m_i}{2}\mathbf{u}_i\left(\frac{D}{Dt}\right)_i \ln T_i + \nabla_i T_i(X_i^2 - \frac{1}{2}).\end{aligned} \tag{107}$$

PROOF:

Let us invoke now Eq.(104). There results:

$$\begin{aligned}\frac{\partial}{\partial t}\lg n_M + \mathbf{v}_i\cdot\boldsymbol{\nabla}_i g_M &= \underbrace{\boxed{\sum_{i=1,N}\left(\tfrac{D}{Dt}\right)_i \ln f}}_{(1)} + \underbrace{\boxed{\mathbf{u}_i\cdot\boldsymbol{\nabla}_i \ln f}}_{(3)} + \left(\underbrace{\boxed{\sum_{i=1,N}\left(\tfrac{D}{Dt}\right)_i}}_{(5)} + \underbrace{\boxed{\mathbf{u}_i\cdot\nabla_i}}_{(6)}\right)\ln T_i\left(X_i^2 - \frac{3}{2}\right) + \\ &+\underbrace{\boxed{\sum_{i=1,N}\left(\tfrac{D\mathbf{V}_j}{Dt}\right)_i\cdot\tfrac{2\mathbf{u}_j}{v_{th,j}^2}}}_{(2)} + \underbrace{\boxed{\mathbf{u}_i\cdot\boldsymbol{\nabla}_i\mathbf{V}_j\cdot\tfrac{2\mathbf{u}_j}{v_{th,j}^2}}}_{(4)}\end{aligned}$$

$$\begin{aligned}\mathbf{K}_{ui}(g_M) &= T_i\nabla_i \ln f + m_{(i)}\mathbf{u}_{(i)}\cdot\nabla_{(i)}\mathbf{V}_i + (m_{(i)}\mathbf{u}_j\cdot\nabla_j\mathbf{V}_i)' + \\ &+\frac{m_i}{2}\mathbf{u}_i\left(\frac{D}{Dt}\right)_i \ln T_i + \nabla_i T_i(X_i^2 - \frac{1}{2}).\end{aligned} \tag{108}$$

$$\begin{aligned}\frac{1}{g_M}\frac{\partial}{\partial\mathbf{v}_i}\cdot\left(g_M\frac{1}{m_i}\mathbf{K}_i(g_M)\right) &= \underbrace{\boxed{-\tfrac{2\mathbf{u}_i}{v_{th,i}^2}\cdot\tfrac{1}{m_i}\mathbf{F}_i(g_M)}}_{(2)} - \frac{2\mathbf{u}_i}{v_{thi}^2}\cdot\left[\underbrace{\boxed{\tfrac{1}{m_i}T_i\nabla_i\ln f}}_{(3)} + \underbrace{\boxed{\mathbf{u}_j\cdot\nabla_j\mathbf{V}_i}}_{(4)} + \underbrace{\boxed{\tfrac{1}{2}\mathbf{u}_i\left(\tfrac{D}{Dt}\right)_i\ln T_i}}_{(5)}\underbrace{\boxed{+\tfrac{1}{m_i}\nabla_i T_i(X_i^2 - \tfrac{1}{2})}}_{(6)}\right] - \\ &+\underbrace{\boxed{\nabla_i\cdot\mathbf{V}_i}}_{(1)} + \underbrace{\boxed{\tfrac{3}{2}\left(\tfrac{D}{Dt}\right)_i\ln T_i}}_{(5)}\underbrace{\boxed{+\mathbf{u}_i\cdot\nabla_i\ln T_i}}_{(6)}\end{aligned}$$

which proves the statement. Q.E.D.

A.BIS - Reduced 1-body IKT

The reduced 1-body IKT is obtained introducing the integral operator

$$H_1 = \int_{\Gamma_1} dx_2 ... \int_{\Gamma_N} dx_N \tag{109}$$

and denoting

$$g_{M,1} = H_1\left\{g_M\right\} \equiv f_1\frac{1}{\pi^{3/2}v_{th,1}^{3/2}}\exp\left\{-X_1^2\right\}. \tag{110}$$

Then IKE yields

$$\frac{\partial}{\partial t}g_{M,1}+\mathbf{v}_1\cdot\boldsymbol{\nabla}_1 g_{M,1}+\frac{\partial}{\partial \mathbf{v}_1}\cdot H_1\left(g_M\frac{1}{m_1}\mathbf{K}_1(g_M)\right)=0, \tag{111}$$

where

$$H_1\left(g_M\frac{1}{m_1}\mathbf{K}_1(g_M)\right)=g_{M,1}\frac{1}{m_1}\mathbf{F}_1+$$
$$+H_1\left(g_M\frac{1}{m_1}\mathbf{K}_{u1}(g_M)\right)$$

It follows

$$H_1\left(g_M\frac{1}{m_1}\mathbf{K}_{u1}(g_M)\right)=H_1 g_M\left\{T_i\nabla_i\ln f+\right. \tag{112}$$
$$\left.+\nabla_i T_i(X_i^2-\frac{1}{2})\right\}=H_1\left\{g_M T_i\nabla_i\ln f\right\}+$$
$$+g_{M,1}\nabla_1 T_1(X_1^2-\frac{1}{2})+H_1\left\{g_M\nabla_j T_j\right\}, \tag{113}$$

namely

$$H_1\left(g_M\frac{1}{m_1}\mathbf{K}_{u1}(g_M)\right)=\frac{1}{f_1}g_{M1}G_1\left\{\frac{1}{f_i}g_{Mi}T_i\nabla_i f\right\}+ \tag{114}$$
$$+g_{M,1}\nabla_1 T_1(X_1^2-\frac{1}{2})+\frac{1}{f_1}g_{M1}G_1\left\{\frac{f}{f_i}g_{Mi}\nabla_i T_i\right\}$$

B. IKT-Schrödinger dynamical system

Let us introduce the phase-space dynamical system defined by IKE, namely

$$\mathbf{x}(t_o)=\mathbf{x}_o\rightarrow\mathbf{x}(t)=T_{t,t_o}\mathbf{x}_o \tag{115}$$

where the evolution operator T_{t,t_o} is generated by the flow of the initial-value problem

$$\dot{\mathbf{r}}\ \equiv\ \frac{d\mathbf{r}}{dt}=\mathbf{v}, \tag{116}$$

$$\dot{\mathbf{v}}\ \equiv\ \frac{d\mathbf{v}}{dt}\equiv\frac{d\dot{\mathbf{r}}}{dt}=\frac{1}{m}\mathbf{K}(g_M), \tag{117}$$

$\mathbf{x}\equiv(\mathbf{r},\mathbf{v})$ and $\mathbf{v}$ denoting respectively the *kinetic state* and the *kinetic velocity* defined by Eqs.(116) and (117). In the remainder we shall require that $\mathbf{x}(t)\equiv\{\mathbf{r}(t),\mathbf{v}(t)\}=T_{t,t_o}\mathbf{x}_o$ satisfies the boundary conditions

$$\mathbf{x}(t_o)\ =\ \mathbf{x}_o, \tag{118}$$
$$\mathbf{x}(t_1)\ =\ \mathbf{x}_1. \tag{119}$$

In the present case (115) is denoted as *IKT-Schrödinger dynamical system.*

C.The search of a variational formulation

Let us pose the problem of the search of a variational formulation of the boundary-value problem for Eqs. (116) and (117): in other words a variational principle of the form

$$\begin{cases}\delta S(\boldsymbol{\xi})=0\\ \forall\delta\boldsymbol{\xi}(t)\end{cases} \tag{120}$$

where the real vector functions $\boldsymbol{\xi}(t)\in\{\boldsymbol{\xi}(t)\}$, $S(\boldsymbol{\xi})$ [variational functional], $\{\boldsymbol{\xi}(t)\}$ [functional class], $\delta\boldsymbol{\xi}(t)$ [synchronous variation of $\boldsymbol{\xi}(t)$)] and $\delta S(\boldsymbol{\xi})$ [synchronous variation of $\delta S(\boldsymbol{\xi}(t))$] are all to be suitably defined.

CASE A:

In case A, Eq.(117) reads

$$\frac{d}{dt}\dot{\mathbf{r}} - \frac{T}{m}\frac{\partial}{\partial \mathbf{r}}\ln f(\mathbf{r},t) - \\ -\frac{q}{m}\left[\mathbf{E}(\mathbf{r},t)+\frac{1}{c}\mathbf{V}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)\right] - \frac{1}{m}\nabla U_{QM}(\mathbf{r},t) - \nabla\mathbf{V}(\mathbf{r},t)\cdot\left[\dot{\mathbf{r}}-\mathbf{V}\right] - \frac{1}{2}\left[\dot{\mathbf{r}}-\mathbf{V}\right]\frac{\partial}{\partial t}\ln T = 0, \tag{121}$$

where $\mathbf{V}(\mathbf{r},t)$ denotes an arbitrary particular solution of the quantum Euler equation [see Eq.(169)], namely

$$\frac{D}{Dt}\mathbf{V}(\mathbf{r},t) = \frac{q}{m}\left[\mathbf{E}(\mathbf{r},t)+\frac{1}{c}\mathbf{V}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)\right] - \frac{1}{m}\nabla U_{QM}(\mathbf{r},t) \tag{122}$$

[this equation can be proven to be itself variational and Hamiltonian (see Appendix A)]. There results

$$\nabla\mathbf{V}(\mathbf{r},t)\cdot\left[\dot{\mathbf{r}}-\mathbf{V}\right] = \nabla\mathbf{V}(\mathbf{r},t)\cdot\dot{\mathbf{r}} - \nabla\frac{1}{2}\mathbf{V}^2(\mathbf{r},t) = \\ = \nabla\mathbf{V}(\mathbf{r},t)\cdot\dot{\mathbf{r}} - \frac{D}{Dt}\mathbf{V}(\mathbf{r},t) + \frac{\partial}{\partial t}\mathbf{V}(\mathbf{r},t) = \\ = \frac{d}{dt}\mathbf{V}(\mathbf{r},t) - \frac{D}{Dt}\mathbf{V}(\mathbf{r},t)\ .$$

Let us introduce the decomposition

$$\mathbf{r} = \mathbf{R} + \boldsymbol{\rho}, \tag{123}$$

where $\{\mathbf{R}(\boldsymbol{\rho}(t),t)\}$ and $\{\boldsymbol{\rho}(t)\}$ and denote respectively the configuration-space Lagrangian trajectories solutions of the equations

$$\frac{d\mathbf{R}}{dt} = \mathbf{V}(\mathbf{R}+\boldsymbol{\rho},t) \equiv \frac{D\mathbf{R}}{Dt}, \tag{124}$$

$$\frac{d\boldsymbol{\rho}}{dt} = \mathbf{v} - \mathbf{V}(\mathbf{r},t) \equiv \mathbf{u}. \tag{125}$$

As a consequence Eq.(121) is reduced to the ODE:

$$\frac{d}{dt}\dot{\boldsymbol{\rho}} = \frac{T}{m}\frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t) + \frac{1}{2}\dot{\boldsymbol{\rho}}\frac{\partial}{\partial t}\ln T.$$

Hence, denoting $T(t_o) = T_o$ (with $T_o > 0$), the same equation can also be written as

$$\frac{d}{dt}\left(\frac{m}{2}\frac{T_o}{T}\dot{\boldsymbol{\rho}}\right) - \frac{T_o}{2}\frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t) = 0, \tag{126}$$

to be considered subject to the boundary conditions

$$\boldsymbol{\rho}(t_i) = \boldsymbol{\rho}_i \tag{127}$$

for $i = 0, 1$. This equation can be viewed as prescribing *the kinetic relative dynamics*, i.e., with respect the local (quantum) fluid element [which moves with velocity $\mathbf{V}(\mathbf{r},t)$].

CASE B

In case B one obtains instead:

$$\frac{d}{dt}\dot{\mathbf{r}}+\frac{T}{m}\frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t)-$$
$$-\frac{q}{m}\left[\mathbf{E}(\mathbf{r},t)+\frac{1}{c}\mathbf{V}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)\right]+\frac{1}{m}\nabla U_{QM}(\mathbf{r},t)+$$
$$+\nabla\mathbf{V}(\mathbf{r},t)\cdot\left[\dot{\mathbf{r}}-\mathbf{V}\right]+\frac{1}{2}\left[\dot{\mathbf{r}}-\mathbf{V}\right]\frac{D}{Dt}\ln T-\frac{1}{m}\nabla T(X^2-\frac{1}{2})=0, \tag{128}$$

As a consequence the equation reduces to the ODE:

$$\frac{d}{dt}\dot{\boldsymbol{\rho}}=\frac{T}{m}\frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t)+\frac{1}{2}\dot{\boldsymbol{\rho}}\frac{D}{Dt}\ln T-\frac{1}{m}\nabla T(X^2-\frac{1}{2})$$

where

$$X^2=\frac{m\dot{\boldsymbol{\rho}}^2}{2T}, \tag{129}$$

namely

$$\frac{d}{dt}\left(\frac{m}{2}\frac{T_o}{T}\dot{\boldsymbol{\rho}}\right)-\frac{T_o}{2}\frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t)+\frac{T_o}{2}\frac{\partial}{\partial\mathbf{r}}\ln T(\frac{m\dot{\boldsymbol{\rho}}^2}{2T}-\frac{1}{2})=0. \tag{130}$$

This equation is manifestly non-variational.

D. Variational formulation for Eq.(126) - The basic results

We intend to prove that the boundary-value problem associated to Eq.(126) is:

1. *variational*
2. *Hamiltonian.*

The result does not pose any constraint on the quantum temperature $T=T(t)$.
The following results hold:

THM.1 - Lagrangian variational principle for Eq.(126)

Let us introduce the following definitions:

1) functional $S_1(\boldsymbol{\rho})$:

$$S_1(\boldsymbol{\rho})=\int_{t_0}^{t_1}dtL_1(\boldsymbol{\rho}(t),\dot{\boldsymbol{\rho}}(t),t), \tag{131}$$

$$L_1(\boldsymbol{\rho},\dot{\boldsymbol{\rho}},t)=\frac{m}{4}\frac{T(t)}{T_o}\dot{\boldsymbol{\rho}}^2+\frac{T^2(t)}{2T_o}\ln f(\mathbf{R}+\boldsymbol{\rho},t)\ ; \tag{132}$$

2) functional classes $\{\boldsymbol{\rho}(t)\}$ and $\{\mathbf{r}(t)\}_R$:

$$\{\boldsymbol{\rho}(t)\}\ =\ \left\{\boldsymbol{\rho}(t):\boldsymbol{\rho}(t)\in C^{(2)}(I);\boldsymbol{\rho}(t_i)=\boldsymbol{\rho}_i\text{ and }\boldsymbol{\rho}(t),\boldsymbol{\rho}_i\in\mathbb{R}^3,i=0,1\right\} \tag{133}$$

$$\{\mathbf{r}(t)\}_R\ =\ \left\{\mathbf{r}(t):\mathbf{r}(t)=\mathbf{R}(t)+\boldsymbol{\rho}(t);\ \mathbf{R}(t)\in C^{(2)}(I),\boldsymbol{\rho}(t)\in\{\boldsymbol{\rho}(t)\},\mathbf{r}(t_i)=\mathbf{r}_i\text{ and }\mathbf{r}(t),\mathbf{r}_i\in\mathbb{R}^3,\ i=0,1\right\}; \tag{134}$$

3) in Eq.(133) the vector function $\mathbf{R}(t)$ is considered uniquely prescribed for all curves $\mathbf{r}(t)$, i.e., independent of che choice of $\boldsymbol{\rho}(t)\in\{\boldsymbol{\rho}(t)\}$;

4) synchronous variation $\delta S_1(\boldsymbol{\rho})$:

$$\delta S_1(\boldsymbol{\rho}) = \frac{d}{d\alpha}\Psi_1(\alpha)\Big|_{\alpha=0} \tag{135}$$

with $\Psi_1(\alpha)$ *the real function defined, for* $\alpha \in]-1,1[$, *as*

$$\Psi_1(\alpha) = \delta S_1(\boldsymbol{\rho}+\alpha\delta\boldsymbol{\rho}) \equiv \int_{t_0}^{t_1} dt L_1(\boldsymbol{\rho}(t)+\alpha\delta\boldsymbol{\rho}(t), \dot{\boldsymbol{\rho}}(t)+\alpha\delta\dot{\boldsymbol{\rho}}(t), t)$$

where $\delta\boldsymbol{\rho}(t) = \boldsymbol{\rho}(t) - \boldsymbol{\rho}_1(t)$, *with* $\boldsymbol{\rho}(t)$ *and* $\boldsymbol{\rho}_1(t)$ *denoting two arbitrary functions belonging to* $\{\boldsymbol{\rho}(t)\}$. *Hence, consistent with the requirements #2 and 3, we let*

$$\begin{aligned} &\Psi_1(\alpha) = \\ &= \int_{t_0}^{t_1} dt \left[\frac{m}{4}\frac{T(t)}{T_o}\left(\dot{\boldsymbol{\rho}}(t)+\alpha\delta\dot{\boldsymbol{\rho}}(t)\right)^2 + \frac{T^2(t)}{2T_o}\ln f(\mathbf{R}(\boldsymbol{\rho}(t),t)+\boldsymbol{\rho}(t)+\alpha\delta\boldsymbol{\rho}(t),t)\right]. \end{aligned} \tag{136}$$

Then it follows that the Lagrangian variational principle

$$\begin{cases} \delta S_1(\boldsymbol{\rho}) = 0 \\ \forall\delta\boldsymbol{\rho}(t) \end{cases} \tag{137}$$

is equivalent to the boundary-value problem (126)-(127).

PROOF

From definitions #1-4 it follows

$$\delta S_1(\boldsymbol{\rho}) = \int_{t_0}^{t_1} dt\delta\boldsymbol{\rho}(t)\cdot\left\{-\frac{d}{dt}\left(\frac{m}{2}\frac{T}{T_o}\dot{\boldsymbol{\rho}}\right) + \frac{T^2}{2T_o}\Big/\frac{\partial}{\partial\boldsymbol{\rho}}\ln f(\mathbf{R}(\boldsymbol{\rho},t)+\boldsymbol{\rho},t)\Big|_{\mathbf{R},t}\right\}; \tag{138}$$

Now we notice that by definition

$$\begin{aligned} \frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{r},t) &\equiv \frac{\partial}{\partial\mathbf{r}}\ln f(\mathbf{R}(\boldsymbol{\rho},t)+\boldsymbol{\rho},t) = \\ &= \frac{\partial}{\partial\boldsymbol{\rho}}\ln f(\mathbf{R}(\boldsymbol{\rho},t)+\boldsymbol{\rho},t)\Big|_{\mathbf{R},t}. \end{aligned} \tag{139}$$

Hence the Euler-Lagrange equations corresponding to the variational principle (137) manifestly coincide with Eq.(126), with $\boldsymbol{\rho}(t)$ to be considered subject to the same boundary conditions (127). Therefore Eqs.(137) and (126) are equivalent. Q.E.D.

THM.2 - Hamiltonian form of Eq.(126)

In validity of THM.1 there results:

a) (Proposition a-THM.2)

the boundary-value problem (126)-(127) admits the modified Hamilton principle

$$\begin{cases} \delta S_{1,H}(\mathbf{z}) = 0 \\ \forall\delta\boldsymbol{\rho}(t), \delta\mathbf{p}_\rho(t) \end{cases} \tag{140}$$

where $S_{1,H}(\mathbf{z})$ *is the Hamiltonian action*

$$S_{1,H}(\mathbf{z}) = \int_{t_0}^{t_1} dt\left[\dot{\boldsymbol{\rho}}(t)\cdot\mathbf{p}_\rho(t) - H(\mathbf{z}(t),t)\right] \tag{141}$$

and $H(\mathbf{z},t)$ the corresponding Hamiltonian function

$$H(\mathbf{z},t) = \frac{T_o}{4mT(t)}\mathbf{p}_\rho^2 - \frac{T^2(t)}{2T_o}\ln f(\mathbf{R}+\boldsymbol{\rho},t); /// \tag{142}$$

b) (Proposition b-THM.2)

the boundary-value problem (126)-(127) admits an Hamiltonian equations defined w.r. to the Hamiltonian (142) and the canonical state $\mathbf{z} = \left(\boldsymbol{\rho}, \mathbf{p}_\rho\right)$. Thus, equation (126) is equivalent to the canonical equations

$$\dot{\boldsymbol{\rho}} = \frac{\partial}{\partial \mathbf{p}_\rho} H(\mathbf{z},t), \tag{143}$$

$$\dot{\mathbf{p}}_\rho = -\frac{\partial}{\partial \boldsymbol{\rho}} H(\mathbf{z},t). \tag{144}$$

PROOF

The proof of Proposition a) is an obvious consequence of THM.1. In fact, the Lagrangian (132) manifestly regular, since by assumption $\frac{m}{4}\frac{T(t)}{T_o} > 0$. Therefore, the transformation $\left\{\boldsymbol{\rho}, \dot{\boldsymbol{\rho}}\right\} \to \{\boldsymbol{\rho}, \mathbf{p}_\rho\}$, with

$$\mathbf{p}_\rho = \frac{\partial L_1(\boldsymbol{\rho}, \dot{\boldsymbol{\rho}}, t)}{\partial \dot{\boldsymbol{\rho}}} = \frac{m}{2}\frac{T(t)}{T_o}\dot{\boldsymbol{\rho}}(t)$$

is a diffeomeorphism. Thus, Eq.(140) is the modified Hamilton variational principle corresponding to the Lagrangian variational principle (137). To prove Proposition b), let us invoke Eq.(142). It follows manifestly that Eqs.(**??**) yield Eq.(126). Q.E.D.

IV. COMPARISON BETWEEN IKT AND THE METHOD OF CONFIGURATION-SPACE CHARACTERISTICS

V. CONCLUSIONS

Motivated by the previous results, relevant for the mathematical investigation of the Schrödinger equation, which concern the discovery of an IKT for the Schrödinger equation, properties of the the underlying dynamical system (the Schrödinger dynamical system), have been investigated. We have found that, that a particular realization of the IKT can be achieved which permits by means its identification with an abstract Hamiltonian system. The present approach has the following main features:

1. the inverse kinetic equation (IKE) has been assumed to be a Vlasov-type kinetic equation, while its solution, i.e., the kinetic PDF, has been required *to be a Maxwelin distriubution endowed with a single kinetic temperature* T, with T required to depend only on time;

2. the IKT achieved in this way is complete, namely all fluid fields are expressed as moments of the kinetic distribution function, while all the hydrodynamic equations are identified with suitable moment equations of IKE.

3. the theory holds for arbitrary quantum fluid fields, i.e., arbitrary initial and boundary conditions for the quantum wave function, as well as arbitrary conservative (both quantum and classical) forces acting for the quantum system.

The result appears relevant for the fluid description of quantum mechanics and a deeper understanding of the underlying statistical (in particular, kinetic) descriptions.

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APPENDIX A: THE METHOD OF CONFIGURATION-SPACE CHARACTERISTICS

A.1 - Formulation for QHE's

As is well known [in the theory of PDE's] *the method of characteristics* is the classical approach to construct local solutions to nonlinear PDE's [for a presentation see Evans, 1988 [56][. This method can be used:

1) to define a Lagrangian representation of QHE's;

2) to cast a suitable subset of the same equations [represented by Eqs.(27) and (30)] in Hamiltonian form.

In particular, the method of characteristics is wellknown in the case of the Hamilton-Jacobi (HJ) equation, namely an equation of the form

$$\frac{\partial S(\mathbf{r},t)}{\partial t} + H(\mathbf{r},\nabla S,t) = 0, \tag{145}$$

where $H(\mathbf{r},\nabla S,t)$ denotes in principle an arbitrary smooth real function. Then, letting

$$\mathbf{p} \equiv \nabla S, \tag{146}$$

its *characteristics* $\mathbf{r}(t)$ are simply the solutions (i.e., the integral curves) of the coupled *Lagrangian equations*

$$\begin{aligned} \mathbf{r}' &= \frac{\partial H(\mathbf{r},\mathbf{p},t)}{\partial \mathbf{p}}, \\ \mathbf{p}' &= -\frac{\partial H(\mathbf{r},\mathbf{p},t)}{\partial \mathbf{r}}, \end{aligned} \tag{147}$$

for $\mathbf{r}(t)$, $\mathbf{p}(t)$, where, $\mathbf{r}'$ and $\mathbf{p}'$ denote suitable derivatives with respect to the variable t and the curves and $\mathbf{r}(t)$, $\mathbf{p}(t)$ satisfy the initial conditions

$$\begin{aligned} \mathbf{r}(t_o) &= \mathbf{r}_o, \\ \mathbf{p}(t_o) &= \mathbf{p}_o. \end{aligned} \tag{148}$$

In such a framework the approach can be extended in a straihtforward way to the quantum HJ equation [i.e., Eq.(166)], where the Hamiltonian H is now of the form

$$H \equiv H_c(\mathbf{r},\nabla S - \frac{q}{c}\mathbf{A},t), \tag{149}$$

simply by letting

$$\mathbf{p} \equiv \nabla S - \frac{q}{c}\mathbf{A},$$

and identifying the derivatives on the l.h.s. of Eqs.(147) with $\frac{D}{Dt}$, i.e., the fluid Lagrangian derivative defined above (28). As a consequence *Eq.(166) delivers the Hamilton equations*

$$\begin{aligned} \frac{D\mathbf{r}}{Dt} &= \frac{\partial H_c(\mathbf{r},\mathbf{p},t)}{\partial \mathbf{p}}, \\ \frac{D\mathbf{p}}{Dt} &= -\frac{\partial H_c(\mathbf{r},\mathbf{p},t)}{\partial \mathbf{r}}, \end{aligned} \tag{150}$$

with the initial conditions (148). These equations are manifestly equivalent to the set of non-canonical equations (27) and (30) expressed in the (non-canonical) variables $(\mathbf{r},\mathbf{V})$.

A.2 - Another form of the Hamiltonian characteristics

The previous equations can also be written in the alternative way in terms of the *kinetic Lagrangian derivative*

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \frac{1}{m}\mathbf{K}\cdot\frac{\partial}{\partial \mathbf{v}}. \tag{151}$$

In this case Eqs. (27) and (30) are replaced respectively by

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}, \tag{152}$$

$$\frac{d\mathbf{V}(\mathbf{r},t)}{dt} \equiv \frac{D\mathbf{V}(\mathbf{r},t)}{Dt} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{V}(\mathbf{r},t) = \frac{1}{m}\mathbf{F}(\mathbf{r},\mathbf{V},t) + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{V}(\mathbf{r},t), \tag{153}$$

where $\mathbf{v}$ and

$$\mathbf{u} = \mathbf{v} - \mathbf{V}(\mathbf{r},t) \tag{154}$$

denote the *kinetic* and *relative kinetic velocities*. Let us now introduce the Hamiltonian function

$$H_1(\mathbf{r},\mathbf{p},\mathbf{u}(t),t) = \frac{1}{2m}\left[\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t) + U_{QM}(\mathbf{r},t) + \mathbf{u}(t)\cdot\left[m\mathbf{V}(\mathbf{r}(t),t) + \frac{q}{c}\mathbf{A}(\mathbf{r}(t),t)\right]. \tag{155}$$

In this case there follows:

THM.3 - Hamiltonian form of QHE

The Hamiltonian equations corresponding to Eqs.(150) read

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \equiv \frac{\partial H_1(\mathbf{r},\mathbf{p},\mathbf{u}(t),t)}{\partial \mathbf{p}}, \tag{156}$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H_1(\mathbf{r},\mathbf{p},\mathbf{u}(t),t)}{\partial \mathbf{r}}. \tag{157}$$

PROOF
The proof follows by invoking the Hamiltonian (155). Q.E.D.

A.3 - Time-evolution of the fluid fields

Let us show, finally, that the the classical Hamiltonian dynamical system generated by Eqs.(**??**),namely the bijection

$$\mathbf{x}_o \to \mathbf{x}(t) = [\mathbf{r}(t), \mathbf{P}(\mathbf{r}(t),t)] \equiv T_{t_o,t}\mathbf{x}_o \tag{158}$$

[with $T_{t_o,t}$ prescribed by Eqs.(**??**) and (**??**)] *uniquely determines the time evolution of the fluid fields* $\{f(\mathbf{r},t), \mathbf{V}(\mathbf{r},t)\}$.
To prove the statement, let us introduce the Liouville equation

$$Lg(\mathbf{x},t) = 0, \tag{159}$$

where L is the Liouville operator

$$L = \frac{\partial}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla} + \frac{\partial}{\partial \mathbf{v}}\cdot\{\mathbf{K}(\mathbf{x},t)\} \tag{160}$$

and the KDF is prescribed so that there results identically

$$f(\mathbf{r},t) = \int_{\mathbb{R}^3} d^3\mathbf{v}\, g(\mathbf{x},t) \tag{161}$$

$$\mathbf{V}(\mathbf{r},t) = \int_{\mathbb{R}^3} d^3\mathbf{v}\mathbf{v}\, g(\mathbf{x},t). \tag{162}$$

As a consequence the corresponding moment equation of Eq.(159) necessarily must coincide respectively with Eqs.(165) and (**??**). Since Eq.(159) can be written in the equivalent integral form

$$g(\mathbf{x}(t),t)=\frac{1}{J(\mathbf{x}(t),t)}g(\mathbf{x}_o,t_o),$$

where

$$J(\mathbf{x}(t),t)=\left|\frac{\partial\mathbf{x}(t)}{\partial\mathbf{x}_o}\right|,$$

while Eqs (161) and (162) hold identically by assumption, it follows that $g(\mathbf{x}(t),t)$ determines the fluid fields at time t [while the initial fluid fields are prescribed by $g(\mathbf{x}_o,t_o)$]. Hence the Liouville equation (159) actually advances in time also the fluid fields.

Then, it is immediate to prove that a particular solution $\{\mathbf{K}(\mathbf{x},t),g(\mathbf{x},t)\}$ is delivered by

$$\begin{cases}\mathbf{K}(\mathbf{x},t)=\frac{1}{m}\mathbf{F}(\mathbf{x},t),\\ g(\mathbf{x},t)=\delta\left(\mathbf{v}-\mathbf{V}(\mathbf{r},t)\right).\end{cases}$$

APPENDICE: VERIFICA QHE'S

Let us derive explicitly the complete set of PDE's, to be fulfilled by a suitable set of fluid fields $\{Z\}$, which correspond to the Schrödinger equation. Invoking the position (12) there follows

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi &= \psi\left[\frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f-\frac{\partial}{\partial t}S\right],\\
\frac{1}{2m}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}\right)^2\psi &= \frac{1}{2m}\left(-i\hbar\nabla-\frac{q}{c}\mathbf{A}\right)\cdot\psi\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S-\frac{q}{c}\mathbf{A}\right]=\\
&= \frac{\psi}{2m}\left[-\frac{\hbar^2}{2}\nabla^2\ln f-i\hbar\nabla^2S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]+\\
&\quad+\frac{\psi q}{2mc}\left[\frac{i\hbar}{2}\mathbf{A}\cdot\nabla\ln f-\mathbf{A}\cdot\nabla S+\frac{q}{c}\left|\mathbf{A}\right|^2\right]+\\
&\quad+\frac{\psi}{2m}\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\left[-\frac{i\hbar}{2}\nabla\ln f+\nabla S\right].
\end{aligned}$$

Hence the imaginary part of the equation yields

$$\begin{aligned}
\frac{i\hbar}{2}\frac{\partial}{\partial t}\ln f &= \frac{1}{2m}\left[-i\hbar\nabla^2S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]+\frac{q}{2mc}\frac{i\hbar}{2}\mathbf{A}\cdot\nabla\ln f+\\
&\quad-\frac{1}{2m}\frac{i\hbar}{2}\nabla\ln f\cdot\nabla S-\frac{1}{2m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\frac{i\hbar}{2}\nabla\ln f=\\
&= \frac{1}{2m}\left[-i\hbar\nabla^2S+\frac{q}{c}i\hbar\nabla\cdot\mathbf{A}\right]-\frac{i\hbar}{2m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\nabla\ln f
\end{aligned}$$

namely

$$\frac{\partial}{\partial t}\ln f+\frac{1}{m}\left[\nabla S-\frac{q}{c}\mathbf{A}\right]\cdot\nabla\ln f+\frac{1}{m}\nabla^2S=\frac{q}{mc}\nabla\cdot\mathbf{A}. \tag{163}$$

Imposing the Coulomb gauge $\nabla\cdot\mathbf{A}=0$ and introducing the (quantum) fluid velocity field $\mathbf{V}=\mathbf{V}(\mathbf{r},t)$:

$$\mathbf{V}=\frac{1}{m}\left(\nabla S-\frac{q}{c}\mathbf{A}\right), \tag{164}$$

one obtains the countinuity equation:

$$\frac{\partial}{\partial t}\ln f+\mathbf{V}\cdot\nabla\ln f+\nabla\cdot\mathbf{V}=0. \tag{165}$$

Similarly the real part of the equation delivers the *quantum Hamilton-Jacobi equation*:

$$\frac{\partial}{\partial t}S + H_c(\mathbf{r},\nabla S - \frac{q}{c}\mathbf{A},t) = 0, \tag{166}$$

where $H_c(\mathbf{r},\nabla S - \frac{q}{c}\mathbf{A},t)$ is the Hamiltonian function

$$H_c(\mathbf{r},\nabla S - \frac{q}{c}\mathbf{A},t) = \frac{1}{2m}\left(\nabla S - \frac{q}{c}\mathbf{A}\right)^2 + U_{QM} + q\phi. \tag{167}$$

Moreover, here U_{QM} denotes the so-called *free-particle quantum potential* [8]

$$U_{QM} = \frac{\hbar^2}{2}\left(\frac{1}{2}\nabla^2 \ln f + \frac{1}{4}\left|\nabla \ln f\right|^2\right). \tag{168}$$

Applying the operator $(\frac{1}{m}\nabla)$ to the previous equation and introducing the position (164) there follows

$$\frac{\partial}{\partial t}\mathbf{V} + \frac{1}{2m^2}\nabla\left(\nabla S - \frac{q}{c}\mathbf{A}\right)^2 = -\frac{q}{mc}\frac{\partial}{\partial t}\mathbf{A} - \frac{1}{m}\nabla U_{QM} - \frac{1}{m}\nabla q\phi.$$

Now we notice that

$$\begin{aligned}\frac{1}{2m^2}\nabla\left(\nabla S - \frac{q}{c}\mathbf{A}\right)^2 &= \frac{1}{m^2}\left(\nabla S - \frac{q}{c}\mathbf{A}\right)\cdot\nabla\left(\nabla S - \frac{q}{c}\mathbf{A}\right) + \frac{1}{m^2}\left(\nabla S - \frac{q}{c}\mathbf{A}\right)\times\left[\nabla\times\left(\nabla S - \frac{q}{c}\mathbf{A}\right)\right] = \\ &= \mathbf{V}\cdot\nabla\mathbf{V} - \frac{q}{mc}\mathbf{V}\times[\nabla\times\mathbf{A}] = \mathbf{V}\cdot\nabla\mathbf{V} - \frac{q}{mc}\mathbf{V}\times\mathbf{B}.\end{aligned}$$

Hence it follows the *quantum Euler equation*:

$$\frac{\partial}{\partial t}\mathbf{V} + \mathbf{V}\cdot\boldsymbol{\nabla}\mathbf{V} = \frac{1}{m}\mathbf{F}(\mathbf{r},t), \tag{169}$$

where $\mathbf{F}(\mathbf{r},t)$ (*quantum force-field*) is the vector field

$$\mathbf{F}(\mathbf{r},t) \equiv q\left\{\mathbf{E} + \frac{1}{c}\mathbf{V}\times\mathbf{B}\right\} - \nabla U_{QM} \tag{170}$$

and

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\mathbf{A} \tag{171}$$

$$\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A} \tag{172}$$

are the EM fields.

The PDE's (165) and (169) are denoted *quantum hydrodynamic equations* (QHE's) and $\{Z\} \equiv \{f, \mathbf{V}\}$ as corresponding *quantum fliid fields*.

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