

# Mapping of the classical kinetic balance equations onto the Schrödinger equation

Adriana I Pesci<sup>1</sup> and Raymond E Goldstein<sup>1,2</sup>

<sup>1</sup> Department of Physics, University of Arizona, Tucson, AZ 85721, USA

<sup>2</sup> Program in Applied Mathematics, University of Arizona, Tucson, AZ 85721, USA

E-mail: pesci@physics.arizona.edu and gold@physics.arizona.edu

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## Abstract

Here we find a mapping onto the Sturm–Liouville operator of the first two balance equations derived from Boltzmann’s equation. This mapping, which is irreversible and valid only for a subclass of solutions, is achieved by applying a Fourier transform to the momentum coordinate. In light of this irreversibility, it is necessary to develop a set of consistent prescriptions to find the probability of any physical quantity in the  $\mathbf{p}$ -conjugate space such that it will coincide with the average over the momentum of the true probabilities obtained from the original Boltzmann equation. The one drawback of this prescription is that it is impossible to predict exactly the precise values of the position  $\mathbf{x}$  and the momentum  $\mathbf{p}$  at the same time. This uncertainty is limited by the relationship that all conjugate variables in a Fourier transform should obey, namely  $\Delta x \Delta p = \eta/2$ , where  $\eta$  is a free parameter of the theory. The prescriptions we have found appear to coincide with the postulates of quantum mechanics, when  $\eta$  is set equal to  $\hbar$ . This procedure seems to provide a statistical representation of quantum mechanics.

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## 1. Introduction

Since the work of Madelung [1], it has been known that the Schrödinger equation is equivalent to Euler’s equations for a fluid with an unusual form of the pressure. This hydrodynamic approach has been studied extensively [2, 3]. In general, the equations of motion of fluids have an underlying kinetic theory, so one might wonder whether this is also true for the case leading to Schrödinger’s equation. In this paper, we present a possible route to this connection.

It is well known that the motion of an ensemble of  $N$  classical particles is governed by Liouville's equation [4],

$$\frac{\partial D}{\partial t} = \{H, D\}, \quad (1)$$

where  $D$  represents the number density of points in phase space and  $H$  is the Hamiltonian of the  $N$ -particle system [5]. Calling  $\Omega$  the volume in phase space and

$$f_N(\mathbf{x}_1, \mathbf{p}_1, \dots, \mathbf{x}_N, \mathbf{p}_N) = \frac{D}{\int_{\Omega} D d\Omega} \quad (2)$$

we can then define for  $1 \leq j < N$  the following functions:

$$f_j(\mathbf{x}^j, \mathbf{p}^j) = \int_{\Omega} f_N(\mathbf{x}^N, \mathbf{p}^N) \prod_{l=j+1}^N d\mathbf{x}_l d\mathbf{p}_l, \quad (3)$$

where  $(\mathbf{x}^N, \mathbf{p}^N) = (\mathbf{x}_1, \mathbf{p}_1, \dots, \mathbf{x}_N, \mathbf{p}_N)$ . These functions are called the reduced probability distributions and correspond to the probability of finding the subsystem of  $j < N$  particles in the phase volume  $\prod_{l=1}^j d\mathbf{x}_l d\mathbf{p}_l$  about the state  $(\mathbf{x}_1, \mathbf{p}_1, \dots, \mathbf{x}_j, \mathbf{p}_j)$ . Using the reduced probability distributions it is possible to recast Liouville's equation as a set of  $N$  coupled nonlinear partial differential equations for the set of  $N$  functions  $\{f_j\}$ . These  $N$  equations are known as the BBKGY hierarchy [6], the first two terms of which (i.e. the equations for  $f_1$  and  $f_2$ ) determine the kinetic and potential energies of an aggregate of particles, and have a crucial role in fluid dynamics. Even though no exact solution to this hierarchy is known, it is possible to decouple the equations in certain cases when some ansatz about the properties of the probability functions is introduced. This decoupling provides us with what is known as the kinetic equations for the system.

One of the most important set of kinetic equations is the one obtained with the Bogoliubov ansatz [6]. This leads to the following equation for the one-particle reduced probability density  $f_1 = f_1(\mathbf{x}_1, \mathbf{p}_1, t)$ :

$$\frac{\partial f_1}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} - \frac{\partial V(\mathbf{x}_1)}{\partial \mathbf{x}_1} \cdot \frac{\partial f_1}{\partial \mathbf{p}_1} = 2\pi \int r_2 dr_2 g \int d\mathbf{p}_2 [f_1(\mathbf{p}'_1) f_1(\mathbf{p}'_2) - f_1(\mathbf{p}_1) f_1(\mathbf{p}_2)], \quad (4)$$

where  $V(\mathbf{x}_1)$  is the external potential averaged over all other spatial coordinates,  $g$  is the magnitude of the relative velocity defined as  $\mathbf{g} = (\mathbf{p}_2 - \mathbf{p}_1)/m$  and where we used  $d\mathbf{x}_2 = r_2 dr_2 d\phi dz$ . This is known as Boltzmann's equation. A well-known theorem states that the integral over  $\mathbf{p}_1$  of the collision integral multiplied by a function  $\varphi(\mathbf{p}_1)$  vanishes if  $\varphi$  satisfies  $\varphi_1 + \varphi_2 = \varphi_{1'} + \varphi_{2'}$ . Choosing  $\varphi = 1$ ,  $\varphi = \mathbf{p}_1$  or  $\varphi = \mathbf{p}_1^2$ , which clearly satisfy this condition, we obtain, respectively, the conservation laws for particle number, momentum and energy, which are necessary conditions for the physical validity of any kinetic equation [6]. Since the collision integral contributions vanish identically, the first two balance equations read

$$\int_{-\infty}^{+\infty} d\mathbf{p} \left( \frac{\partial f_1}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}} - \frac{\partial V(\mathbf{x})}{\partial \mathbf{x}} \cdot \frac{\partial f_1}{\partial \mathbf{p}} \right) = 0 \quad (5)$$

and

$$\int_{-\infty}^{+\infty} \mathbf{p} d\mathbf{p} \left( \frac{\partial f_1}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}} - \frac{\partial V(\mathbf{x})}{\partial \mathbf{x}} \cdot \frac{\partial f_1}{\partial \mathbf{p}} \right) = 0, \quad (6)$$

where we have dropped the subindex 1 from the coordinates  $\mathbf{x}_1$  and  $\mathbf{p}_1$ . Notice that the last term of the first equation vanishes, since it can be integrated to yield a surface term that will tend

to zero due to the convergence properties of  $f_1$ . In fact,  $-\int_{-\infty}^{+\infty} d\mathbf{p}(\partial V(\mathbf{x})/\partial \mathbf{x}) \cdot (\partial f_1/\partial \mathbf{p}) = -(\partial V(\mathbf{x})/\partial \mathbf{x}) \cdot \int_{-\infty}^{+\infty} d\mathbf{p}(\partial f_1/\partial \mathbf{p}) = -(\partial V(\mathbf{x})/\partial \mathbf{x}) \cdot f_1|_{-\infty}^{+\infty} \rightarrow 0$ . And in the last equation this same term can be integrated by parts to yield  $-\int_{-\infty}^{+\infty} d\mathbf{p} \mathbf{p}(\partial V(\mathbf{x})/\partial \mathbf{x}) \cdot (\partial f_1/\partial \mathbf{p}) = (\partial V(\mathbf{x})/\partial \mathbf{x}) \cdot \int_{-\infty}^{+\infty} d\mathbf{p} f_1$  where again we have used the fact that the surface terms vanish. It is not possible to calculate the average  $\langle \overleftrightarrow{\mathbf{p}\mathbf{p}} \rangle$  that appears in the second term of equation (6) without explicit knowledge of the distribution function  $f_1$ . This term defines the pressure tensor and is the only term that depends on the collision integral, through  $f_1$ . A standard method of calculation of  $f_1$  is the Chapman–Enskog expansion that perturbatively incorporates the collision integral. The zeroth order term yields the standard Euler equation of fluid dynamics with a diagonal pressure tensor, while the first correction yields the viscous terms of the Navier–Stokes equation.

## 2. Mapping

We now introduce into our two balance equations the following representation for  $f_1$ :

$$f_1(\mathbf{x}, \mathbf{p}, t) = \frac{1}{(2\pi\eta)^3} \int_{-\infty}^{+\infty} \exp\left(-i\frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) \hat{f}(\mathbf{x}, \mathbf{y}, t) d\mathbf{y}, \quad (7)$$

where  $\hat{f}(\mathbf{x}, \mathbf{y}, t)$  is, of course, given by

$$\hat{f}(\mathbf{x}, \mathbf{y}, t) = \int_{-\infty}^{+\infty} \exp\left(i\frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}. \quad (8)$$

With these definitions and after some straightforward algebra the balance equations can be written as

$$\frac{1}{(2\pi\eta)^3} \iint_{-\infty}^{+\infty} d\mathbf{p} d\mathbf{y} \exp\left(-i\frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) \left[ \frac{\partial \hat{f}}{\partial t} + \frac{\eta}{im} \frac{\partial}{\partial \mathbf{x}} \cdot \frac{\partial \hat{f}}{\partial \mathbf{y}} \right] = 0 \quad (9)$$

and

$$\begin{aligned} & \frac{1}{(2\pi\eta)^3} \iint_{-\infty}^{+\infty} d\mathbf{p} d\mathbf{y} \exp\left(-i\frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) \\ & \times \left[ \frac{\partial}{\partial t} \left( \frac{\eta}{i} \frac{\partial \hat{f}}{\partial \mathbf{y}} \right) - \frac{\eta^2}{m} \frac{\partial}{\partial \mathbf{x}} \cdot \left( \frac{\overleftrightarrow{\partial^2 \hat{f}}}{\partial \mathbf{y} \partial \mathbf{y}} \right) + \frac{\partial}{\partial \mathbf{y}} \left( \mathbf{y} \cdot \frac{\partial V}{\partial \mathbf{x}} \hat{f} \right) \right] = 0. \end{aligned} \quad (10)$$

Using the identity

$$\frac{\partial}{\partial \mathbf{y}} \left( \mathbf{y} \cdot \frac{\partial V}{\partial \mathbf{x}} \hat{f} \right) = \frac{\partial V}{\partial \mathbf{x}} \hat{f} + \mathbf{y} \cdot \frac{\partial}{\partial \mathbf{y}} \left( \frac{\partial V}{\partial \mathbf{x}} \hat{f} \right) \quad (11)$$

and after performing the  $\mathbf{p}$ -integrals that yield delta functions on  $\mathbf{y}$  we obtain:

$$\int_{-\infty}^{+\infty} d\mathbf{y} \delta(\mathbf{y}) \left[ \frac{\partial \hat{f}}{\partial t} + \frac{\eta}{im} \frac{\partial}{\partial \mathbf{x}} \cdot \frac{\partial \hat{f}}{\partial \mathbf{y}} \right] = 0 \quad (12)$$

and

$$\int_{-\infty}^{+\infty} d\mathbf{y} \delta(\mathbf{y}) \left[ \frac{\partial}{\partial t} \left( \frac{\eta}{i} \frac{\partial \hat{f}}{\partial \mathbf{y}} \right) - \frac{\eta^2}{m} \frac{\partial}{\partial \mathbf{x}} \cdot \left( \frac{\overleftrightarrow{\partial^2 \hat{f}}}{\partial \mathbf{y} \partial \mathbf{y}} \right) + \frac{\partial V}{\partial \mathbf{x}} \hat{f} + \mathcal{O}(\mathbf{y}) \right] = 0. \quad (13)$$

It is clear that the results of these integrals are given by the limit for  $\mathbf{y} \rightarrow 0$  of the integrands,

$$\lim_{\mathbf{y} \rightarrow 0} \left[ \frac{\partial \hat{f}}{\partial t} + \frac{\eta}{im} \frac{\partial}{\partial \mathbf{x}} \cdot \frac{\partial \hat{f}}{\partial \mathbf{y}} \right] = 0, \quad (14)$$

$$\lim_{\mathbf{y} \rightarrow 0} \left[ \frac{\partial}{\partial t} \left( \frac{\eta}{i} \frac{\partial \hat{f}}{\partial \mathbf{y}} \right) - \frac{\eta^2}{m} \frac{\partial}{\partial \mathbf{x}} \cdot \left( \frac{\overleftrightarrow{\partial^2 \hat{f}}}{\partial \mathbf{y} \partial \mathbf{y}} \right) + \frac{\partial V}{\partial \mathbf{x}} \hat{f} \right] = 0. \quad (15)$$

These limits are quite interesting since, except for multiplicative constants, they are identical to the limits that Fröhlich [7–9] encountered when deriving the equations of hydrodynamics from quantum mechanics in the reduced density matrix formalism. In continuing our analysis, we could follow his derivation exactly, but it is simpler and more intuitive to use the properties of  $\hat{f}$ . Notice that the first two limits necessary for the first balance equation correspond to the following averages:

$$\begin{aligned} \lim_{\mathbf{y} \rightarrow 0} \hat{f} &= \lim_{\mathbf{y} \rightarrow 0} \int_{-\infty}^{+\infty} \exp\left(i \frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} \\ &= \int_{-\infty}^{+\infty} f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} = \frac{\rho(\mathbf{x}, t)}{m}, \end{aligned} \quad (16)$$

$$\begin{aligned} \lim_{\mathbf{y} \rightarrow 0} \frac{\partial \hat{f}}{\partial \mathbf{y}} &= \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{y}} \int_{-\infty}^{+\infty} \exp\left(i \frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} \\ &= \frac{i}{\eta} \int_{-\infty}^{+\infty} \mathbf{p} f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} \\ &= \frac{i}{\eta} \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t), \end{aligned} \quad (17)$$

where we have defined the mean velocity  $\mathbf{u}$  as the average, over the momentum  $\mathbf{p}$  alone, of  $\mathbf{p}/m$ , where  $m$  is the mass. Replacing these values into the first balance equation it is straightforward to obtain the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \mathbf{u})}{\partial \mathbf{x}} = 0. \quad (18)$$

The second equation then transforms into

$$\frac{1}{m} \frac{\partial(\rho \mathbf{u})}{\partial t} - \frac{\eta^2}{m} \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{x}} \cdot \left( \frac{\overleftrightarrow{\partial^2 \hat{f}}}{\partial \mathbf{y} \partial \mathbf{y}} \right) + \frac{\rho}{m} \frac{\partial V}{\partial \mathbf{x}} = 0. \quad (19)$$

Now we are left with the not-so-simple task of evaluating the limit of the tensor in the second term. As in the discussion following equation (6), evaluation of this pressure tensor requires some knowledge of  $\hat{f}$ . This task is greatly simplified if we first study the symmetries of  $\hat{f}$  and any possible constraints that may arise from its equations of motion. To proceed, we turn our attention to equations (9) and (10). First, we integrate them over the variable  $\mathbf{x}$  and then make the canonical change of variables  $\mathbf{y} = \mathbf{x}' - \mathbf{x}''$  and  $\mathbf{x} = (\mathbf{x}' + \mathbf{x}'')/2$ , which satisfies

the following relationships:

$$\begin{aligned} \mathbf{x}' &= \mathbf{x} + \frac{\mathbf{y}}{2}, \\ \mathbf{x}'' &= \mathbf{x} - \frac{\mathbf{y}}{2}, \\ \frac{\partial}{\partial \mathbf{y}} &= \frac{1}{2} \left( \frac{\partial}{\partial \mathbf{x}'} - \frac{\partial}{\partial \mathbf{x}''} \right), \\ \frac{\partial}{\partial \mathbf{x}} &= \left( \frac{\partial}{\partial \mathbf{x}'} + \frac{\partial}{\partial \mathbf{x}''} \right). \end{aligned} \quad (20)$$

We can now rewrite the term with the potential  $V$  making use of the derivative by definition, the change of variables (20) and the fact that  $\lim_{\mathbf{y} \rightarrow 0} \equiv \lim_{\mathbf{x}' \rightarrow \mathbf{x}''}$

$$\begin{aligned} \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{y}} \left( \mathbf{y} \cdot \frac{\partial V}{\partial \mathbf{x}} \hat{f} \right) &= \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{y}} \left( \hat{f} \mathbf{y} \cdot \frac{V(\mathbf{x}') - V(\mathbf{x}'')}{(\mathbf{x}' - \mathbf{x}'')} \right) \\ &= \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{y}} \left( \hat{f} \mathbf{y} \cdot \frac{V(\mathbf{x} + \mathbf{y}/2) - V(\mathbf{x} - \mathbf{y}/2)}{\mathbf{y}} \right) \\ &= \lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial \mathbf{y}} \left( \hat{f} \left[ V\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) - V\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \right] \right) \\ &= \lim_{\mathbf{x}' \rightarrow \mathbf{x}''} \frac{1}{2} \left( \frac{\partial}{\partial \mathbf{x}'} - \frac{\partial}{\partial \mathbf{x}''} \right) (\hat{f} [V(\mathbf{x}') - V(\mathbf{x}'')]). \end{aligned} \quad (21)$$

After integrating over  $\mathbf{p}$  and  $\mathbf{x}'$ , and replacing (21) into (9) and (10) they become

$$\int d\mathbf{x}'' \lim_{\mathbf{x}' \rightarrow \mathbf{x}''} \left[ i\eta \frac{\partial \hat{f}}{\partial t} + \frac{\eta^2}{2m} \left( \frac{\partial^2 \hat{f}}{\partial \mathbf{x}^2} - \frac{\partial^2 \hat{f}}{\partial \mathbf{x}''^2} \right) \right] = 0 \quad (22)$$

and

$$\int d\mathbf{x}'' \lim_{\mathbf{x}' \rightarrow \mathbf{x}''} \frac{1}{2} \left( \frac{\partial}{\partial \mathbf{x}'} - \frac{\partial}{\partial \mathbf{x}''} \right) \left[ \frac{\eta}{i} \frac{\partial \hat{f}}{\partial t} - \frac{\eta^2}{2m} \left( \frac{\partial^2 \hat{f}}{\partial \mathbf{x}^2} - \frac{\partial^2 \hat{f}}{\partial \mathbf{x}''^2} \right) + (V(\mathbf{x}') - V(\mathbf{x}'')) \hat{f} \right] = 0. \quad (23)$$

Notice that in the limit  $\mathbf{y} \rightarrow 0$ , which corresponds to  $\mathbf{x}' \rightarrow \mathbf{x}''$ ,  $\mathbf{x}' = \mathbf{x}'' \equiv \mathbf{x}$ . The fact that the symmetries of  $\hat{f}$  can be obtained from the balance equations is the consequence of two important points. The first is that the main mechanism driving the equation is the nonlinearity arising from what will eventually become the convective derivative. If that nonlinearity were not present we would be left with nothing to study. Second, the Fourier transform has linearized the nonlinear term, making it separable in each variable, thus enhancing the intrinsic symmetries of the original equation. In fact, the left-hand side of Boltzmann's equation, even though highly nonlinear, presents a remarkable symmetry regarding the variables  $\mathbf{x}$  and  $\mathbf{p}$ ; it is clear that the left-hand side remains invariant under the exchange  $\mathbf{x} \leftrightarrow \mathbf{p}$ :

$$\frac{\partial f_1}{\partial t} + \frac{d\mathbf{x}}{dt} \cdot \frac{\partial f_1}{\partial \mathbf{x}} + \frac{d\mathbf{p}}{dt} \cdot \frac{\partial f_1}{\partial \mathbf{p}}. \quad (24)$$

This symmetry is most apparent in the new variables, and translates into the fact that equations (22) and (23) can be satisfied up to  $\mathcal{O}(\mathbf{y})$  by a function  $\hat{f}(\mathbf{x}', \mathbf{x}'', t)$  that has the property of being separable. Thus,

$$\hat{f}(\mathbf{x}', \mathbf{x}'', t) = h'(\mathbf{x}', t) h''(\mathbf{x}'', t). \quad (25)$$

We must point out that separable solutions correspond only to a subclass of solutions of the original equation. In fact, if the initial and/or boundary conditions of the problem to be

solved are not separable the solution will not be separable either. It is nonetheless instructive to consider the subset of separable solutions because it is *only* this subclass that leads to Schrödinger's equation<sup>3</sup>. Another important feature of the solutions to equations (22) and (23) is that regardless of its separability the limit  $\mathbf{y} \rightarrow 0$  of the function  $\hat{f}$  must be real since it coincides with the average over the momentum of the reduced probability function  $f_1$ ; this is the real quantity that we have labelled  $\rho/m$ . However, before the limit is taken  $\hat{f}(\mathbf{x}', \mathbf{x}'', t)$  is a complex function that can be written in terms of a magnitude  $\sigma$  and a phase shift  $e^{i\phi}$ . This phase must vanish in the limit  $\mathbf{y} \rightarrow 0$  so that  $\hat{f}$  will be real in this limit. Thus, we write  $\hat{f}$  as

$$\hat{f}(\mathbf{x}', \mathbf{x}'', t) = \sigma(\mathbf{x}', \mathbf{x}'', t) e^{i\phi(\mathbf{x}', \mathbf{x}'', t)}. \quad (26)$$

Replacing this expression for  $\hat{f}$  into our tensor we can write its  $k, l$ -component as

$$\lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial y_k} \frac{\partial}{\partial y_l} \hat{f}(\mathbf{x}', \mathbf{x}'', t) = \lim_{\mathbf{y} \rightarrow 0} e^{i\phi} \left[ \frac{\partial^2 \sigma}{\partial y_k \partial y_l} - \sigma \frac{\partial \phi}{\partial y_k} \frac{\partial \phi}{\partial y_l} + i \left( \frac{\partial \phi}{\partial y_l} \frac{\partial \sigma}{\partial y_k} + \frac{\partial \phi}{\partial y_k} \frac{\partial \sigma}{\partial y_l} + \sigma \frac{\partial^2 \phi}{\partial y_k \partial y_l} \right) \right]. \quad (27)$$

As we pointed out before, the imaginary part of this expression must vanish. This will constrain  $\sigma$  and  $\phi$  to be functions with given symmetries: first,  $(\partial^2 \phi / \partial y_k \partial y_l)$  must vanish. This requirement is satisfied if  $\phi(\mathbf{x}', \mathbf{x}'', t) = -\phi(\mathbf{x}'', \mathbf{x}', t)$ , i.e.  $\phi$  is antisymmetric in the variables  $\mathbf{x}'$  and  $\mathbf{x}''$ . And second, since the first derivative of  $\phi$  will not vanish due to the fact that  $\phi$  is antisymmetric, the remaining terms will vanish if  $(\partial \sigma / \partial y_n)$  vanishes for  $n = k, l$ . This condition is satisfied if we require that  $\sigma(\mathbf{x}', \mathbf{x}'', t) = \sigma(\mathbf{x}'', \mathbf{x}', t)$ , i.e.  $\sigma$  is symmetric in the variables  $\mathbf{x}'$  and  $\mathbf{x}''$ . Due to these symmetry conditions we can immediately determine the value of  $(\partial \phi / \partial y_k)$  for any  $k$ . Since  $\lim_{\mathbf{y} \rightarrow 0} (\partial \hat{f} / \partial y_k) = \lim_{\mathbf{y} \rightarrow 0} e^{i\phi} [(\partial \sigma / \partial y_k) + i\sigma (\partial \phi / \partial y_k)]$  and  $\lim_{\mathbf{y} \rightarrow 0} (\partial \sigma / \partial y_k) = 0$  by symmetry, then

$$\lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial y_k} \hat{f}(\mathbf{x}', \mathbf{x}'', t) = \lim_{\mathbf{y} \rightarrow 0} i\sigma \frac{\partial \phi}{\partial y_k} = \frac{1}{\eta} m u_k \quad (28)$$

and, thus,

$$\lim_{\mathbf{y} \rightarrow 0} \frac{\partial}{\partial y_k} \frac{\partial}{\partial y_l} \hat{f}(\mathbf{x}', \mathbf{x}'', t) = -\frac{1}{\eta^2} m \rho u_k u_l + \lim_{\mathbf{y} \rightarrow 0} \frac{\partial^2 \sigma}{\partial y_k \partial y_l}, \quad (29)$$

where  $u_k$  and  $u_l$  are the  $k$  and  $l$  components of the average velocity  $\mathbf{u}(\mathbf{x}, t)$ . Finally, we can write the remainder of our tensor using the separability property. We can write  $\sigma$  as a product of two functions  $g_1(\mathbf{x}', t)$  and  $g_2(\mathbf{x}'', t)$ . Since  $\sigma$  must also be symmetric,  $g_1$  and  $g_2$  must be equal up to a multiplicative constant that can be normalized, so we can set, in the limit  $\mathbf{y} \rightarrow 0$ ,  $g_1(\mathbf{x}, t) = g_2(\mathbf{x}, t) = g(\mathbf{x}, t)$ . When these results are substituted into (29) we obtain

$$\begin{aligned} \lim_{\mathbf{y} \rightarrow 0} \frac{\partial^2 \sigma}{\partial y_k \partial y_l} &= \frac{g^2}{4} \left[ \frac{2}{mg} \frac{\partial^2 (mg)}{\partial x_k \partial x_l} - \frac{2}{(mg)^2} \frac{\partial (mg)}{\partial x_k} \frac{\partial (mg)}{\partial x_l} \right] \\ &= \frac{1}{4m} \rho(\mathbf{x}, t) \frac{\partial^2 \ln \rho(\mathbf{x}, t)}{\partial x_k \partial x_l}, \end{aligned} \quad (30)$$

where we have used

$$\lim_{\mathbf{y} \rightarrow 0} \hat{f} = \lim_{\mathbf{y} \rightarrow 0} \sigma e^{i\phi} = \lim_{\mathbf{y} \rightarrow 0} \sigma = \frac{\rho(\mathbf{x}, t)}{m} \quad (31)$$

<sup>3</sup> We find Feynman's description (1951 *Phys. Rev.* **84** 108) of his own work quite applicable here. 'The mathematics is not completely satisfactory. No attempt has been made to maintain mathematical rigor. The excuse is not that it is expected that rigorous demonstrations can be easily supplied. Quite the contrary, it is believed that to put the present methods on a rigorous basis may be quite a difficult task, beyond the abilities of the author.'

in keeping with the definition introduced in equation (16). We should point out that this tensor was first derived by Kaniadakis [3] in a different context. Finally, our two balance equations in Fourier space read:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (32)$$

and

$$\frac{\partial}{\partial t}(m\rho\mathbf{u}) + \nabla \cdot \left[ \rho \left( m\mathbf{u}\mathbf{u} - \frac{\eta^2}{4m} \frac{\overleftrightarrow{\partial^2 \ln \rho}}{\partial \mathbf{x} \partial \mathbf{x}} \right) \right] + \rho \nabla V = 0, \quad (33)$$

where  $\nabla \equiv \partial/\partial \mathbf{x}$ . It is interesting to notice that the only difference between this pair of balance equations and the ones obtained with the usual method of averaging without Fourier transforming is the presence of the Kaniadakis tensor instead of an arbitrary pressure tensor. From this point on, finishing the mapping onto the Sturm–Liouville operator is a task whose individual parts have been done many times before. For completeness, we will summarize the main steps of the mapping closely following Kaniadakis [3].

First, the pair of equations we found is transformed into the standard form of Euler's equations for a non-viscous fluid with an unusual pressure tensor by using the continuity equation to eliminate the time derivative of  $\rho$ . This yields the result

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \frac{\eta^2}{4m^2 \rho} \nabla \cdot \left( \rho \frac{\overleftrightarrow{\partial^2 \ln \rho}}{\partial \mathbf{x} \partial \mathbf{x}} \right) + \frac{1}{m} \nabla V = 0. \quad (34)$$

When we compare this equation to the standard Euler equation we notice that the pressure has become the term proportional to  $\eta^2$  (recall that the pressure is related to the standard deviation of the velocity) and that its very particular form is a direct consequence of having assumed separability for  $\hat{f}$ . Once we have rewritten our equations in the standard form, we use the notation  $Q = \ln \rho$  and the classical definition of the action  $S$  in terms of the momentum in the Hamilton–Jacobi formalism;  $\tilde{\mathbf{p}} = \nabla S$ . Since we are working in Cartesian coordinates  $\tilde{\mathbf{p}} = m\mathbf{u}$ . Substituting this into our two balance equations, after considerable algebra we find

$$\frac{\partial Q}{\partial t} + \frac{1}{m} \nabla S \cdot \nabla Q + \frac{1}{m} \nabla^2 S = 0 \quad (35)$$

and

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 - \frac{\eta^2}{4m} \left( \nabla^2 Q + \frac{1}{2} (\nabla Q)^2 \right) + V = 0. \quad (36)$$

Then, multiplying the first equation by  $\frac{1}{2}$ , the second by  $\eta/i$ , and adding them we can write [1,2]

$$\frac{\eta}{i} \frac{\partial Z}{\partial t} = \frac{\eta^2}{2m} (\nabla^2 Z + (\nabla Z)^2), \quad (37)$$

where we have defined  $Z = (Q/2) + (\eta/i)S$ . Finally, we perform a standard Hopf–Cole transformation  $Z = \ln \Psi$  to obtain the Sturm–Liouville operator:

$$-\frac{\eta^2}{2m} \nabla^2 \Psi + V(\mathbf{x})\Psi = i\eta \frac{\partial \Psi}{\partial t}. \quad (38)$$

At this point, we can solve this equation for a given potential and in principle we would have the reduced one-particle probability in  $\mathbf{p}$ -conjugate space from the fact that

$$\rho(\mathbf{x}, t) = |\Psi(\mathbf{x}, t)|^2 = \Psi(\mathbf{x}, t)\Psi^*(\mathbf{x}, t), \quad (39)$$

where the asterisk indicates the complex conjugate. This seems to be a simple enough task, however as we mentioned before the mapping is irreversible; we cannot recover  $f_1(\mathbf{x}, \mathbf{p}, t)$ . In fact, the closest approximation to the original reduced probability distribution that can be constructed looks rather similar to the Wigner function [10] of quantum mechanics:

$$\begin{aligned} f_1^{(W)}(\mathbf{x}, \mathbf{p}, t) &= \frac{1}{(2\pi\eta)^3} \int_{-\infty}^{+\infty} e^{-i(\mathbf{p}\cdot\mathbf{y})/\eta} \hat{f}(\mathbf{x}, \mathbf{y}, t) d\mathbf{y} \\ &= \frac{1}{(2\pi\eta)^3} \int_{-\infty}^{+\infty} e^{-i(\mathbf{p}\cdot\mathbf{y})/\eta} \Psi\left(\mathbf{x} + \frac{1}{2}\mathbf{y}, t\right) \Psi^*\left(\mathbf{x} - \frac{1}{2}\mathbf{y}, t\right) d\mathbf{y}. \end{aligned} \quad (40)$$

This function will give the correct probability as a function of  $\mathbf{x}$  when integrated over  $\mathbf{p}$  and will give the correct probability as a function of  $\mathbf{p}$  when integrated over  $\mathbf{x}$  but, clearly, it is not equal to the true reduced probability density  $f_1$ . In fact, as well known from discussions of the Wigner function,  $f_1^{(W)}$  may even become negative for some values of the variables. This discrepancy is due to the fact that  $\hat{f}$  has been constructed using *only* information given by the first two kinetic equations, without any input from the others. To have all the information necessary to reconstruct  $f_1$  fully, it would be necessary to know every single moment (of the infinitely many) of the Boltzmann equations. To claim that anti-transforming the  $\hat{f}$  we found retains any resemblance with the full probability  $f_1$  would be similar to claiming that the polynomial built with the first two coefficients of the Taylor expansion of a function would be equivalent to the said function everywhere. On the other hand, since we have the exact value of the function  $\hat{f}$  for  $\mathbf{y} \rightarrow 0$ , it is correct to say that the probabilities obtained in this limit are the same as the ones in the original problem in that particular case. Thus, since we cannot retrieve  $f_1$  completely, we are unfortunately confined to make all our calculations in the  $\mathbf{p}$ -conjugate space. This can only be done if we find a way to evaluate the averages we need and recover as much information as possible without undoing the mapping.

We continue by studying some of the features of the transformations we used. Examining (36) we are tempted to think that setting  $\eta = 0$  would give us the Hamilton–Jacobi equation for a single particle. However, this would leave the role of equation (35) unexplained. Since our original starting point was an ensemble of classical particles, equation (36) can only be viewed as the equation of motion of the velocity potential of this ensemble. Another issue that comes to mind is the fact that we have performed several integrations by parts involving the function  $\hat{f}$ . In each one of these integrations we assumed that  $\lim_{\mathbf{x} \rightarrow \pm L} \hat{f} \rightarrow 0$  for  $L \rightarrow \pm\infty$  so that the surface integrals would vanish. Were this not the case the mapping would be rendered invalid. This is almost never a problem since this property can be fulfilled for most cases by imposing the appropriate boundary conditions on  $\Psi$ . A notable exception to this is the case of zero external potential (i.e.  $V(\mathbf{x}) = 0$ ), since  $\Psi$  cannot be made to vanish as  $L \rightarrow \pm\infty$ . It is possible in some very special cases to salvage the situation if only the averages are of interest. Then we need to confine our transform to integration between  $(-L, +L)$  and, only at the end of the calculation, after the averages were calculated, take the limit  $L \rightarrow \infty$ .

Another interesting feature of this mapping has already been pointed out by others [3], but is nonetheless worthwhile to review. The last transformation, known as Hopf–Cole, involves the logarithm of a complex function

$$Z = \frac{\ln \rho}{2} + \frac{\eta}{i} S = \ln \Psi. \quad (41)$$

This is not a single valued transformation, since  $\ln \Psi = \ln |\Psi| + i(\theta_0 + 2l\pi)$ , where  $l$  is an integer. This puts some restrictions on  $S$  and hence on  $\mathbf{u}$  since we defined previously  $\mathbf{u} = (1/m)\nabla S$ . As pointed out by Kaniadakis the consequence of introducing the complex variable  $\Psi$  is that



the velocity  $\mathbf{u}$  and hence its associated momentum defined as  $\tilde{\mathbf{p}} = m\mathbf{u}$  must satisfy the condition

$$\Delta S = \oint \tilde{\mathbf{p}} \, d\mathbf{x} = 2\pi n\eta, \quad (42)$$

where  $n$  is an integer.

Finally, we will derive the prescription to evaluate the averages in the  $\mathbf{p}$ -conjugate space. Since we have not changed the meaning of the variable  $\mathbf{x}$  anywhere in the calculation (recall that in the limit  $\mathbf{y} \rightarrow 0$  not only  $\mathbf{x}' = \mathbf{x}''$ , but also they are both equal to  $\mathbf{x}$ ), it is clear how to compute the averages for physical quantities that only depend on the position  $\mathbf{x}$ :

$$\begin{aligned} \langle \mathbf{x}^n \rangle &= \frac{\int \mathbf{x}^n f_1(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{x} \, d\mathbf{p}}{\int f_1(\mathbf{x}, \mathbf{p}, t) \, d\mathbf{p} \, d\mathbf{x}} \\ &= \frac{\int \mathbf{x}^n (\lim_{\mathbf{y} \rightarrow 0} m \hat{f}) \, d\mathbf{x}}{\int (\lim_{\mathbf{y} \rightarrow 0} m \hat{f}) \, d\mathbf{x}} \\ &= \frac{\int \Psi \mathbf{x}^n \Psi^* \, d\mathbf{x}}{\int \Psi \Psi^* \, d\mathbf{x}}. \end{aligned} \quad (43)$$

However this is not the case for those quantities that depend on the momentum  $\mathbf{p}$ . It is possible to show (see appendix A) that the average of an integer power of the momentum  $\mathbf{p}$  is given by

$$\langle \mathbf{p}^n \rangle = \frac{\int \Psi^* (-i\eta \nabla)^n \Psi \, d\mathbf{x}}{\int \Psi \Psi^* \, d\mathbf{x}}. \quad (44)$$

Notice that this is the true momentum  $\mathbf{p}$  from the original Boltzmann equation and *not* the momentum  $\tilde{\mathbf{p}} = m\mathbf{u}$  that we defined above. In fact,  $\tilde{\mathbf{p}}(\mathbf{x}, t)$  is the value of  $\mathbf{p}$  after the Fourier transform and the average in the original variable  $\mathbf{p}$  has already been performed. It is true, however, that  $\langle \mathbf{p} \rangle = \langle \tilde{\mathbf{p}} \rangle$ .

By making use of expression (44) it is possible to prove that the average of a physical quantity  $A(\mathbf{x}, \mathbf{p}, t)$  is given by (see appendix A)

$$\langle A \rangle = \frac{\int \Psi^* \hat{A}(\mathbf{x}, \mathbf{p}_F, t) \Psi \, d\mathbf{x}}{\int \Psi \Psi^* \, d\mathbf{x}}, \quad (45)$$

where we have defined the operator  $\mathbf{p}_F = -i\eta \nabla$  to represent the resulting momentum in Fourier space after the average over all possible momenta has been done.

An interesting issue that we wish to address relates to the relative importance of each of the terms in equation (34) because this is the determining factor in the applicability of perturbative methods. The easiest way to determine the relative order of each term is by a rescaling of the variables so that the equation becomes dimensionless. We introduce the following rescalings:

$$\begin{aligned} \nabla &= \frac{1}{Y} \tilde{\nabla}, & V &= V_0 \tilde{V}, \\ \mathbf{u} &= U_0 \tilde{\mathbf{u}}, & t &= \frac{Y}{U_0} \tilde{t}, \\ \rho &= \frac{1}{Y^3} \tilde{\rho}, & \mathbf{x} &= Y \tilde{\mathbf{x}}, \end{aligned} \quad (46)$$

where  $Y$ ,  $V_0$  and  $U_0$  are the characteristic length, potential and velocity, respectively. Introducing this rescaling into equation (34) we obtain

$$\left( \frac{mU_0^2}{V_0} \right) \left[ \frac{\partial \tilde{\mathbf{u}}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\mathbf{u}} \right] - \frac{\eta^2}{4mV_0Y^2\tilde{\rho}} \tilde{\nabla} \cdot \left( \tilde{\rho} \frac{\overleftrightarrow{\partial^2 \ln \tilde{\rho}}}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right) + \tilde{\nabla} \tilde{V}(\tilde{\mathbf{x}}) = 0. \quad (47)$$

When the characteristic kinetic and potential energies are of the same order (i.e.  $(mU_0^2/V_0) \simeq 1$ ) we can define the following dimensionless quantity, the Shelley number:

$$Sh = \frac{\eta}{2(mV_0)^{1/2}Y} = \frac{\eta}{2P_0Y}, \quad (48)$$

where  $P_0$  is a characteristic momentum. Then we can rewrite (48) as

$$\left[ \frac{\partial \tilde{\mathbf{u}}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\mathbf{u}} \right] - (Sh)^2 \frac{1}{\tilde{\rho}} \tilde{\nabla} \cdot \left( \tilde{\rho} \frac{\overleftrightarrow{\partial^2 \ln \tilde{\rho}}}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right) + \tilde{\nabla} \tilde{V}(\tilde{\mathbf{x}}) = 0. \quad (49)$$

Since the term proportional to  $Sh^2$  is the highest derivative in the equation of motion, any perturbation scheme will be singular. This equation strongly suggests the existence of a boundary layer where the small value of the Shelley number is counterbalanced by a large value of the highest derivative. In general, it will be necessary to use matched asymptotic techniques to obtain an adequate solution valid everywhere. Moreover, if we first set  $Sh = 0$  and find the solution afterwards, the results obtained will not be able to represent faithfully the true behaviour of the full solution in the limit  $Sh \rightarrow 0$ . This singular behaviour is hardly surprising since the limit  $Sh \rightarrow 0$  corresponds to the limit  $\mathbf{y} \rightarrow 0$  and  $\eta \rightarrow 0$  in the Fourier transforms (7), (8), obviously a quite singular limit. A last interesting detail is that, as clearly can be observed from the way in which  $Sh$  appears in the equation of motion, most perturbative schemes will only produce even powers of the parameter  $\eta$ .

One last important point relates to Frölich's derivation of the equations of hydrodynamics in the reduced density matrix formalism. In his case, the starting point for the derivation was the equation of motion for the first-order quantum reduced probability function known as the first-order reduced density matrix, which is constructed from the wave functions, solutions of the time dependent Schrödinger equation. The equations that Frölich obtains in the particular case of isotropic ideal fluids are identical to (18) and (19) when replacing  $\eta = \hbar$ . Since the tensor Frölich derived operates on a function that naturally has the symmetries required to ultimately yield the Kaniadakis tensor, it is clear that an aggregate of quantum particles will evolve according to a Sturm–Liouville operator, which in this case corresponds exactly to the time dependent Schrödinger equation since the constant  $\eta$  is  $\hbar$  in Frölich's case. This clearly means that aggregates of quantum particles behave like quantum objects themselves, as is well known in superfluids, superconductors, etc.

### 3. Conclusions

Using Boltzmann's equation obtained through the Bogoliubov ansatz applied to the BBKGY hierarchy, we connected the equation of motion of an ensemble of  $N$  classical particles to the Sturm–Liouville operator. The main consequences of such a mapping, achieved by taking a limit to the Fourier transform on  $\mathbf{p}$  of the Boltzmann equation, are

- (1) The new equation of motion in  $\mathbf{p}$ -conjugate space is

$$-\frac{\eta^2}{2m} \nabla^2 \Psi + V(\mathbf{x}) \Psi = i\eta \frac{\partial \Psi}{\partial t} \quad (50)$$

and the probability in  $\mathbf{p}$ -conjugate space is a function of  $\mathbf{x}$  only, given by  $\rho(\mathbf{x}, t) = \Psi(\mathbf{x}, t) \Psi^*(\mathbf{x}, t)$ , where  $\Psi(\mathbf{x}, t)$  is a solution of the equation of motion (50) and  $\Psi^*(\mathbf{x}, t)$  its conjugate.

(2) The average of any physical quantity  $A(\mathbf{x}, \mathbf{p}; t)$  in the original problem can be found by calculating

$$\langle A(\mathbf{x}, \mathbf{p}; t) \rangle = \frac{\int_{-\infty}^{+\infty} d\mathbf{x} \Psi^* \hat{A}(\mathbf{x}, \mathbf{p}_F; t) \Psi}{\int \Psi \Psi^* d\mathbf{x}}. \quad (51)$$

where  $\mathbf{p}_F = -i\eta \nabla$ .

Notice that an immediate consequence of the definition for  $\mathbf{p}_F$  is that the equation of motion can be written as

$$\left[ \frac{\mathbf{p}_F^2}{2m} + V(\mathbf{x}) \right] \Psi = i\eta \frac{\partial \Psi}{\partial t}. \quad (52)$$

The term in square brackets in (52) corresponds to the energy stored in the streamline described by equation (34). Thus, we can define  $E_F = \mathbf{p}_F^2/2m + V(\mathbf{x})$ . With this definition and using (52) we can establish the correspondence  $E_F = i\eta(\partial/\partial t)$ .

(3) We have lost the ability to recover  $f_1(\mathbf{x}, \mathbf{p}, t)$ . This precludes us from predicting values of  $\mathbf{p}$  when in conjugate space. Due to the intrinsic properties of the Fourier transform with regard to conjugate variables the following relationship must hold:

$$\Delta p \Delta x = \frac{\eta}{2}, \quad (53)$$

where  $\Delta p$  and  $\Delta x$  represent the standard deviations of  $\mathbf{p}$  and  $\mathbf{x}$ , respectively.

Notice that by substituting  $\eta = \hbar$  the rules we have derived read like the postulates of quantum mechanics.

In closing, we would also like to point out the wonderful coincidence of having started with an equation due to a theorem proven by Joseph Liouville in 1838, and having transformed it into a linear differential equation whose properties and solvability conditions were finally understood thanks to Jacques Sturm and Joseph Liouville himself.

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## Appendix A

To prove equation (44) we begin by expressing the average of  $\mathbf{p}$  in terms of  $\hat{f}$ ,

$$\begin{aligned} \lim_{y \rightarrow 0} \frac{\partial^n \hat{f}}{\partial \mathbf{y}^n} &= \lim_{y \rightarrow 0} \frac{\partial^n}{\partial \mathbf{y}^n} \int_{-\infty}^{+\infty} \exp\left(i \frac{\mathbf{p} \cdot \mathbf{y}}{\eta}\right) f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} \\ &= \left(\frac{i}{\eta}\right)^n \int_{-\infty}^{+\infty} \mathbf{p}^n f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}. \end{aligned} \quad (54)$$

Then,

$$\begin{aligned} \langle \mathbf{p}^n \rangle &= \frac{\iint_{-\infty}^{+\infty} \mathbf{p}^n f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x}}{\iint_{-\infty}^{+\infty} f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x}} \\ &= (-i\eta)^n \frac{\int_{-\infty}^{+\infty} d\mathbf{x} m \lim_{y \rightarrow 0} \partial^n \hat{f} / \partial \mathbf{y}^n}{\int_{-\infty}^{+\infty} d\mathbf{x} m \lim_{y \rightarrow 0} \hat{f}}. \end{aligned} \quad (55)$$

As we have shown before,  $m \lim_{y \rightarrow 0} \hat{f} = \rho(\mathbf{x}, t)$ , so we only have to calculate the numerator in our expression. We do so by using the canonical change of variables given by (20), so that

$$\begin{aligned} \frac{\partial^n}{\partial \mathbf{y}^n} &= \frac{1}{2^n} \left( \frac{\partial}{\partial \mathbf{x}'} - \frac{\partial}{\partial \mathbf{x}''} \right)^n \\ &= \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} \left( \frac{\partial}{\partial \mathbf{x}'} \right)^k \left( -\frac{\partial}{\partial \mathbf{x}''} \right)^{(n-k)}. \end{aligned} \quad (56)$$

Once more we will invoke the separability of  $\hat{f}$  in the form

$$\hat{f}(\mathbf{x}', \mathbf{x}'', t) = h'(\mathbf{x}', t) h''(\mathbf{x}'', t). \quad (57)$$

Notice that  $h'$  and  $h''$  are complex functions given by  $h' = g_1 e^{i\phi'}$  and  $h'' = g_2 e^{i\phi''}$  and  $\phi(\mathbf{x}', \mathbf{x}'', t) = \phi'(\mathbf{x}', t) + \phi''(\mathbf{x}'', t)$ . Then, replacing into the integral of the numerator we obtain

$$\begin{aligned} \int_{-\infty}^{+\infty} d\mathbf{x} m \lim_{y \rightarrow 0} \frac{\partial^n \hat{f}}{\partial \mathbf{y}^n} &= \int_{-\infty}^{+\infty} d\mathbf{x} \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} m \lim_{y \rightarrow 0} \left( \frac{\partial h'}{\partial \mathbf{x}'} \right)^k \left( -\frac{\partial h''}{\partial \mathbf{x}''} \right)^{(n-k)} \\ &= \int_{-\infty}^{+\infty} d\mathbf{x} \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} \frac{\partial^k \Psi}{\partial \mathbf{x}^k} (-1)^{(n-k)} \frac{\partial^{(n-k)} \Psi^*}{\partial \mathbf{x}^{(n-k)}}, \end{aligned} \quad (58)$$

where we have used the identities

$$\begin{aligned} m \lim_{y \rightarrow 0} \hat{f}(\mathbf{x}', \mathbf{x}'', t) &= m \lim_{y \rightarrow 0} h'(\mathbf{x}', t) h''(\mathbf{x}'', t) \\ &= \rho(\mathbf{x}, t) \equiv \Psi \Psi^* \end{aligned} \quad (59)$$

and called  $m^{1/2} \lim_{y \rightarrow 0} h'(\mathbf{x}', t) = \Psi(\mathbf{x}, t)$  and  $m^{1/2} \lim_{y \rightarrow 0} h''(\mathbf{x}'', t) = \Psi^*(\mathbf{x}, t)$ . Then, after integrating by parts  $(n - k)$  times the derivatives of  $\Psi^*$ , we obtain

$$\int_{-\infty}^{+\infty} d\mathbf{x} \Psi^* \frac{\partial^n \Psi}{\partial \mathbf{x}^n}, \quad (60)$$

where we have used the fact that  $\sum_{k=0}^n \binom{n}{k} = 2^n$ . Finally, replacing these results into (55) and changing the notation to  $\partial/\partial \mathbf{x} \equiv \nabla$ , the expression for  $\langle \mathbf{p}^n \rangle$  reads

$$\langle \mathbf{p}^n \rangle = \frac{\int \Psi^* (-i\eta \nabla)^n \Psi d\mathbf{x}}{\int \Psi \Psi^* d\mathbf{x}}. \quad (61)$$

To prove (45) we write the physical magnitude  $A(\mathbf{x}, \mathbf{p}, t)$  through its series representation,

$$A(\mathbf{x}, \mathbf{p}, t) = \sum_{n,m} A_{nm} \mathbf{x}^n \mathbf{p}^m, \quad (62)$$

where the coefficients  $A_{nm}$  are functions of time. Then, its average is given by

$$\begin{aligned} \langle A \rangle &= \frac{\int \int_{-\infty}^{+\infty} \sum_{n,m} A_{nm} \mathbf{x}^n \mathbf{p}^m f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x}}{\int \int_{-\infty}^{+\infty} f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x}} \\ &= \frac{\sum_{n,m} A_{nm} \int_{-\infty}^{+\infty} d\mathbf{x} \mathbf{x}^n \int_{-\infty}^{+\infty} d\mathbf{p} \mathbf{p}^m f_1(\mathbf{x}, \mathbf{p}, t)}{\int \int_{-\infty}^{+\infty} f_1(\mathbf{x}, \mathbf{p}, t) d\mathbf{p} d\mathbf{x}}. \end{aligned} \quad (63)$$

Now, using (60) we can rewrite this average as

$$\begin{aligned}
\langle A \rangle &= \frac{\sum_{n,m} A_{nm} \int_{-\infty}^{+\infty} d\mathbf{x} \mathbf{x}^n \Psi^* (-i\eta \nabla)^m \Psi}{\int \Psi \Psi^* d\mathbf{x}} \\
&= \frac{\int_{-\infty}^{+\infty} d\mathbf{x} \Psi^* \left[ \sum_{n,m} A_{nm} \mathbf{x}^n (-i\eta \nabla)^m \right] \Psi}{\int \Psi \Psi^* d\mathbf{x}} \\
&= \frac{\int_{-\infty}^{+\infty} d\mathbf{x} \Psi^* \hat{A}(\mathbf{x}, \mathbf{p}_F, t) \Psi}{\int \Psi \Psi^* d\mathbf{x}}, \tag{64}
\end{aligned}$$

where  $\mathbf{p}_F = -i\eta \nabla$ .

## Appendix B

Here we show an interesting feature of the BBKGY hierarchy, which even though not fully relevant to this paper, is nonetheless quite intriguing.

The equation that governs the  $s$ -particle probability function in the classical BBKGY hierarchy is given by

$$\begin{aligned}
\frac{\partial f_s}{\partial t} + \sum_{\ell=1}^s \frac{\mathbf{p}_\ell}{m} \cdot \frac{\partial f_s}{\partial \mathbf{x}_\ell} + \sum_{\ell < j}^s -\frac{\partial u_{\ell j}}{\partial \mathbf{x}_\ell} \cdot \left( \frac{\partial f_s}{\partial \mathbf{p}_\ell} - \frac{\partial f_s}{\partial \mathbf{p}_j} \right) \\
+(N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \sum_{\ell=1}^s -\frac{\partial u_{\ell, s+1}}{\partial \mathbf{x}_\ell} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_\ell} = 0, \tag{65}
\end{aligned}$$

where  $u_{ij}$  is the inter-particle potential between the particles  $i$  and  $j$ , which only depends on the distance between those particles.

Given the results obtained by introducing Fourier transforms into the momentum averages of Boltzmann's equation, one could ask about the outcome of such a procedure when applied to the momentum average of any one member of the full BBKGY hierarchy:

$$\begin{aligned}
\int \prod_{k=1}^s d\mathbf{p}_k \left[ \frac{\partial f_s}{\partial t} + \sum_{\ell=1}^s \frac{\mathbf{p}_\ell}{m} \cdot \frac{\partial f_s}{\partial \mathbf{x}_\ell} + \sum_{\ell < j}^s -\frac{\partial u_{\ell j}}{\partial \mathbf{x}_\ell} \cdot \left( \frac{\partial f_s}{\partial \mathbf{p}_\ell} - \frac{\partial f_s}{\partial \mathbf{p}_j} \right) \right. \\
\left. + (N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \sum_{\ell=1}^s -\frac{\partial u_{\ell, s+1}}{\partial \mathbf{x}_\ell} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_\ell} \right] = 0. \tag{66}
\end{aligned}$$

Thus, we generalize our previous mapping by introducing the following transforms:

$$f_s(\mathbf{X}_s, \mathbf{P}_s, t) = \frac{1}{(2\pi\eta)^{3s}} \int_{-\infty}^{+\infty} \exp\left(-\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) \hat{f}_s(\mathbf{X}_s, \mathbf{Y}_s, t) d\mathbf{Y}_s \tag{67}$$

and

$$\hat{f}_s(\mathbf{X}_s, \dots, \mathbf{Y}_s, t) = \int_{-\infty}^{+\infty} \exp\left(\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) f_s(\mathbf{X}_s, \mathbf{P}_s, t) d\mathbf{P}_s, \tag{68}$$

where we have introduced the short-hand notation  $\mathbf{X}_s = (\mathbf{x}_1, \dots, \mathbf{x}_s)$ ,  $\mathbf{Y}_s = (\mathbf{y}_1, \dots, \mathbf{y}_s)$ ,  $\mathbf{P}_s = (\mathbf{p}_1, \dots, \mathbf{p}_s)$ ,  $d\mathbf{Y}_s = \prod_{\ell=1}^s d\mathbf{y}_\ell$  and  $d\mathbf{P}_s = \prod_{\ell=1}^s d\mathbf{p}_\ell$ . Also, from now on we will not write explicitly the  $\mathbf{X}_s$ ,  $\mathbf{Y}_s$  and  $\mathbf{P}_s$  dependence of  $f_s$  and  $\hat{f}_s$  unless needed for clarity.

When these definitions are replaced into each term of (66) and the usual algebraic steps are followed we obtain:

$$\frac{\partial f_s}{\partial t} = \frac{1}{(2\pi\eta)^{3s}} \int_{-\infty}^{+\infty} d\mathbf{Y}_s \exp\left(-\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) \frac{\partial \hat{f}_s}{\partial t} \tag{69}$$

for the first term,

$$\sum_{\ell=1}^s \frac{\mathbf{p}_\ell}{m} \cdot \frac{\partial f_s}{\partial \mathbf{x}_\ell} = \frac{1}{(2\pi\eta)^{3s}} \int_{-\infty}^{+\infty} d\mathbf{Y}_s \exp\left(-\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) \sum_{\ell=1}^s \frac{i\eta}{m} \frac{\partial}{\partial \mathbf{y}_\ell} \cdot \frac{\partial \hat{f}_s}{\partial \mathbf{x}_\ell} \quad (70)$$

for the second term, using the symmetry relation  $\partial u_{\ell j} / \partial \mathbf{x}_\ell = -\partial u_{\ell j} / \partial \mathbf{x}_j$ ,

$$\begin{aligned} \sum_{\ell < j}^s -\frac{\partial u_{\ell j}}{\partial \mathbf{x}_\ell} \cdot \left( \frac{\partial f_s}{\partial \mathbf{p}_\ell} - \frac{\partial f_s}{\partial \mathbf{p}_j} \right) &= \frac{1}{(2\pi\eta)^{3s}} \sum_{\ell < j}^s \int_{-\infty}^{+\infty} d\mathbf{Y}_s \frac{i}{\eta} \left[ \mathbf{y}_\ell \cdot \frac{\partial u_{\ell j}}{\partial \mathbf{x}_\ell} + \mathbf{y}_j \cdot \frac{\partial u_{\ell j}}{\partial \mathbf{x}_j} \right] \\ &\times \hat{f}_s \exp\left(-\frac{i}{\eta} \sum_{k=1}^s \mathbf{p}_k \cdot \mathbf{y}_k\right) \end{aligned} \quad (71)$$

for the third term and

$$\begin{aligned} (N-s) \int d\mathbf{x}_{s+1} d\mathbf{p}_{s+1} \sum_{\ell=1}^s -\frac{\partial u_{\ell, s+1}}{\partial \mathbf{x}_\ell} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_\ell} &= \frac{1}{(2\pi\eta)^{3(s+1)}} \sum_{\ell=1}^s \int d\mathbf{p}_{s+1} d\mathbf{x}_{s+1} \\ &\times \int_{-\infty}^{+\infty} d\mathbf{Y}_{s+1} \exp\left(-\frac{i}{\eta} \sum_{k=1}^{s+1} \mathbf{p}_k \cdot \mathbf{y}_k\right) \frac{i}{\eta} \left[ \mathbf{y}_\ell \cdot \frac{\partial u_{\ell, s+1}}{\partial \mathbf{x}_\ell} \right] \hat{f}_{s+1} \end{aligned} \quad (72)$$

for the fourth term.

Now we introduce the usual canonical change of variables  $\mathbf{y}_j = \mathbf{x}'_j - \mathbf{x}''_j$  and  $\mathbf{x}_j = (\mathbf{x}'_j + \mathbf{x}''_j)/2$ . The first term remains the same and the second term can be rewritten as

$$\frac{1}{(2\pi\eta)^{3s}} \int_{-\infty}^{+\infty} d\mathbf{Y}_s \exp\left(-\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) \sum_{\ell=1}^s -\frac{1}{i\eta} \left[ -\frac{\eta^2}{2m} \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell'^2} - \left(-\frac{\eta^2}{2m}\right) \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell''^2} \right]. \quad (73)$$

For the third and fourth terms we notice that

$$\begin{aligned} \mathbf{y}_\ell \cdot \frac{\partial u_{\ell j}}{\partial \mathbf{x}_\ell} + \mathbf{y}_j \cdot \frac{\partial u_{\ell j}}{\partial \mathbf{x}_j} &= u\left(\mathbf{x}_\ell + \frac{\Delta \mathbf{x}_\ell}{2}, \mathbf{x}_j + \frac{\Delta \mathbf{x}_j}{2}\right) - u\left(\mathbf{x}_\ell - \frac{\Delta \mathbf{x}_\ell}{2}, \mathbf{x}_j - \frac{\Delta \mathbf{x}_j}{2}\right) + \mathcal{O}(\mathbf{y}_\ell, \mathbf{y}_j) \\ &= u(\mathbf{x}'_\ell, \mathbf{x}'_j) - u(\mathbf{x}''_\ell, \mathbf{x}''_j) + \mathcal{O}(\mathbf{y}_\ell, \mathbf{y}_j). \end{aligned} \quad (74)$$

Thus, the third and fourth terms can be rewritten, up to order  $\mathcal{O}(\mathbf{Y}_{s+1})$ , as

$$\frac{1}{(2\pi\eta)^{3s}} \sum_{\ell < j}^s \int_{-\infty}^{+\infty} d\mathbf{Y}_s \exp\left(-\frac{i}{\eta} \sum_{k=1}^s \mathbf{p}_k \cdot \mathbf{y}_k\right) \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_j) - u(\mathbf{x}''_\ell, \mathbf{x}''_j)] \hat{f}_s \quad (75)$$

and

$$\begin{aligned} \frac{1}{(2\pi\eta)^{3(s+1)}} \sum_{\ell=1}^s \int d\mathbf{p}_{s+1} d\mathbf{x}_{s+1} \int_{-\infty}^{+\infty} d\mathbf{Y}_{s+1} \exp\left(-\frac{i}{\eta} \sum_{k=1}^{s+1} \mathbf{p}_k \cdot \mathbf{y}_k\right) \\ \times \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_{s+1}) - u(\mathbf{x}''_\ell, \mathbf{x}''_{s+1})] \hat{f}_{s+1}, \end{aligned} \quad (76)$$

respectively. In equation (76), the integral on  $\mathbf{p}_{s+1}$  can be calculated since the only dependence on this variable appears in the exponential:

$$\frac{1}{(2\pi\eta)^3} \int_{-\infty}^{+\infty} d\mathbf{p}_{s+1} \exp\left(-\frac{i}{\eta} \mathbf{p}_{s+1} \cdot \mathbf{y}_{s+1}\right) = \delta(\mathbf{y}_{s+1}). \quad (77)$$

Since  $\delta(\mathbf{y}_{s+1}) = \delta(\mathbf{x}'_{s+1} - \mathbf{x}''_{s+1})$ ,

$$\int_{-\infty}^{+\infty} d\mathbf{x}_{s+1} \int_{-\infty}^{+\infty} d\mathbf{Y}_{s+1} \delta(\mathbf{y}_{s+1}) = \int_{-\infty}^{+\infty} d\mathbf{x}'_{s+1} d\mathbf{x}''_{s+1} \delta(\mathbf{x}'_{s+1} - \mathbf{x}''_{s+1}). \quad (78)$$

Finally, replacing identity (78) in the last term and collecting all the results we obtain for the Fourier transform of the  $s$ -term in the BBKGY hierarchy:

$$\begin{aligned} & \frac{1}{(2\pi\eta)^{3s}} \int_{-\infty}^{+\infty} d\mathbf{P}_s \int_{-\infty}^{+\infty} d\mathbf{Y}_s \exp\left(-\frac{i}{\eta} \sum_{\ell=1}^s \mathbf{p}_\ell \cdot \mathbf{y}_\ell\right) \\ & \times \left\{ \frac{\partial \hat{f}_s}{\partial t} + \sum_{\ell=1}^s -\frac{1}{i\eta} \left[ -\frac{\eta^2}{2m} \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell'^2} - \left(-\frac{\eta^2}{2m}\right) \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell''^2} \right] \right. \\ & + \sum_{\ell < j}^s \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_j) - u(\mathbf{x}''_\ell, \mathbf{x}''_j)] \hat{f}_s \\ & + (N-s) \sum_{\ell=1}^s \int_{-\infty}^{+\infty} d\mathbf{x}'_{s+1} d\mathbf{x}''_{s+1} \delta(\mathbf{x}'_{s+1} - \mathbf{x}''_{s+1}) \\ & \left. \times \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_{s+1}) - u(\mathbf{x}''_\ell, \mathbf{x}''_{s+1})] \hat{f}_{s+1} \right\} + \mathcal{O}(Y_s) = 0. \quad (79) \end{aligned}$$

We can now use the well-known fact that for any function  $F(\mathbf{Y}_s, \mathbf{X}_s)$

$$\begin{aligned} & \frac{1}{(2\pi\eta)^3} \int_{-\infty}^{+\infty} d\mathbf{p}_k \int_{-\infty}^{+\infty} d\mathbf{y}_k \exp\left(-\frac{i}{\eta} \mathbf{p}_k \cdot \mathbf{y}_k\right) F(\mathbf{Y}_s, \mathbf{X}_s) \\ & = \int_{-\infty}^{+\infty} d\mathbf{y}_k \delta(\mathbf{y}_k) F(\mathbf{Y}_s, \mathbf{X}_s) = \lim_{y_k \rightarrow 0} F(\mathbf{Y}_s, \mathbf{X}_s) \end{aligned} \quad (80)$$

taking into account that  $\lim_{Y_s \rightarrow 0} \equiv \lim_{\mathbf{X}'_s \rightarrow \mathbf{X}''_s}$  and replacing (80) for each value of  $k$  into (79) we obtain

$$\begin{aligned} & \lim_{\mathbf{X}'_s \rightarrow \mathbf{X}''_s} \left\{ \frac{\partial \hat{f}_s}{\partial t} + \sum_{\ell=1}^s -\frac{1}{i\eta} \left[ -\frac{\eta^2}{2m} \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell'^2} - \left(-\frac{\eta^2}{2m}\right) \frac{\partial^2 \hat{f}_s}{\partial \mathbf{x}_\ell''^2} \right] \right. \\ & + \sum_{\ell < j}^s \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_j) - u(\mathbf{x}''_\ell, \mathbf{x}''_j)] \hat{f}_s \\ & + (N-s) \sum_{\ell=1}^s \int_{-\infty}^{+\infty} d\mathbf{x}'_{s+1} d\mathbf{x}''_{s+1} \delta(\mathbf{x}'_{s+1} - \mathbf{x}''_{s+1}) \\ & \left. \times \left(-\frac{1}{i\eta}\right) [u(\mathbf{x}'_\ell, \mathbf{x}'_{s+1}) - u(\mathbf{x}''_\ell, \mathbf{x}''_{s+1})] \hat{f}_{s+1} \right\} = 0, \quad (81) \end{aligned}$$

where we have omitted the corrections  $\mathcal{O}(Y_s)$  because they vanish when we take the limit.

If we replace in (81), as we have done before,  $\eta \equiv \hbar$  and also relabel  $\rho_s \equiv \hat{f}_s$ , the expression inside the curly brackets coincides, except for the limiting operation, with the equation that governs the  $s$ th member of the quantum hierarchy for the density matrix  $\rho_s(\mathbf{X}'_s, \mathbf{X}''_s)$  [6]. We should point out, though, that results calculated with the density matrix only have physical meaning when at the end of such calculation the limit  $\mathbf{x}'_j \rightarrow \mathbf{x}''_j, \forall j$  is taken. Therefore, any averages obtained from either  $\hat{f}_s$  or  $\rho_s$  should be identical. This would also seem to indicate that the solutions for  $\hat{f}_s$  could be separable in this limit since the solutions for  $\rho_s$  satisfy this property. While this argument by no means constitutes a proof of the existence of separable solutions for  $\hat{f}_s$  it is encouraging in that direction.

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