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Many-particle quantum hydrodynamics: Exact equations and pressure tensors

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In the first part of this paper, the many-particle quantum hydrodynamics equations for a system containing many particles of different sorts are derived exactly from the many-particle Schrödinger equation, including the derivation of the many-particle continuity equations, many-particle Ehrenfest equations of motion, and many-particle quantum Cauchy equations for any of the different particle sorts and for the total particle ensemble. The new point in our analysis is that we consider a set of arbitrary particles of different sorts in the system. In the many-particle quantum Cauchy equations, there appears a quantity called the pressure tensor. In the second part of this paper, we analyze two versions of this tensor in depth: the Wyatt pressure tensor and the Kuzmenkov pressure tensor. There are different versions because there is a gauge freedom for the pressure tensor similar to that for potentials. We find that the interpretation of all the quantities contributing to the Wyatt pressure tensor is understandable, but for the Kuzmenkov tensor it is difficult. Furthermore, the transformation from Cartesian coordinates to cylindrical coordinates for the Wyatt tensor can be done in a clear way, but for the Kuzmenkov tensor it is rather cumbersome.

Subject Index A60, A63, A64, J19

1. Introduction

Quantum hydrodynamics (QHD) is a concept that was developed in 1926 by Madelung (Refs. [1,2]). He transformed the Schrödinger equation for a single particle into the corresponding QHD equations. It was further developed by Bohm in 1952 (Refs. [3,4]). The motivation to name this field QHD is that by applying it one finds differential equations with a similar form to the well-known differential equations in classical hydrodynamics, like the continuity equation or the Navier–Stokes equation (Ref. [5], pp. 2 and 45). Such equations related to QHD were analyzed for systems where the wave function was a single or quasi-single particle wave function in several papers (Refs. [1–4,6–22]). First ideas for many-particle quantum hydrodynamics (MPQHD) were already discussed by Bohm (Ref. [3]). In addition, MPQHD was analyzed using the energy density functional method (Refs. [23–25]), a time-dependent Hartree–Fock ansatz (Ref. [26–28]), and a non-stationary non-linear Schrödinger equation ansatz for quantum plasma physics (Refs. [29,30]). Furthermore, in 1999, Kuzmenkov and Maksimov developed a method where equations for mass, momentum, and energy balance for MPQHD were derived for exact non-relativistic many-particle wave functions without regarding the particle spin (Ref. [31]). Later, the method was further developed by Kuzmenkov and his colleagues to investigate spin effects (Refs. [32,33]) and Bose–Einstein condensates (Ref. [34]). Moreover, applications of this method were discussed, for example related to electrons in graphene (Ref. [35]) and plasma effects (Ref. [36–41]). In particular, Ref. [38] briefly mentions how to apply MPQHD when several sorts of particles are present, and the MPQHD equations stated in Refs. [38–41] describe the special case of two particle sorts in a plasma. In Refs. [38–40] these two sorts are electrons and a single ion sort, and in Ref. [41] the two sorts are electrons and positrons.

In Sect. 2 of this paper, we are aiming at developing further the methods described in Refs. [31,38] by rigorously deriving the MPQHD equations for the case that the particle ensemble includes several sorts of particles; in particular, in our general ansatz we do not restrict the number of particle sorts and we do not specify the types of the particle sorts. As we want to focus there on the main points, we neglect spin effects in our calculations, and at the end of Sect. 2 we briefly mention the effects of external electromagnetic fields. In addition, in our calculations in Sect. 2 we mention a quantity called the pressure tensor. One can find different versions of this pressure tensor in the literature (Refs. [13,23,28,31]); an explanation for this variety can be found in Ref. [13]. In Sect. 3, we pick up the pressure tensor version given in Ref. [31] and name it the "Kuzmenkov pressure tensor". In addition, the discussion about QHD in Ref. [42], pp. 30f, is our motivation to introduce another pressure tensor version called the "Wyatt pressure tensor". We analyze how these tensors can be interpreted physically. Moreover, we discuss for which of these two tensors a transformation from Cartesian coordinates into cylindrical coordinates can be done more easily.

2. Basic physics of exact MPQHD

Here, the basic physics for many-particle quantum hydrodynamics (MPQHD) is analyzed. A particle ensemble consisting of different particle sorts is examined, and a many-particle continuity equation (MPCE), a many-particle Ehrenfest equation of motion (MPEEM), and a many-particle quantum Cauchy equation (MPQCE) is derived each for the total ensemble of particles and for a particular sort of particle. The MPCEs are equations related to mass conservation, the MPEEMs are equations related to the time evolution of mass flux densities, and the MPQCEs are equations related to the momentum balance. For these derivations, several quantities have to be defined first.

2.1. *Definitions*

We assume that there are N_S sorts of particles, and that A,B,C stand for any number $\in \{1, 2, \ldots, N_S\}$ related to one sort of particle. For brevity, we denote any Ath sort of particle also as the sort of particle A or just as sort A. The $N(\mathrm{A})$ particles of any sort A shall be indistinguishable. In particular, each particle of sort A has the same mass m_{A} and the same charge e_{A}. In this publication, spin effects are not considered; for a more general analysis with spin effects one would have to consider that each particle of sort A has a spin s_{A}.

The ansatz to treat particles of the same sort as indistinguishable does not diminish the generality of the following analysis, for this reason: If there are sorts of particles where the individual particles can be distinguished, this can be implemented in the calculations below by treating each of these particles as a whole sort of particle of its own. In this sense, the following analysis is valid both for distinguishable and for indistinguishable particles.

Moreover, all the subsequent analysis in this paper is correct for these three cases: (1) All particles are fermions. (2) All particles are bosons. (3) The particles of some sorts are fermions, and the particles of the remaining sorts are bosons. We mention that in Ref. [31], one can find a discussion where the question is analyzed as to how the property of the particles being either bosons or fermions influences quantum hydrodynamics. Hereby, the many-particle wave function is decomposed within the Hartree–Fock method as a sum over many-particle eigenfunctions in the occupation number space. As a result, for such a decomposition of the many-particle wave function one needs to make a distinction between the cases that the particles are bosons or fermions; since we will not make a decomposition of the many-particle wave function into its eigenfunctions within the analysis in our paper, however, all the equations in our paper are valid both for bosons and for fermions.

The position vector of the ith particle of sort A (so $i \in 1, 2, \ldots, N(\mathrm{A})$) is $\vec{q}_i^{\,\mathrm{A}}$; this particle is called (A, i) particle. Moreover,

$$\vec{Q} = \left(\vec{q}_1^{\,1}, \vec{q}_2^{\,1}, \ldots, \vec{q}_{N(1)}^{\,1}, \vec{q}_1^{\,2}, \ldots, \vec{q}_{N(2)}^{\,2}, \ldots, \vec{q}_1^{\,N_S}, \ldots, \vec{q}_{N(N_S)}^{\,N_S}\right) \tag{1}$$

is the complete set of particle coordinates, and $\Psi(\vec{Q}, t)$ is the normalized total wave function of the system.

The particles shall be exposed only to forces arising from a real-valued two-particle potential (e.g., a Coulomb potential):

$$V_{ij}^{\mathrm{AB}} = \begin{cases} V^{\mathrm{AB}}(|\vec{q}_i^{\,\mathrm{A}} - \vec{q}_j^{\,\mathrm{B}}|) & \text{for } (i \neq j) \quad \text{or} \quad (\mathrm{A} \neq \mathrm{B}), \\ 0 & \text{for } (i = j) \quad \text{and} \quad (\mathrm{A} = \mathrm{B}), \end{cases} \tag{2}$$

where we regard that the two-particle potential does not couple a particle with itself by the distinction of cases in the equation above.

This two-particle potential has the symmetry properties

$$V_{ij}^{\mathrm{AB}} = V_{ji}^{\mathrm{BA}}, \tag{3}$$

$$\nabla_i^{\mathrm{A}} V_{ij}^{\mathrm{AB}} = -\nabla_j^{\mathrm{B}} V_{ji}^{\mathrm{BA}}, \tag{4}$$

where ∇_i^{A} is the nabla operator relative to the coordinate $\vec{q}_i^{\,\mathrm{A}}$. Later, we will explain what happens if external fields are present.

The canonical momentum operator $\hat{\vec{p}}_i^{\,\mathrm{A}}$ relative to the coordinate $\vec{q}_i^{\,\mathrm{A}}$ is

$$\hat{\vec{p}}_i^{\,\mathrm{A}} = \frac{\hbar}{\mathrm{i}} \nabla_i^{\mathrm{A}}. \tag{5}$$

Then, the Schrödinger equation of the system is given by

$$\mathrm{i}\hbar \, \frac{\partial \Psi(\vec{Q}, t)}{\partial t} = \hat{H}(\vec{Q}) \; \Psi(\vec{Q}, t), \tag{6}$$

with a Hamiltonian

$$\hat{H}(\vec{Q}) = \sum_{\mathrm{A}=1}^{N_S} \sum_{i=1}^{N(\mathrm{A})} \frac{\left(\hat{\vec{p}}_i^{\,\mathrm{A}}\right)^2}{2m_{\mathrm{A}}} + \frac{1}{2} \sum_{\mathrm{A}=1}^{N_S} \sum_{i=1}^{N(\mathrm{A})} \sum_{\mathrm{B}=1}^{N_S} \sum_{j=1}^{N(\mathrm{B})} V_{ij}^{\mathrm{AB}}. \tag{7}$$

The next quantity we define is the volume element $\mathrm{d}\vec{Q}$ for all particles; it is given by:

$$\mathrm{d}\vec{Q} = \prod_{\mathrm{A}=1}^{N_S} \left(\prod_{i=1}^{N(\mathrm{A})} \mathrm{d}\vec{q}_i^{\,\mathrm{A}} \right). \tag{8}$$

The volume element $\mathrm{d}\vec{Q}_i^{\mathrm{A}}$ for all coordinates except for coordinate $\vec{q}_i^{\,\mathrm{A}}$ is then defined by:

$$\mathrm{d}\vec{Q}_i^{\mathrm{A}} = \frac{\mathrm{d}\vec{Q}}{\mathrm{d}\vec{q}_i^{\,\mathrm{A}}}. \tag{9}$$

Note that $\mathrm{d}\vec{q}_i^{\,\mathrm{A}}$ is a volume element and not a vector, so its appearance in the denominator is correct. We now define the total particle density $D(\vec{Q},t)$ by

$$D(\vec{Q},t) = \left|\Psi(\vec{Q},t)\right|^2. \tag{10}$$

For the case of a single particle, Eq. (10) is equivalent to the equation for the particle density in a single-particle system in quantum mechanics textbooks (see Ref. [43], pp. 38f and Ref. [44], p. 4).

Using the definitions above and the indistinguishability of the particles of each sort, we introduce the total one-particle mass density $\rho_m^{\mathrm{tot}}(\vec{q},t)$:

$$\rho_m^{\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} m_{\mathrm{A}} \sum_{i=1}^{N(\mathrm{A})} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\; D(\vec{Q},t) \tag{11}$$

$$= \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t). \tag{12}$$

Moreover, $\vec{Q}_i^{\mathrm{A}}(\vec{q})$ means that in the particle coordinate set $\vec{Q}$ given by Eq. (1), the coordinate vector $\vec{q}_i^{\,\mathrm{A}}$ is set to $\vec{q}$.

Because of Eq. (12), it is clear that the one-particle mass density of the Ath sort $\rho_m^{\mathrm{A}}(\vec{q},t)$ is given by:

$$\rho_m^{\mathrm{A}}(\vec{q},t) = N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t), \tag{13}$$

and

$$\rho_m^{\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} \rho_m^{\mathrm{A}}(\vec{q},t). \tag{14}$$

Here, we introduce mass densities instead of just particle densities because the use of mass densities makes the MPEEMs and MPQCEs more compact. For the same reason, we introduce in the following mass current densities instead of just particle current densities.

Thus, as the next quantity, we define the total particle mass current density $\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t)$ as:

$$\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} \sum_{i=1}^{N(\mathrm{A})} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\; \Re\left[\Psi^*(\vec{Q},t)\; \hat{\vec{p}}_i^{\,\mathrm{A}}\; \Psi(\vec{Q},t)\right]. \tag{15}$$

Regarding the definition of the canonical momentum operator $\hat{\vec{p}}_i^{\,\mathrm{A}}$ of the (A,i) particle in Eq. (5) and the indistinguishability of the particles of each sort, we can transform Eq. (15) into

$$\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t) = \hbar \sum_{\mathrm{A}=1}^{N_S} \sum_{i=1}^{N(\mathrm{A})} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\; \Im\left[\Psi^*(\vec{Q},t)\; \nabla_i^{\mathrm{A}}\Psi(\vec{Q},t)\right] \tag{16}$$

$$= \hbar \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A}) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; \Im\left[\Psi^*(\vec{Q},t)\; \nabla_1^{\mathrm{A}}\Psi(\vec{Q},t)\right]. \tag{17}$$

For the case of a single-particle system, Eq. (17) turns into the definition of the particle current density (Ref. [43], pp. 144f and Ref. [44], p. 24).

Furthermore, Eqs. (15)–(17) make clear that the mass current density $\vec{j}_m^{\rm A}(\vec{q},t)$ of all the particles of sort A is given by:

$$\vec{j}_m^{\rm A}(\vec{q},t) = \sum_{i=1}^{N(\rm A)} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_i^{\,\rm A})\; \Re\left[\Psi^*(\vec{Q},t)\; \hat{\vec{p}}_i^{\,\rm A}\; \Psi(\vec{Q},t)\right] \tag{18}$$

$$= \hbar\, N(\rm A) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\rm A})\; \Im\left[\Psi^*(\vec{Q},t)\; \nabla_1^{\rm A}\Psi(\vec{Q},t)\right], \tag{19}$$

so

$$\vec{j}_m^{\rm tot}(\vec{q},t) = \sum_{\rm A=1}^{N_S} \vec{j}_m^{\rm A}(\vec{q},t). \tag{20}$$

Moreover, we note that because of Eq. (18), the quantity $\vec{j}_m^{\rm A}(\vec{q},t)$ can be interpreted as the expectation value of this operator $\hat{\vec{j}}_m^{\rm A}(\vec{Q},\vec{q})$ (Ref. [31]):

$$\hat{\vec{j}}_m^{\rm A}(\vec{Q},\vec{q}) = \frac{1}{2}\sum_{i=1}^{N(\rm A)} \left[\delta(\vec{q}-\vec{q}_i^{\,\rm A})\hat{\vec{p}}_i^{\,\rm A} + \hat{\vec{p}}_i^{\,\rm A}\delta(\vec{q}-\vec{q}_i^{\,\rm A})\right], \tag{21}$$

$$\vec{j}_m^{\rm A}(\vec{q},t) = \int \mathrm{d}\vec{Q}\; \Psi^*(\vec{Q},t)\; \hat{\vec{j}}_m^{\rm A}(\vec{Q},\vec{q})\; \Psi(\vec{Q},t). \tag{22}$$

As the next step, for the particles of sort A, we define the mean particle velocity $\vec{v}^{\rm A}(\vec{q},t)$ for all positions $\vec{q}$, where $\rho_m^{\rm A}(\vec{q},t) \neq 0$:

$$\vec{v}^{\rm A}(\vec{q},t) = \frac{\vec{j}_m^{\rm A}(\vec{q},t)}{\rho_m^{\rm A}(\vec{q},t)}. \tag{23}$$

For all positions $\vec{q}_0$, where $\rho_m^{\rm A}(\vec{q}_0,t) = 0$, we define:

$$\vec{v}^{\rm A}(\vec{q}_0,t) = \lim_{\vec{q}\to\vec{q}_0} \frac{\vec{j}_m^{\rm A}(\vec{q},t)}{\rho_m^{\rm A}(\vec{q},t)}. \tag{24}$$

Now we use the representation (Ref. [2,3])

$$\Psi(\vec{Q},t) = a(\vec{Q},t)\exp\left[\frac{\mathrm{i}S(\vec{Q},t)}{\hbar}\right] \tag{25}$$

for the wave function $\Psi(\vec{Q},t)$, where $a(\vec{Q},t)$ and $S(\vec{Q},t)$ are real-valued, continuous, and differentiable functions, and they define the velocity $\vec{w}_i^{\rm A}(\vec{Q},t)$ of the $(\rm A, i)$ particle by

$$\vec{w}_i^{\rm A}(\vec{Q},t) = \frac{1}{m_{\rm A}}\nabla_i^{\rm A} S(\vec{Q},t). \tag{26}$$

Note that for the velocity of the $(\rm A, i)$ particle we assigned the letter w, and for the mean particle velocity for particles of sort A we assigned the letter v, because then the MPQHD equations will be similar to the classical hydrodynamic equations in textbooks. These equations can be found, for example, in Ref. [5], pp. 2f, 11f, and 44f. As Madelung already realized in 1927 (Ref. [2]) for the case of a single-particle system, a direct consequence of the definition in Eq. (26) for the velocity $\vec{w}_i^{\rm A}(\vec{Q},t)$ of the $(\rm A, i)$ particle is that the rotation of this velocity relative to the coordinate $\vec{q}_i^{\,\rm A}$ vanishes:

$$\nabla_i^{\rm A} \times \vec{w}_i^{\rm A}(\vec{Q},t) = \vec{0}. \tag{27}$$

The definition above for $\vec{w}_i^{\rm A}(\vec{Q},t)$ can now be used to do the following transformation of the term $\Im\left[\Psi^*(\vec{Q},t)\nabla_1^{\rm A}\Psi(\vec{Q},t)\right]$ appearing in Eq. (17) for $\vec{j}_m^{\rm tot}(\vec{q},t)$:

$$\begin{aligned}\Im\left[\Psi^*(\vec{Q},t)\ \nabla_1^{\rm A}\Psi(\vec{Q},t)\right] &= \Im\left[\underbrace{a(\vec{Q},t)\ \nabla_1^{\rm A}a(\vec{Q},t)}_{\in\mathbb{R}} + \frac{\rm i}{\hbar}\underbrace{a(\vec{Q},t)^2\ \nabla_1^{\rm A}S(\vec{Q},t)}_{=D(\vec{Q},t)\ m_{\rm A}\ \vec{w}_1^{\rm A}(\vec{Q},t)}\right]\\ &= \frac{m_{\rm A}}{\hbar}D(\vec{Q},t)\ \vec{w}_1^{\rm A}(\vec{Q},t).\end{aligned} \tag{28}$$

With this transformation, we find the following form for $\vec{j}_m^{\rm tot}(\vec{q},t)$:

$$\vec{j}_m^{\rm tot}(\vec{q},t) = \sum_{\rm A=1}^{N_S} N({\rm A})\, m_{\rm A}\int {\rm d}\vec{Q}_1^{\rm A}\ D(\vec{Q}_1^{\rm A}(\vec{q}),t)\ \vec{w}_1^{\rm A}(\vec{Q}_1^{\rm A}(\vec{q}),t). \tag{29}$$

Thus, the mass current density $\vec{j}_m^{\rm A}(\vec{q},t)$ for particles of sort A is given by:

$$\vec{j}_m^{\rm A}(\vec{q},t) = N({\rm A})\, m_{\rm A}\int {\rm d}\vec{Q}_1^{\rm A}\ D(\vec{Q}_1^{\rm A}(\vec{q}),t)\ \vec{w}_1^{\rm A}(\vec{Q}_1^{\rm A}(\vec{q}),t). \tag{30}$$

Equation (30) is a logical result for $\vec{j}_m^{\rm A}(\vec{q},t)$ because it can be explained in the following way: For the situation that the (A, 1) particle is located at $\vec{q}$ and we average over the positions of all the other particles, it is intuitive that the corresponding mass flux density of the (A, 1) particle is given by the integral of the term $D(\vec{Q}_1^{\rm A}(\vec{q}),t)\ \vec{w}_1^{\rm A}(\vec{Q}_1^{\rm A}(\vec{q}),t)$ over the infinitesimal ${\rm d}\vec{Q}_1^{\rm A}$ multiplied by $m_{\rm A}$. Since the $N({\rm A})$ particles of sort A cannot be distinguished from each other, the flux density $\vec{j}_m^{\rm A}(\vec{q},t)$ for the $N({\rm A})$ particles of sort A is then just $N({\rm A})$ times this integral.

As a further quantity, we define the relative velocity $\vec{u}_i^{\rm A}(\vec{Q},t)$ of the $({\rm A},i)$ particle as:

$$\vec{u}_i^{\rm A}(\vec{Q},t) = \vec{w}_i^{\rm A}(\vec{Q},t) - \vec{v}^{\rm A}(\vec{q}_i^{\rm A},t). \tag{31}$$

The motivation to name it relative velocity is that $\vec{u}_i^{\rm A}(\vec{Q},t)$ is the velocity of the $({\rm A},i)$ particle relative to $\vec{v}^{\rm A}(\vec{q}_i^{\rm A},t)$. Moreover, $\vec{u}_i^{\rm A}(\vec{Q},t)$ has the following property: The $({\rm A},i)$ particle shall be in the position $\vec{q}_i^{\rm A}=\vec{q}$, so $\vec{Q}=\vec{Q}_i^{\rm A}(\vec{q})$, and we average $\vec{u}_i^{\rm A}(\vec{Q},t)$ over all positions which the other particles can occupy. Hereby, we weight $\vec{u}_i^{\rm A}(\vec{Q},t)$ with the probability $D(\vec{Q},t)$ that the positions of all particles are given by $\vec{Q}$. This average for the relative velocity $\vec{u}_i^{\rm A}(\vec{Q},t)$ vanishes. In the following calculation, the vanishing of this average is shown, and we use in this calculation Eqs. (13) and (30):

$$\begin{aligned}\int {\rm d}\vec{Q}\ \delta(\vec{q}-\vec{q}_i^{\rm A})\ D(\vec{Q},t)\ \vec{u}_i^{\rm A}(\vec{Q},t) &= \int {\rm d}\vec{Q}_i^{\rm A}\ D(\vec{Q}_i^{\rm A}(\vec{q}),t)\ \vec{u}_i^{\rm A}(\vec{Q}_i^{\rm A}(\vec{q}),t)\\ = \int {\rm d}\vec{Q}_1^{\rm A}\ D(\vec{Q}_1^{\rm A}(\vec{q}),t)\ \vec{u}_1^{\rm A}(\vec{Q}_1^{\rm A}(\vec{q}),t) &= \int {\rm d}\vec{Q}_1^{\rm A}\ D(\vec{Q}_1^{\rm A}(\vec{q}),t)\ \left(\vec{w}_1^{\rm A}(\vec{Q}_1^{\rm A}(\vec{q}),t) - \vec{v}^{\rm A}(\vec{q},t)\right)\end{aligned}$$

$$= \underbrace{\int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\ D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t)\ \vec{w}_1^{\mathrm{A}}(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t)}_{=\frac{1}{N(\mathrm{A})\,m_{\mathrm{A}}}\vec{j}_m^{\mathrm{A}}(\vec{q},t)} - \underbrace{\left[\int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\ D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t)\right]}_{=\frac{1}{N(\mathrm{A})\,m_{\mathrm{A}}}\rho_m^{\mathrm{A}}(\vec{q},t)} \vec{v}^{\mathrm{A}}(\vec{q},t)$$

$$= \frac{1}{N(\mathrm{A})\,m_{\mathrm{A}}}\left(\vec{j}_m^{\mathrm{A}}(\vec{q},t) - \rho_m^{\mathrm{A}}(\vec{q},t)\ \vec{v}^{\mathrm{A}}(\vec{q},t)\right) = \vec{0}. \tag{32}$$

In this context, we also call the relative velocities $\vec{u}_i^{\mathrm{A}}(\vec{Q},t)$ the fluctuating velocities, but note that this is a fluctuation relative to coordinate dependencies and not to time dependencies.

Moreover, we can define new quantities related to the total ensemble of particles analogously to the velocities $\vec{v}^{\mathrm{A}}(\vec{q},t)$ and $\vec{u}_i^{\mathrm{A}}(\vec{Q},t)$.

The first one is the mean particle velocity $\vec{v}^{\,\mathrm{tot}}(\vec{q},t)$ for the total particle ensemble. For all positions $\vec{q}$ where $\rho_m^{\mathrm{tot}}(\vec{q},t) \neq 0$, it is:

$$\vec{v}^{\,\mathrm{tot}}(\vec{q},t) = \frac{\vec{j}_m^{\mathrm{tot}}(\vec{q},t)}{\rho_m^{\mathrm{tot}}(\vec{q},t)}, \tag{33}$$

and for all positions $\vec{q}_0$, where $\rho_m^{\mathrm{tot}}(\vec{q}_0,t) = 0$, it is:

$$\vec{v}^{\,\mathrm{tot}}(\vec{q}_0,t) = \lim_{\vec{q}\to\vec{q}_0} \frac{\vec{j}_m^{\mathrm{tot}}(\vec{q},t)}{\rho_m^{\mathrm{tot}}(\vec{q},t)}. \tag{34}$$

The second one is another relative velocity of the (A,i) particle named $\vec{\mathrm{u}}_i^{\mathrm{A}}(\vec{Q},t)$:

$$\vec{\mathrm{u}}_i^{\mathrm{A}}(\vec{Q},t) := \vec{w}_i^{\mathrm{A}}(\vec{Q},t) - \vec{v}^{\,\mathrm{tot}}(\vec{q}_i^{\,\mathrm{A}},t). \tag{35}$$

Note that $\vec{\mathrm{u}}_i^{\mathrm{A}}(\vec{Q},t)$ is the relative velocity of the (A,i) particle to $\vec{v}^{\,\mathrm{tot}}(\vec{q}_i^{\,\mathrm{A}},t)$, while $\vec{u}_i^{\mathrm{A}}(\vec{Q},t)$ is the relative velocity of this particle to $\vec{v}^{\mathrm{A}}(\vec{q}_i^{\,\mathrm{A}},t)$. We emphasize that this is an expansion beyond Refs. [31, 38], where just one kind of relative particle velocity was defined.

2.2. *Derivation of the MPCE*

Now we derive the many-particle continuity equation (MPCE) both for all particles and for particles of a certain sort A. This can be done in an analogous way to the derivation of the continuity equation for a single-particle wave function in quantum mechanics textbooks (Ref. [43], pp. 144f and Ref. [44], p. 24). Therefore, we calculate the time derivative of $\rho_m^{\mathrm{A}}(\vec{q},t)$ by inserting the Schrödinger equation Eq. (6) into Eq. (13):

$$\frac{\partial \rho_m^{\mathrm{A}}(\vec{q},t)}{\partial t} = N(\mathrm{A})\,m_{\mathrm{A}} \int \mathrm{d}\vec{Q}_1^{\mathrm{A}} \left(\frac{\partial \Psi^*(\vec{Q}_1(\vec{q}),t)}{\partial t}\ \Psi(\vec{Q}_1(\vec{q}),t) + \Psi^*(\vec{Q}_1(\vec{q}),t)\ \frac{\partial \Psi(\vec{Q}_1(\vec{q}),t)}{\partial t}\right)$$

$$= \frac{2N(\mathrm{A})\,m_{\mathrm{A}}}{\hbar} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}_1^{\,\mathrm{A}})\ \Im\left[\Psi^*(\vec{Q},t)\ \hat{H}(\vec{Q})\ \Psi(\vec{Q},t)\right]. \tag{36}$$

We evaluate the imaginary part appearing in Eq. (36) with Eqs. (5) and (7):

$$\Im\left(\Psi^*\ \hat{H}\ \Psi\right) = \Im\left(-\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})} \Psi^* \frac{\hbar^2}{2m_{\mathrm{B}}} \triangle_j^{\mathrm{B}}\ \Psi + \frac{1}{2}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\sum_{\mathrm{C}=1}^{N_S}\sum_{k=1}^{N(\mathrm{C})} \underbrace{\Psi^* V_{jk}^{\mathrm{BC}} \Psi}_{\in\mathbb{R}}\right.$$

$$= -\sum_{B=1}^{N_S}\sum_{j=1}^{N(B)} \frac{\hbar^2}{2m_B} \Im\Big[\nabla_j^B\left(\Psi^*\nabla_j^B\Psi\right) - \underbrace{\left(\nabla_j^B\Psi^*\right)\left(\nabla_j^B\Psi\right)}_{\in\mathbb{R}}\Big]$$

$$= -\sum_{B=1}^{N_S}\sum_{j=1}^{N(B)} \frac{\hbar^2}{2m_B} \Im\left[\nabla_j^B\left(\Psi^*\nabla_j^B\Psi\right)\right], \tag{37}$$

where $\triangle_j^B$ is the Laplace operator relative to the coordinate $\vec{q}_j^{\,B}$.

As a next step, we insert Eq. (37) into Eq. (36), and then the summand for the case $\{B = A, j = 1\}$ is extracted from the double sum over B, j. We can then transform the integration over the coordinate $\vec{q}_j^{\,B}$ for all the remaining summands with the divergence theorem into an integral over the system boundary surface where the wave function vanishes. So, these remaining summands vanish, and only the extracted summand of the double sum for the case $\{B = A, j = 1\}$ remains:

$$\begin{aligned}\frac{\partial\rho_m^A(\vec{q},t)}{\partial t} &= -\hbar N(A)\, m_A \sum_{B=1}^{N_S}\sum_{j=1}^{N(B)} \frac{1}{m_B}\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\Im\left[\nabla_j^B\left(\Psi^*\nabla_j^B\Psi\right)\right]\\
&= -\hbar N(A)\, m_A\Bigg\{\frac{1}{m_A}\int d\vec{Q}_1^A\int d\vec{q}_1^{\,A}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\Im\left[\nabla_1^A\left(\Psi^*\nabla_1^A\Psi\right)\right]\\
&\quad + \sum_{\substack{B=1\\ \{B,j\}\neq\{A,1\}}}^{N_S}\sum_{j=1}^{N(B)} \frac{1}{m_B}\int d\vec{Q}_j^B\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\Im\Big[\underbrace{\int d\vec{q}_j^{\,B}\;\nabla_j^B\left(\Psi^*\nabla_j^B\Psi\right)}_{=0}\Big]\Bigg\}\\
&= -\,\hbar N(A)\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\Im\left[\nabla_1^A\left(\Psi^*\nabla_1^A\Psi\right)\right].\end{aligned} \tag{38}$$

Finally, regarding the δ-function in Eq. (38), we can substitute the outer nabla operator ∇_1^A in the imaginary part by a ∇ operator related to the coordinate $\vec{q}$ in the following manner:

$$\frac{\partial\rho_m^A(\vec{q},t)}{\partial t} = -\nabla\left\{\hbar N(A)\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\Im\left[\Psi^*(\vec{Q},t)\;\nabla_1^A\Psi(\vec{Q},t)\right]\right\}. \tag{39}$$

Because of Eq. (19), which describes the mass flux density $\vec{j}_m^A(\vec{q},t)$ for all particles of sort A, the equation above is then the MPCE for these particles:

$$\frac{\partial\rho_m^A(\vec{q},t)}{\partial t} = -\nabla\vec{j}_m^A(\vec{q},t). \tag{40}$$

By summing the MPCE for particles of a certain sort A over all sorts of particles, we get, using Eqs. (14) and (20), the MPCE for all particles:

$$\frac{\partial\rho_m^{tot}(\vec{q},t)}{\partial t} = -\nabla\vec{j}_m^{tot}(\vec{q},t). \tag{41}$$

We note here that Eqs. (40) and (41) are MPCEs, where mass densities and mass flux densities appear. Corresponding MPCEs for particle densities and particle flux densities can be derived.

2.3. *Derivation of the MPEEM*

As our next task, we start with the derivation of the many-particle Ehrenfest equation of motion (MPEEM) both for all particles and for particles of a certain sort A. Therefore, we calculate the time derivative of the flux density $\vec{j}_m^{\mathrm{A}}(\vec{q},t)$ for sort A. We do not regard the indistinguishability of the particles of each sort at the start of the following calculation but we will take this point into account later, because by applying this approach some details in this derivation can be treated more systematically. Thus, we start with the time derivative of Eq. (18) instead of Eq. (19) and transform it, using Eq. (5) for the momentum operator:

$$\begin{aligned}
\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t} &= \sum_{i=1}^{N(\mathrm{A})} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\ \frac{\partial}{\partial t} \Re\left[\Psi^*(\vec{Q},t)\ \hat{\vec{p}}_i^{\,\mathrm{A}}\ \Psi(\vec{Q},t)\right] \\
&= \sum_{i=1}^{N(\mathrm{A})} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}}) \frac{\partial}{\partial t} \Im\left[\hbar\ \Psi^*(\vec{Q},t)\ \nabla_i^{\mathrm{A}} \Psi(\vec{Q},t)\right].
\end{aligned} \tag{42}$$

Now, we transform the time derivative term in Eq. (42). Here, $q_{j\beta}^{\mathrm{B}}$ are the Cartesian components of the vector $\vec{q}_j^{\,\mathrm{B}}$. So, the index β is an element of the set $K_{\mathrm{Ca}} = \{x, y, z\}$:

$$\begin{aligned}
\hbar\ \frac{\partial}{\partial t} \Im\left[\Psi^* \nabla_i^{\mathrm{A}} \Psi\right] &= \hbar\ \Im\left[\left(\frac{\partial \Psi^*}{\partial t}\right) \nabla_i^{\mathrm{A}} \Psi + \Psi^* \nabla_i^{\mathrm{A}} \left(\frac{\partial \Psi}{\partial t}\right)\right] \\
&= \hbar\ \Im\left[\left(\frac{1}{\mathrm{i}\hbar} \hat{H} \Psi\right)^* \nabla_i^{\mathrm{A}} \Psi + \Psi^* \nabla_i^{\mathrm{A}} \left(\frac{1}{\mathrm{i}\hbar} \hat{H} \Psi\right)\right] \\
&= \Re\left\{\left[-\sum_{\mathrm{B}=1}^{N_S} \sum_{j=1}^{N(\mathrm{B})} \frac{\hbar^2}{2m_{\mathrm{B}}} \left(\triangle_j^{\mathrm{B}} \Psi^*\right) + \frac{1}{2} \sum_{\mathrm{B}=1}^{N_S} \sum_{j=1}^{N(\mathrm{B})} \sum_{\mathrm{C}=1}^{N_S} \sum_{k=1}^{N(\mathrm{C})} \Psi^* V_{jk}^{\mathrm{BC}}\right] (\nabla_i^{\mathrm{A}} \Psi)\right. \\
&\quad \left. + \Psi^* \nabla_i^{\mathrm{A}} \left[\sum_{\mathrm{B}=1}^{N_S} \sum_{j=1}^{N(\mathrm{B})} \frac{\hbar^2}{2m_{\mathrm{B}}} \triangle_j^{\mathrm{B}}\ \Psi - \frac{1}{2} \sum_{\mathrm{B}=1}^{N_S} \sum_{j=1}^{N(\mathrm{B})} \sum_{\mathrm{C}=1}^{N_S} \sum_{k=1}^{N(\mathrm{C})} V_{jk}^{\mathrm{BC}} \Psi\right]\right\} \\
&= \Re\left\{\sum_{\mathrm{B},j} \frac{\hbar^2}{2m_{\mathrm{B}}} \left[\Psi^* \nabla_i^{\mathrm{A}} \left(\triangle_j^{\mathrm{B}} \Psi\right) - \left(\triangle_j^{\mathrm{B}} \Psi^*\right) (\nabla_i^{\mathrm{A}} \Psi)\right]\right. \\
&\quad \left. + \frac{1}{2} \sum_{\mathrm{B},\mathrm{C},j,k} \Psi^* \left[V_{jk}^{\mathrm{BC}} \nabla_i^{\mathrm{A}} \Psi - \nabla_i^{\mathrm{A}} \left(V_{jk}^{\mathrm{BC}} \Psi\right)\right]\right\} \\
&= \Re\left\{\sum_{\mathrm{B},j} \frac{\hbar^2}{2m_{\mathrm{B}}} \sum_{\beta \in K_{\mathrm{Ca}}} \left[\Psi^* \nabla_i^{\mathrm{A}} \left(\frac{\partial^2 \Psi}{\partial q_{j\beta}^{\mathrm{B}} \partial q_{j\beta}^{\mathrm{B}}}\right) - \left(\frac{\partial^2 \Psi^*}{\partial q_{j\beta}^{\mathrm{B}} \partial q_{j\beta}^{\mathrm{B}}}\right) (\nabla_i^{\mathrm{A}} \Psi)\right]\right\} \\
&\quad - \frac{1}{2} |\Psi|^2 \sum_{\mathrm{B},\mathrm{C},j,k} \nabla_i^{\mathrm{A}} V_{jk}^{\mathrm{BC}} \\
&= \Re\left\{\sum_{\mathrm{B},j} \frac{\hbar^2}{2m_{\mathrm{B}}} \sum_{\beta \in K_{\mathrm{Ca}}} \left\{\frac{\partial}{\partial q_{j\beta}^{\mathrm{B}}} \left[\Psi^* \nabla_i^{\mathrm{A}} \left(\frac{\partial \Psi}{\partial q_{j\beta}^{\mathrm{B}}}\right)\right] - \left(\frac{\partial \Psi^*}{\partial q_{j\beta}^{\mathrm{B}}}\right) \nabla_i^{\mathrm{A}} \left(\frac{\partial \Psi}{\partial q_{j\beta}^{\mathrm{B}}}\right)\right.\right. \\
&\quad \left.\left. - \frac{\partial}{\partial q_{j\beta}^{\mathrm{B}}} \left[\left(\frac{\partial \Psi^*}{\partial q_{j\beta}^{\mathrm{B}}}\right) (\nabla_i^{\mathrm{A}} \Psi)\right] + \left(\frac{\partial \Psi^*}{\partial q_{j\beta}^{\mathrm{B}}}\right) \frac{\partial}{\partial q_{j\beta}^{\mathrm{B}}} (\nabla_i^{\mathrm{A}} \Psi)\right\}\right\} \\
&\quad - \frac{1}{2} D \sum_{\mathrm{B},\mathrm{C},j,k} \left(\delta_{ij} \delta_{\mathrm{AB}} \nabla_i^{\mathrm{A}} V_{ik}^{\mathrm{AC}} + \delta_{ik} \delta_{\mathrm{AC}} \nabla_i^{\mathrm{A}} V_{ji}^{\mathrm{BA}}\right)
\end{aligned} \tag{43}$$

$$= \Re\left\{\sum_{\mathrm{B},j}\frac{\hbar^2}{2m_{\mathrm{B}}}\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q^{\mathrm{B}}_{j\beta}}\left[\Psi^*\nabla^{\mathrm{A}}_i\left(\frac{\partial\Psi}{\partial q^{\mathrm{B}}_{j\beta}}\right)-\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{B}}_{j\beta}}\right)\left(\nabla^{\mathrm{A}}_i\Psi\right)\right]\right\}$$
$$- D\sum_{\mathrm{B},j}\nabla^{\mathrm{A}}_i V^{\mathrm{AB}}_{ij}. \tag{44}$$

With this result, we get the following intermediate result for $\frac{\partial\vec{j}^{\mathrm{A}}_m(\vec{q},t)}{\partial t}$:

$$\frac{\partial\vec{j}^{\mathrm{A}}_m(\vec{q},t)}{\partial t} = \sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_i)\frac{\hbar^2}{2m_{\mathrm{B}}}$$
$$\times\;\Re\left\{\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q^{\mathrm{B}}_{j\beta}}\left[\Psi^*\nabla^{\mathrm{A}}_i\left(\frac{\partial\Psi}{\partial q^{\mathrm{B}}_{j\beta}}\right)-\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{B}}_{j\beta}}\right)\left(\nabla^{\mathrm{A}}_i\Psi\right)\right]\right\}$$
$$-\sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_i)\;D\;\nabla^{\mathrm{A}}_i V^{\mathrm{AB}}_{ij}. \tag{45}$$

The term in the last line of Eq. (45) is the force density $\vec{f}^{\,\mathrm{A}}(\vec{q},t)$ for all particles of sort A; it is caused by the two-particle potential V^{AB}_{ij}:

$$\vec{f}^{\,\mathrm{A}}(\vec{q},t) = \sum_{i=1}^{N(\mathrm{A})}\left[-\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_i)\;D(\vec{Q},t)\;\nabla^{\mathrm{A}}_i V^{\mathrm{AB}}_{ij}\right]. \tag{46}$$

Note that in spite of Eq. (4) the summands in the triple sum are not antisymmetric relative to a permutation of $\{\mathrm{A},i\}\leftrightarrow\{\mathrm{B},j\}$ because of the argument $\vec{q}-\vec{q}^{\,\mathrm{A}}_i$ in the δ-function. This is related to the fact that the term in squared brackets in Eq. (46) is the force density for the (A,i) particle.

As the next step, we do a case-by-case analysis by splitting in Eq. (46) the sum over the sorts of particles B into a sum over the summands for $\mathrm{B}\neq\mathrm{A}$ and the remaining summand for $\mathrm{B}=\mathrm{A}$:

$$\vec{f}^{\,\mathrm{A}}(\vec{q},t) = -\sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1,\mathrm{B}\neq\mathrm{A}}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_i)\;D(\vec{Q},t)\;\nabla^{\mathrm{A}}_i V^{\mathrm{AB}}_{ij}$$
$$-\sum_{i=1}^{N(\mathrm{A})}\sum_{j=1}^{N(\mathrm{A})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_i)\;D(\vec{Q},t)\;\nabla^{\mathrm{A}}_i V^{\mathrm{AA}}_{ij}\,. \tag{47}$$

The first line in Eq. (47) is related to the case $\mathrm{B}\neq\mathrm{A}$, and the second line in this equation is related to the case $\mathrm{B}=\mathrm{A}$.

The interaction of a particle with itself is excluded because in Eq. (2) we defined $V^{\mathrm{AA}}_{ii}=0$. Thus, a particle of sort A can interact with $(N(\mathrm{A})-1)$ particles of its own sort and with $N(\mathrm{B})$ particles of sort B if $\mathrm{B}\neq\mathrm{A}$. Therefore, we evaluate the indistinguishability between particles of one sort in the following manner:

We substitute the sum over i in each of the first and second lines of Eq. (47) by its summand for $i=1$ multiplied by $N(\mathrm{A})$. Moreover, in the first line, we substitute the sum over j by its summand for

$j = N(\mathrm{B})$ multiplied by $N(\mathrm{B})$, and in the second line, we substitute the sum over j by its summand for $j = N(\mathrm{A})$ multiplied by $(N(\mathrm{A}) - 1)$. Combining these substitutions with the definition in Eq. (2) for the potential terms V_{ij}^{AB} leads to this result:

$$\vec{f}^{\,\mathrm{A}}(\vec{q}, t) = -\,N(\mathrm{A}) \left[\sum_{\mathrm{B}=1, \mathrm{B} \neq \mathrm{A}}^{N_S} N(\mathrm{B}) \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}), t)\; \nabla V^{\mathrm{AB}}(|\vec{q} - \vec{q}_{N(\mathrm{B})}^{\,B}|) \right]$$
$$-\; N(\mathrm{A})\,(N(\mathrm{A}) - 1) \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}), t)\; \nabla V^{\mathrm{AB}}(|\vec{q} - \vec{q}_{N(\mathrm{A})}^{\,\mathrm{A}}|). \tag{48}$$

The reader might wonder why we choose the last summand for $j = N(\mathrm{A})$ or $j = N(\mathrm{B})$, respectively, for the substitution of the sums over j in Eq. (47) and not, in a more obvious approach, the first summand for $j = 1$. The reason for this is that we have to make sure that we choose two different particles of sort A as representative particles for the consideration of the two-particle interaction between particles of sort A since the interaction of a particle with itself is excluded.

Here, the transformation of the second line of Eq. (47) into the term appearing in the second line of Eq. (48) can be interpreted in this manner: The $(\mathrm{A}, 1)$ particle and the $(\mathrm{A}, N(\mathrm{A}))$ particle are chosen as representative particles for the two-particle interaction between particles of sort A. This choice is appropriate because for $N(\mathrm{A}) > 1$, the $(\mathrm{A}, 1)$ particle and the $(\mathrm{A}, N(\mathrm{A}))$ particle are different particles. The $(\mathrm{A}, 1)$ particle and the $(\mathrm{A}, N(\mathrm{A}))$ particle are the same particle for the special case $N(\mathrm{A}) = 1$, however, but this case is still evaluated in Eq. (48) correctly, since for $N(\mathrm{A}) = 1$, the factor $(N(\mathrm{A}) - 1)$ in the second line of Eq. (48) is zero; thus we can say that for $N(\mathrm{A}) = 1$ the single particle of sort A cannot interact with other particles of sort A.

The above explanation gives a clear reason why we choose $j = N(\mathrm{A})$ instead of $j = 1$ for the transformation of the term appearing in the second line of Eq. (47). However, we could have used $j = 1$ for the transformation of the term appearing in the first line of Eq. (47) because it is related to interactions between particles of different sorts. But there we still used the last summand for $j = N(\mathrm{B})$ because, as a consequence, we can now combine the two lines in Eq. (48) in this compact final result for $\vec{f}^{\,\mathrm{A}}(\vec{q}, t)$:

$$\vec{f}^{\,\mathrm{A}}(\vec{q}, t) = -\,N(\mathrm{A}) \left[\sum_{\mathrm{B}=1}^{N_S} (N(\mathrm{B}) - \delta_{\mathrm{AB}}) \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}), t)\; \nabla V^{\mathrm{AB}}(|\vec{q} - \vec{q}_{N(\mathrm{B})}^{\,B}|) \right]. \tag{49}$$

As an additional result, we can now calculate the total force density $\vec{f}^{\,\mathrm{tot}}(\vec{q}, t)$ for all particles; it is given by:

$$\vec{f}^{\,\mathrm{tot}}(\vec{q}, t) = \sum_{\mathrm{A}=1}^{N_S} \vec{f}^{\,\mathrm{A}}(\vec{q}, t) \tag{50}$$
$$= -\sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})$$
$$\times \left[\sum_{\mathrm{B}=1}^{N_S} (N(\mathrm{B}) - \delta_{\mathrm{AB}}) \int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}), t)\; \nabla V^{\mathrm{AB}}(|\vec{q} - \vec{q}_{N(\mathrm{B})}^{\,\mathrm{B}}|) \right]. \tag{51}$$

In Ref. [38], a particle ensemble for two sorts of particles, namely electrons and one ion sort, is examined, and, for this case, the Coulomb force density for the electrons is shown. Equation (49) is a generalization of this result for an arbitrary number N_S of sorts of particles and any two-particle potential that can be described by Eq. (2).

Having discussed the force density term $\vec{f}^{\,\mathrm{A}}(\vec{q},t)$ in the intermediate result in Eq. (45) for $\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t}$, we will now analyze the remaining term.

Therefore, we define a vector $\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)$,

$$\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha) = \frac{\hbar^2}{2m_{\mathrm{B}}}\Re\left[\Psi^*\frac{\partial}{\partial q_{i\alpha}^{\mathrm{A}}}\left(\nabla_j^{\mathrm{B}}\Psi\right) - \nabla_j^{\mathrm{B}}\Psi^*\left(\frac{\partial\Psi}{\partial q_{i\alpha}^{\mathrm{A}}}\right)\right], \tag{52}$$

with a β component

$$x_{j\beta}^{\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha) = \frac{\hbar^2}{2m_{\mathrm{B}}}\Re\left[\Psi^*\frac{\partial}{\partial q_{i\alpha}^{\mathrm{A}}}\left(\frac{\partial\Psi}{\partial q_{j\beta}^{\mathrm{B}}}\right) - \left(\frac{\partial\Psi^*}{\partial q_{j\beta}^{\mathrm{B}}}\right)\left(\frac{\partial\Psi}{\partial q_{i\alpha}^{\mathrm{A}}}\right)\right]. \tag{53}$$

For the following calculation, it is advantageous to choose the notation above for the vector $\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)$ because here, gradient terms $\nabla_j^{\mathrm{B}}\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)$ of this vector appear. Therefore, we emphasize the dependence of the vector $\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)$ on j and B by writing j as a subscript and B as a superscript. Moreover, the remaining terms $\vec{Q},\mathrm{A},i$ and α are listed as additional parameters in brackets for the vector $\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)$.

With the definition in Eq. (52), the α component of $\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t}$ is given by:

$$\begin{aligned}\frac{\partial j_{m,\alpha}^{\mathrm{A}}(\vec{q},t)}{\partial t} &= f_\alpha^{\mathrm{A}}(\vec{q},t) + \sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}}) \\ &\quad\times \sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q_{i\beta}^{\mathrm{B}}}\left\{\frac{\hbar^2}{2m_{\mathrm{B}}}\Re\left[\Psi^*\frac{\partial}{\partial q_{i\alpha}^{\mathrm{A}}}\left(\frac{\partial\Psi}{\partial q_{j\beta}^{\mathrm{B}}}\right) - \left(\frac{\partial\Psi^*}{\partial q_{j\beta}^{\mathrm{B}}}\right)\left(\frac{\partial\Psi}{\partial q_{i\alpha}^{\mathrm{A}}}\right)\right]\right\} \\ &= f_\alpha^{\mathrm{A}}(\vec{q},t) + \sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\;\nabla_j^{\mathrm{B}}\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha).\end{aligned} \tag{54}$$

Now a case-by-case analysis is done for two different summand types in the triple sum over i,j, and B: For the first type, the tuple $\{\mathrm{A},i\}$ is not equal to the tuple $\{\mathrm{B},j\}$, and for the second type, these two tuples are equal. By separating these two summand types, we get:

$$\begin{aligned}\frac{\partial j_{m,\alpha}^{\mathrm{A}}(\vec{q},t)}{\partial t} &= f_\alpha^{\mathrm{A}}(\vec{q},t) \\ &\quad+ \sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{\substack{j=1\\ \{\mathrm{B},j\}\neq\{\mathrm{A},i\}}}^{N(\mathrm{B})}\int \mathrm{d}\vec{Q}_j^{\mathrm{B}}\;\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\int \mathrm{d}\vec{q}_j^{\,\mathrm{B}}\;\nabla_j^{\mathrm{B}}\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha) \\ &\quad+ \sum_{i=1}^{N(\mathrm{A})}\int \mathrm{d}\vec{Q}_i^{\mathrm{A}}\int \mathrm{d}\vec{q}_i^{\,\mathrm{A}}\;\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\;\left[\nabla_j^{\mathrm{B}}\vec{x}_j^{\,\mathrm{B}}(\vec{Q},\mathrm{A},i,\alpha)\right]_{\{\mathrm{B},j\}=\{\mathrm{A},i\}}.\end{aligned} \tag{55}$$

In the middle line of the equation above, a volume integral appears over the coordinate $\vec{q}_j^{\,\mathrm{B}}$. Using the divergence theorem, this integral can be converted into an integral of the system boundary surface where the wave function vanishes, so the full term in the middle line vanishes. However, the term in the last line does not vanish because the integrand for the integral over the coordinate $\vec{q}_i^{\,\mathrm{A}}$ contains the δ-function $\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})$. This context leads to:

$$\begin{aligned}\frac{\partial j^{\mathrm{A}}_{m,\alpha}(\vec{q},t)}{\partial t} &= f^{\mathrm{A}}_{\alpha}(\vec{q},t)\\ &\quad -\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q_\beta}\left\{-\sum_{i=1}^{N(\mathrm{A})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\frac{\hbar^2}{2m_{\mathrm{A}}}\Re\left[\Psi^*\frac{\partial}{\partial q^{\mathrm{A}}_{i\alpha}}\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{i\beta}}\right)-\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{A}}_{i\beta}}\right)\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{i\alpha}}\right)\right]\right\}.\end{aligned}\tag{56}$$

Then, we take into account the indistinguishability of the particles of one sort and find the following result for $\frac{\partial j^{\mathrm{A}}_{m,\alpha}(\vec{q},t)}{\partial t}$:

$$\begin{aligned}\frac{\partial j^{\mathrm{A}}_{m,\alpha}(\vec{q},t)}{\partial t} &= f^{\mathrm{A}}_{\alpha}(\vec{q},t)\\ &\quad -\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q_\beta}\left\{-N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\frac{\hbar^2}{2m_{\mathrm{A}}}\Re\left[\Psi^*\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\beta}}\right)-\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{A}}_{1\beta}}\right)\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\alpha}}\right)\right]\right\}.\end{aligned}\tag{57}$$

In the equation above, in the curly brackets, the components $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ of what is called the momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$ for particles of sort A appear:

$$\begin{aligned}\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) = &-N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\\ &\times\frac{\hbar^2}{2m_{\mathrm{A}}}\Re\left[\Psi^*\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\beta}}\right)-\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{A}}_{1\beta}}\right)\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\alpha}}\right)\right].\end{aligned}\tag{58}$$

By applying the formula $\Re(z)=(z+z^*)/2$ on the real part appearing in Eq. (58), we recognize the symmetry

$$\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)=\Pi^{\mathrm{A}}_{\beta\alpha}(\vec{q},t).\tag{59}$$

Thus, using Eqs. (58) and (59), we find that Eq. (57) can be written as:

$$\frac{\partial j^{\mathrm{A}}_{m,\alpha}(\vec{q},t)}{\partial t}=f^{\mathrm{A}}_{\alpha}(\vec{q},t)-\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial}{\partial q_\beta}\Pi^{\mathrm{A}}_{\beta\alpha}(\vec{q},t).\tag{60}$$

Here, we note that the divergence $\nabla\underline{\underline{T}}(\vec{q})$ of any second-rank tensor $\underline{\underline{T}}(\vec{q})$ is given by:

$$\nabla\underline{\underline{T}}(\vec{q})=\sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}}\frac{\partial T_{\alpha\beta}(\vec{q})}{\partial q_\alpha}\vec{e}_\beta.\tag{61}$$

The equation corresponding to Eq. (60) for the vector $\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t}$ is the sought MPEEM for all particles of sort A, and by applying Eq. (61) we can write this equation in the following form:

$$\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t} = \vec{f}^{\,\mathrm{A}}(\vec{q},t) - \nabla \underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t). \tag{62}$$

Our motivation to name the equation above the many-particle Ehrenfest equation of motion is the following: In Eq. (21), we defined the operator $\hat{\vec{j}}_m^{\mathrm{A}}(\vec{Q},\vec{q})$, and we can interpret the quantity $\vec{j}_m^{\mathrm{A}}(\vec{q},t)$ as the expectation value for it. So, the Ehrenfest theorem (Ref. [45] and Ref. [46], pp. 28ff) predicates that we can calculate the time derivative of the mass flux density for particles of sort A by this equation:

$$\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t} = \frac{\mathrm{i}}{\hbar} \int \mathrm{d}\vec{Q}\ \Psi^*(\vec{Q},t)\ \left[\hat{H}(\vec{Q}), \hat{\vec{j}}_m^{\mathrm{A}}(\vec{Q},\vec{q})\right]\ \Psi(\vec{Q},t). \tag{63}$$

Indeed, by combining Eqs. (42) and (43), one can realize that the equation above is equivalent to our result in Eq. (62) for $\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t}$. This concept of applying the Ehrenfest theorem to derive quantum hydrodynamical equations was already discussed by Epstein in Ref. [47].

As the next step, we discuss the fact that Eq. (58) is not our final result for the tensor components $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$. Instead, we will show two different ways to express them. For the first of these two ways, we note that with the definition in Eq. (5) for the canonical momentum operator $\hat{\vec{p}}_i^{\,\mathrm{A}}$ of the (A,i) particle, Eq. (58) can be rewritten as:

$$\begin{aligned}
\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) &= N(\mathrm{A}) \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}}) \times\ \frac{1}{2m_{\mathrm{A}}} \Re\left[\Psi^*\left(\hat{p}^{\mathrm{A}}_{1\alpha}\hat{p}^{\mathrm{A}}_{1\beta}\Psi\right) + \left(\hat{p}^{\mathrm{A}}_{1\beta}\Psi\right)^*\left(\hat{p}^{\mathrm{A}}_{1\alpha}\Psi\right)\right] \\
&= N(\mathrm{A}) \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\ \frac{1}{4m_{\mathrm{A}}} \\
&\quad \times \left[\Psi^*\left(\hat{p}^{\mathrm{A}}_{1\beta}\hat{p}^{\mathrm{A}}_{1\alpha}\Psi\right) + \left(\hat{p}^{\mathrm{A}}_{1\beta}\Psi\right)^*\left(\hat{p}^{\mathrm{A}}_{1\alpha}\Psi\right) + \left(\hat{p}^{\mathrm{A}}_{1\alpha}\Psi\right)^*\left(\hat{p}^{\mathrm{A}}_{1\beta}\Psi\right) + \left(\hat{p}^{\mathrm{A}}_{1\beta}\hat{p}^{\mathrm{A}}_{1\alpha}\Psi\right)^*\Psi\right]
\end{aligned} \tag{64}$$

To find the second way to express the tensor components $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$, we now transform two terms appearing in Eq. (58) using Eqs. (25) and (26). Here we have the transformation of the first term:

$$\begin{aligned}
\Re\left[\Psi^*\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\beta}}\right)\right] &= \Re\left\{a e^{-\mathrm{i}S/\hbar}\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left[\frac{\partial}{\partial q^{\mathrm{A}}_{1\beta}}\left(a e^{\mathrm{i}S/\hbar}\right)\right]\right\} \\
&= \Re\left[a\frac{\partial^2 a}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}} - \frac{1}{\hbar^2}a^2\frac{\partial S}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial S}{\partial q^{\mathrm{A}}_{1\beta}}\right. \\
&\quad \left. + \frac{\mathrm{i}}{\hbar}a\left(\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial S}{\partial q^{\mathrm{A}}_{1\beta}} + \frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}\frac{\partial S}{\partial q^{\mathrm{A}}_{1\alpha}} + a\frac{\partial^2 S}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}\right)\right] \\
&= -\,a^2\left(\frac{m_{\mathrm{A}}^2}{\hbar^2}w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta} - \frac{1}{a}\frac{\partial^2 a}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}\right).
\end{aligned} \tag{65}$$

And the transformation for the second term is:

$$
\begin{aligned}
-\Re\left[\left(\frac{\partial\Psi^*}{\partial q^{\mathrm{A}}_{1\beta}}\right)\left(\frac{\partial\Psi}{\partial q^{\mathrm{A}}_{1\alpha}}\right)\right] &= -\Re\left[\left(\frac{\partial\left(ae^{-\mathrm{i}S/\hbar}\right)}{\partial q^{\mathrm{A}}_{1\beta}}\right)\left(\frac{\partial\left(ae^{\mathrm{i}S/\hbar}\right)}{\partial q^{\mathrm{A}}_{1\alpha}}\right)\right] \\
&= -\Re\left\{\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}} + \frac{1}{\hbar^2}a^2\frac{\partial S}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial S}{\partial q^{\mathrm{A}}_{1\beta}}\right. \\
&\quad \left. + \frac{\mathrm{i}}{\hbar}a\left[\left(\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}\right)\left(\frac{\partial S}{\partial q^{\mathrm{A}}_{1\alpha}}\right) - \left(\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\right)\left(\frac{\partial S}{\partial q^{\mathrm{A}}_{1\beta}}\right)\right]\right\} \\
&= -a^2\left(\frac{m_{\mathrm{A}}^2}{\hbar^2}w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta} + \frac{1}{a^2}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}\right).
\end{aligned} \tag{66}
$$

Thus, by inserting Eqs. (65) and (66) into Eq. (58), we get as an intermediate result for the tensor elements:

$$
\begin{aligned}
\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) &= N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1) \\
&\quad \times\; a^2\left[m_{\mathrm{A}}w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta} - \frac{\hbar^2}{2m_{\mathrm{A}}}\left(\frac{1}{a}\frac{\partial^2 a}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}} - \frac{1}{a^2}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}\right)\right].
\end{aligned} \tag{67}
$$

Regarding $a^2 = D$, it can be derived that:

$$
\begin{aligned}
\frac{1}{2}\frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}} &= \frac{1}{2}\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{1}{D}\frac{\partial D}{\partial q^{\mathrm{A}}_{1\beta}}\right) = \frac{1}{2}\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{1}{a^2}\frac{\partial a^2}{\partial q^{\mathrm{A}}_{1\beta}}\right) \\
&= \frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{1}{a}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}\right) = \frac{1}{a}\frac{\partial^2 a}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}} - \frac{1}{a^2}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\alpha}}\frac{\partial a}{\partial q^{\mathrm{A}}_{1\beta}}.
\end{aligned} \tag{68}
$$

So we can write Eq. (67) in the following form, which is the second way to express $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$:

$$
\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) = N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\;D\left(m_{\mathrm{A}}w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta} - \frac{\hbar^2}{4m_{\mathrm{A}}}\frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}\right). \tag{69}
$$

Having found this result for $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$, we can define the elements $\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ of the momentum flow density tensor for all particles by:

$$
\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S}\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) \tag{70}
$$

$$
= \sum_{\mathrm{A}=1}^{N_S}N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\;D\left(m_{\mathrm{A}}w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta} - \frac{\hbar^2}{4m_{\mathrm{A}}}\frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}\right). \tag{71}
$$

Moreover, both the matrix elements $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ for a particular sort of particle A and the matrix elements $\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ for all particles can each be split into a classical part (cl) and a quantum part (qu):

$$
\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) = \Pi^{\mathrm{A,cl}}_{\alpha\beta}(\vec{q},t) + \Pi^{\mathrm{A,qu}}_{\alpha\beta}(\vec{q},t), \tag{72}
$$

$$
\Pi^{\mathrm{A,cl}}_{\alpha\beta}(\vec{q},t) = N(\mathrm{A})\,m_{\mathrm{A}}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\;D\;w^{\mathrm{A}}_{1\alpha}w^{\mathrm{A}}_{1\beta}, \tag{73}
$$

$$\Pi^{\mathrm{A,qu}}_{\alpha\beta}(\vec{q},t) = -\,\hbar^2 \frac{N(\mathrm{A})}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D \frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}, \tag{74}$$

$$\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t) = \Pi^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t) + \Pi^{\mathrm{tot,qu}}_{\alpha\beta}(\vec{q},t), \tag{75}$$

$$\Pi^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} \Pi^{\mathrm{A,cl}}_{\alpha\beta}(\vec{q},t) \;=\; \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D\ w^{\mathrm{A}}_{1\alpha} w^{\mathrm{A}}_{1\beta}, \tag{76}$$

$$\Pi^{\mathrm{tot,qu}}_{\alpha\beta}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} \Pi^{\mathrm{A,qu}}_{\alpha\beta}(\vec{q},t) \;=\; -\,\hbar^2 \sum_{\mathrm{A}=1}^{N_S} \frac{N(\mathrm{A})}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D \frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}. \tag{77}$$

So, the classical momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{A,cl}}(\vec{q},t)$ for the specific sort of particle A is related to a dyadic product of the velocity $\vec{w}^{\mathrm{A}}_1(\vec{Q},t)$ of the (A, 1) particle with itself:

$$\underline{\underline{\Pi}}^{\mathrm{A,cl}}(\vec{q},t) = N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D\ \left(\vec{w}^{\mathrm{A}}_1 \otimes \vec{w}^{\mathrm{A}}_1\right). \tag{78}$$

According to this point, the classical momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{tot,cl}}(\vec{q},t)$ for the total particle ensemble is related to dyadic products $\vec{w}^{\mathrm{A}}_1 \otimes \vec{w}^{\mathrm{A}}_1$ for all sorts of particles $\mathrm{A} \in \{1,\dots,N_S\}$:

$$\underline{\underline{\Pi}}^{\mathrm{tot,cl}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D\ \left(\vec{w}^{\mathrm{A}}_1 \otimes \vec{w}^{\mathrm{A}}_1\right). \tag{79}$$

This relation of the classical tensors $\underline{\underline{\Pi}}^{\mathrm{A,cl}}(\vec{q},t)$, $\underline{\underline{\Pi}}^{\mathrm{tot,cl}}(\vec{q},t)$ to dyadic products of particle velocities is an analog to the calculation of the momentum flow density tensor $\underline{\underline{\Pi}}$ in classical hydrodynamics: The equation which is a classical analog to the MPEEM can be found in Ref. [48], p. 32 and Ref. [49], p. 21. Viewing this equation, one can realize that in classical hydrodynamics, the momentum flow density tensor $\underline{\underline{\Pi}}$ contains dyadic products of particle velocities. So, this is why we name $\underline{\underline{\Pi}}^{\mathrm{A,cl}}(\vec{q},t)$, $\underline{\underline{\Pi}}^{\mathrm{tot,cl}}(\vec{q},t)$ classical tensors.

As a consequence of Eqs. (74) and (77), compact forms also exist for the quantum tensors $\underline{\underline{\Pi}}^{\mathrm{A,qu}}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{\mathrm{tot,qu}}(\vec{q},t)$:

$$\underline{\underline{\Pi}}^{\mathrm{A,qu}}(\vec{q},t) = -\,\hbar^2 \frac{N(\mathrm{A})}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D\ \left(\nabla^{\mathrm{A}}_1 \otimes \nabla^{\mathrm{A}}_1\right) \ln D, \tag{80}$$

$$\underline{\underline{\Pi}}^{\mathrm{tot,qu}}(\vec{q},t) = -\,\hbar^2 \sum_{\mathrm{A}=1}^{N_S} \frac{N(\mathrm{A})}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\ D\ \left(\nabla^{\mathrm{A}}_1 \otimes \nabla^{\mathrm{A}}_1\right) \ln D. \tag{81}$$

The term $\nabla^{\mathrm{A}}_1 \otimes \nabla^{\mathrm{A}}_1$ appearing in the two equations above is a dyadic product of the nabla operator ∇^{A}_1 for the (A, 1) particle. In contrast to the classical parts, both the quantum tensor $\underline{\underline{\Pi}}^{\mathrm{A,qu}}(\vec{q},t)$ for a certain sort of particle A and the quantum tensor $\underline{\underline{\Pi}}^{\mathrm{tot,qu}}(\vec{q},t)$ for the total particle ensemble are related only to properties of $D(\vec{Q},t)$, and they vanish in the limit $\hbar \to 0$. Therefore we name these tensors quantum tensors.

Finally, we can find, using Eqs. (72), (75), and (78)–(81), these compact forms for the tensors $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{\mathrm{tot}}(\vec{q},t)$:

$$\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t) = N(\mathrm{A}) \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\ D\ \times \left[m_{\mathrm{A}} \left(\vec{w}_1^{\,\mathrm{A}} \otimes \vec{w}_1^{\,\mathrm{A}} \right) - \frac{\hbar^2}{4m_{\mathrm{A}}} \left(\nabla_1^{\mathrm{A}} \otimes \nabla_1^{\mathrm{A}} \right) \ln D \right], \tag{82}$$

$$\underline{\underline{\Pi}}^{\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} \underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t) \tag{83}$$

$$= \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A}) \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\ D\ \times \left[m_{\mathrm{A}} \left(\vec{w}_1^{\,\mathrm{A}} \otimes \vec{w}_1^{\,\mathrm{A}} \right) - \frac{\hbar^2}{4m_{\mathrm{A}}} \left(\nabla_1^{\mathrm{A}} \otimes \nabla_1^{\mathrm{A}} \right) \ln D \right]. \tag{84}$$

As the next task, we sum the MPEEM for a certain sort of particle in Eq. (62) over all particle sorts $\mathrm{A} \in \{1, \ldots, N_S\}$. Then we note Eqs. (20), (50), and (83) for the quantities $\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t)$, $\vec{f}^{\,\mathrm{tot}}(\vec{q},t)$, and $\underline{\underline{\Pi}}^{\mathrm{tot}}(\vec{q},t)$, thus finding the MPEEM for all particles:

$$\frac{\partial \vec{j}_m^{\,\mathrm{tot}}(\vec{q},t)}{\partial t} = \vec{f}^{\,\mathrm{tot}}(\vec{q},t) - \nabla \underline{\underline{\Pi}}^{\mathrm{tot}}(\vec{q},t). \tag{85}$$

Therefore, there is an MPEEM both for all particles and for each sort of particle. The MPEEM for all sorts of particles in Eq. (85) can be solved numerically to find $\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t)$ if one knows $\vec{f}^{\,\mathrm{tot}}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{\mathrm{tot}}(\vec{q},t)$. In an analogous manner, the MPEEM for a certain sort of particle A in Eq. (62) can be solved numerically if $\vec{f}^{\,\mathrm{A}}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$ are known. Although one might wonder why this idea is interesting, since one can also calculate the mass current density $\vec{j}_m^{\,\mathrm{A}}(\vec{q},t)$ directly with Eq. (19) or the mass current density $\vec{j}_m^{\,\mathrm{tot}}(\vec{q},t)$ with Eq. (17), this is an important option for the numerical application of MPQHD. The reason for this is that there are cases of molecular systems where only a wave function $\Psi^{\mathrm{BO}}(\vec{Q},t)$ within the Born–Oppenheimer approximation is available and the direct calculation method for electronic mass current densities fails (Ref. [50]). Therefore, one has to search for alternative approaches to calculate the electronic mass current densities, and solving the MPEEM in Ref. (62) numerically for the case that the electrons of the molecular system are the particles of sort A could be an option.

Having derived the MPEEM both for all particles and for each sort of particle, we will now derive the corresponding MPQCEs.

2.4. *Derivation of the MPQCE*

The starting point for the derivation of the many-particle quantum Cauchy equation (MPQCE) for particles of sort A is the corresponding MPEEM in Eq. (62):

Taking into account the MPCE in Eq. (40) for particles of sort A, we transform the term $\frac{\partial \vec{j}_m^{\,\mathrm{A}}(\vec{q},t)}{\partial t}$ appearing in Eq. (62) (where $\vec{e}_\alpha, \alpha \in K_{\mathrm{Ca}}$ are the Cartesian unit vectors):

$$\begin{aligned} \frac{\partial \vec{j}_m^{\,\mathrm{A}}(\vec{q},t)}{\partial t} &= \frac{\partial}{\partial t}\left(\rho_m^{\mathrm{A}} \vec{v}^{\,\mathrm{A}}\right) = \frac{\partial \rho_m^{\mathrm{A}}}{\partial t} \vec{v}^{\,\mathrm{A}} + \rho_m^{\mathrm{A}} \frac{\partial \vec{v}^{\,\mathrm{A}}}{\partial t} \\ &= -\left(\nabla \vec{j}_m^{\,\mathrm{A}}\right) \vec{v}^{\,\mathrm{A}} + \rho_m^{\mathrm{A}} \frac{\partial \vec{v}^{\,\mathrm{A}}}{\partial t} \\ &= -\sum_{\alpha \in K_{\mathrm{Ca}}} \vec{e}_\alpha \left[v_\alpha^{\mathrm{A}} \left(\nabla \vec{j}_m^{\,\mathrm{A}} \right) \right] + \rho_m^{\mathrm{A}} \frac{\partial \vec{v}^{\,\mathrm{A}}}{\partial t} \end{aligned}$$

$$= -\sum_{\alpha\in K_{\mathrm{Ca}}} \vec{e}_\alpha \left[\nabla \left(\vec{j}_m^{\mathrm{A}} v_\alpha^{\mathrm{A}}\right)\right] + \underbrace{\sum_{\alpha\in K_{\mathrm{Ca}}} \vec{e}_\alpha \left[\vec{j}_m^{\mathrm{A}} \left(\nabla v_\alpha^{\mathrm{A}}\right)\right]}_{=\left(\rho_m^{\mathrm{A}}\vec{v}^{\mathrm{A}}\nabla\right)\vec{v}^{\mathrm{A}}} + \rho_m^{\mathrm{A}} \frac{\partial \vec{v}^{\mathrm{A}}}{\partial t}$$

$$= \rho_m^{\mathrm{A}} \left[\frac{\partial}{\partial t} + \left(\vec{v}^{\mathrm{A}}\nabla\right)\right]\vec{v}^{\mathrm{A}} - \sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}} \vec{e}_\alpha \left[\frac{\partial}{\partial q_\beta}\left(\rho_m^{\mathrm{A}} v_\beta^{\mathrm{A}} v_\alpha^{\mathrm{A}}\right)\right]$$

$$= \rho_m^{\mathrm{A}} \left[\frac{\partial}{\partial t} + \left(\vec{v}^{\mathrm{A}}\nabla\right)\right]\vec{v}^{\mathrm{A}} - \sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}} \frac{\partial\left(\rho_m^{\mathrm{A}} v_\alpha^{\mathrm{A}} v_\beta^{\mathrm{A}}\right)}{\partial q_\alpha}\vec{e}_\beta. \tag{86}$$

Applying the definition in Eq. (61) for tensor divergences and the notation used before for dyadic products, we get:

$$\frac{\partial \vec{j}_m^{\mathrm{A}}(\vec{q},t)}{\partial t} = \rho_m^{\mathrm{A}} \left[\frac{\partial}{\partial t} + \left(\vec{v}^{\mathrm{A}}\nabla\right)\right]\vec{v}^{\mathrm{A}} - \nabla\left[\rho_m^{\mathrm{A}}\left(\vec{v}^{\mathrm{A}}\otimes\vec{v}^{\mathrm{A}}\right)\right]. \tag{87}$$

Then, we insert Eq. (87) into Eq. (62) and find:

$$\rho_m^{\mathrm{A}} \left[\frac{\partial}{\partial t} + \left(\vec{v}^{\mathrm{A}}\nabla\right)\right]\vec{v}^{\mathrm{A}} = \vec{f}^{\,\mathrm{A}} - \nabla\left[\underline{\underline{\Pi}}^{\mathrm{A}} - \rho_m^{\mathrm{A}}\left(\vec{v}^{\mathrm{A}}\otimes\vec{v}^{\mathrm{A}}\right)\right]. \tag{88}$$

Now we introduce a new quantity called the pressure tensor $\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ for the sort of particle A:

$$\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t) = \underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t) - \rho_m^{\mathrm{A}}(\vec{q},t)\left[\vec{v}^{\mathrm{A}}(\vec{q},t)\otimes\vec{v}^{\mathrm{A}}(\vec{q},t)\right]. \tag{89}$$

More properties of this tensor are discussed in Sect. 2.5.

So, we get the MPQCE for the sort of particle A by combining Eqs. (88) and (89):

$$\rho_m^{\mathrm{A}}(\vec{q},t) \left[\frac{\partial}{\partial t} + \left(\vec{v}^{\mathrm{A}}(\vec{q},t)\nabla\right)\right]\vec{v}^{\mathrm{A}}(\vec{q},t) = \vec{f}^{\,\mathrm{A}}(\vec{q},t) - \nabla\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t). \tag{90}$$

Now we discuss why we name the equation above the many-particle quantum Cauchy equation:

In classical hydrodyamics, there is a differential equation named Cauchy's equation of motion, which is related to the momentum balance in a liquid. It is given by (see Ref. [51], p. 205 and Ref. [52]):

$$\rho_m(\vec{q},t)\frac{d\vec{v}(\vec{q},t)}{dt} = \vec{f}(\vec{q},t) + \nabla\underline{\underline{\sigma}}(\vec{q},t). \tag{91}$$

In the equation above, the quantity $\underline{\underline{\sigma}}(\vec{q},t)$ is the stress tensor. Moreover, the term $\frac{d\vec{v}(\vec{q},t)}{dt}$ is the total rate of change of the velocity and it is given by (Ref. [51], pp. 4–6):

$$\frac{d\vec{v}(\vec{q},t)}{dt} = \left[\frac{\partial}{\partial t} + \left(\vec{v}(\vec{q},t)\nabla\right)\right]\vec{v}(\vec{q},t). \tag{92}$$

This equation shows that the total rate of change of the velocity $\frac{d\vec{v}(\vec{q},t)}{dt}$ is given by the sum of two terms: The first term $\frac{\partial\vec{v}(\vec{q},t)}{\partial t}$ is the local rate of change of the velocity at a fixed position $\vec{q}$, and the second term $\left(\vec{v}(\vec{q},t)\nabla\right)\vec{v}(\vec{q},t)$ is related to the effect that the flow transports the fluid elements to other positions where the velocity of the streaming can differ.

If we now identify

$$\underline{\underline{\sigma}}(\vec{q},t) = -\underline{\underline{p}}(\vec{q},t), \tag{93}$$

and insert Eqs. (92) and (93) into Cauchy's equation of motion in Eq. (91), we realize that Cauchy's equation of motion indeed takes the form of the MPQCE in Eq. (90). So, the MPQCE, which we derived with basic quantum mechanics, is a quantum analog to Cauchy's equation of motion known in classical hydrodynamics.

We mention that in classical hydrodynamics, Cauchy's equation of motion becomes the Navier–Stokes equation by applying the approximation

$$\nabla\underline{\underline{\sigma}}(\vec{q},t) \approx -\nabla P(\vec{q},t) + \eta\,\Delta\vec{v}(\vec{q},t) + \left(\zeta + \frac{\eta}{3}\right)\nabla\left(\nabla\vec{v}(\vec{q},t)\right), \tag{94}$$

where $P(\vec{q},t)$ is the scalar pressure, and ζ and η are called coefficients of viscosity. So, the Navier–Stokes equation has the following form (Ref. [5], pp. 44f):[1]

$$\begin{aligned}\rho_m(\vec{q},t)&\left[\frac{\partial}{\partial t} + (\vec{v}(\vec{q},t)\nabla)\right]\vec{v}(\vec{q},t)\\ &= \vec{f}(\vec{q},t) - \nabla P(\vec{q},t) + \eta\,\Delta\vec{v}(\vec{q},t) + \left(\zeta + \frac{\eta}{3}\right)\nabla\left(\nabla\vec{v}(\vec{q},t)\right).\end{aligned} \tag{95}$$

In Ref. [9], Harvey called the MPQCE in Eq. (90) for the case of a quantum system for a single particle the "quantum-mechanical Navier–Stokes equation". However, we think that this analogy is less precise than the analogy of the MPQCE in Eq. (90) to Cauchy's equation of motion in Eq. (91). The reason for this is that the analogy of the tensor gradient term $-\nabla\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ appearing in the MPQCE in Eq. (90) to the tensor gradient term $\nabla\underline{\underline{\sigma}}(\vec{q},t) = -\nabla\underline{\underline{p}}(\vec{q},t)$ in Cauchy's equation of motion is much closer than the analogy of the mentioned tensor gradient term $-\nabla\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ to the complicated term $-\nabla P(\vec{q},t) + \eta\,\Delta\vec{v}(\vec{q},t) + (\zeta + \frac{\eta}{3})\nabla(\nabla\vec{v}(\vec{q},t))$ in the Navier–Stokes equation in Eq. (95).

As the next step, we derive the MPQCE for all particles. The MPQCEs that are specific for a certain sort of particle are non-linear differential equations because of the non-linear term $\rho_m^{\mathrm{A}}\left(\vec{v}^{\mathrm{A}}\nabla\right)\vec{v}^{\mathrm{A}}$ in Eq. (90). Therefore, we cannot derive the MPQCE for all particles just by summing up all the MPQCEs specific for a certain sort of particle.

Here, one realizes a contrast to the derivation of the MPCE and the MPEEM for the total particle ensemble [see Eqs. (41) and (85)], which could be derived by summing all the corresponding equations for the particular sorts of particles [see Eqs. (40) and (62)]. This context is related to the point that both the MPCE and the MPEEM for a particular sort of particle and the corresponding equations for the total particle ensemble are linear differential equations for which the superposition principle is true, which says that linear combinations of their solutions form new solutions of these equations.

However, the following derivation for the MPQCE for all particles is still quite similar to the derivation of Eq. (90) because the MPQCE for all particles can be derived from the MPEEM in Eq. (85) for all particles in an analogous manner to the way the MPQCE in Eq. (90) specific to a certain sort of particle can be derived from the MPEEM in Eq. (62) for a certain sort of particle.

[1] In Ref. [5], pp. 44f, a Navier–Stokes equation is derived where the force density $\vec{f}$ is neglected, but one can find in the literature other versions of the Navier–Stokes equation with a non-vanishing $\vec{f}$ (Ref. [51], p. 208). Moreover, one can realize easily by comparing the calculations in Ref. [5], p. 3 and Ref. [5], pp. 44f how one can derive a Navier–Stokes equation that includes a force density $\vec{f}$.

Therefore, we find a new expression for the time derivative term $\frac{\partial \vec{j}_m^{\text{tot}}(\vec{q},t)}{\partial t}$ in Eq. (85), and doing so, we insert the MPCE from Eq. (41) for all particles:

$$
\begin{aligned}
\frac{\partial \vec{j}_m^{\text{tot}}(\vec{q},t)}{\partial t} &= \frac{\partial}{\partial t}\left(\rho_m^{\text{tot}}\vec{v}^{\,\text{tot}}\right) = \frac{\partial \rho_m^{\text{tot}}}{\partial t}\vec{v}^{\,\text{tot}} + \rho_m^{\text{tot}}\frac{\partial \vec{v}^{\,\text{tot}}}{\partial t} \\
&= -\left(\nabla \vec{j}_m^{\text{tot}}\right)\vec{v}^{\,\text{tot}} + \rho_m^{\text{tot}}\frac{\partial \vec{v}^{\,\text{tot}}}{\partial t} \\
&= -\sum_{\alpha\in K_{\text{Ca}}} \vec{e}_\alpha \left[v_\alpha^{\text{tot}}\left(\nabla \vec{j}_m^{\text{tot}}\right)\right] + \rho_m^{\text{tot}}\frac{\partial \vec{v}^{\,\text{tot}}}{\partial t} \\
&= -\sum_{\alpha\in K_{\text{Ca}}} \vec{e}_\alpha \left[\nabla\left(\vec{j}_m^{\text{tot}} v_\alpha^{\text{tot}}\right)\right] + \underbrace{\sum_{\alpha\in K_{\text{Ca}}} \vec{e}_\alpha \left[\vec{j}_m^{\text{tot}}\left(\nabla v_\alpha^{\text{tot}}\right)\right]}_{=\left(\rho_m^{\text{tot}}\vec{v}^{\,\text{tot}}\nabla\right)\vec{v}^{\,\text{tot}}} + \rho_m^{\text{tot}}\frac{\partial \vec{v}^{\,\text{tot}}}{\partial t} \\
&= \rho_m^{\text{tot}}\left[\frac{\partial}{\partial t} + \left(\vec{v}^{\,\text{tot}}\nabla\right)\right]\vec{v}^{\,\text{tot}} - \sum_{\alpha\in K_{\text{Ca}}}\sum_{\beta\in K_{\text{Ca}}} \vec{e}_\alpha \left[\frac{\partial}{\partial q_\beta}\left(\rho_m^{\text{tot}} v_\beta^{\text{tot}} v_\alpha^{\text{tot}}\right)\right] \\
&= \rho_m^{\text{tot}}\left[\frac{\partial}{\partial t} + \left(\vec{v}^{\,\text{tot}}\nabla\right)\right]\vec{v}^{\,\text{tot}} - \sum_{\alpha\in K_{\text{Ca}}}\sum_{\beta\in K_{\text{Ca}}} \frac{\partial\left(\rho_m^{\text{tot}} v_\alpha^{\text{tot}} v_\beta^{\text{tot}}\right)}{\partial q_\alpha}\vec{e}_\beta.
\end{aligned} \tag{96}
$$

Regarding the tensor divergence definition in Eq. (61), we now write the last term in the equation above as a tensor divergence:

$$
\frac{\partial \vec{j}_m^{\text{tot}}(\vec{q},t)}{\partial t} = \rho_m^{\text{tot}}\left[\frac{\partial}{\partial t} + \left(\vec{v}^{\,\text{tot}}\nabla\right)\right]\vec{v}^{\,\text{tot}} - \nabla\left[\rho_m^{\text{tot}}\left(\vec{v}^{\,\text{tot}}\otimes\vec{v}^{\,\text{tot}}\right)\right]. \tag{97}
$$

After that, we use Eq. (97) for a transformation of Eq. (85) and find:

$$
\rho_m^{\text{tot}}\left[\frac{\partial}{\partial t} + \left(\vec{v}^{\,\text{tot}}\nabla\right)\right]\vec{v}^{\,\text{tot}} = \vec{f}^{\,\text{tot}} - \nabla\left[\underline{\underline{\Pi}}^{\text{tot}} - \rho_m^{\text{tot}}\left(\vec{v}^{\,\text{tot}}\otimes\vec{v}^{\,\text{tot}}\right)\right]. \tag{98}
$$

Here, a new quantity is introduced called the pressure tensor $\underline{\underline{p}}^{\text{tot}}(\vec{q},t)$ for the total particle ensemble:

$$
\underline{\underline{p}}^{\text{tot}}(\vec{q},t) = \underline{\underline{\Pi}}^{\text{tot}}(\vec{q},t) - \rho_m^{\text{tot}}(\vec{q},t)\left[\vec{v}^{\,\text{tot}}(\vec{q},t)\otimes\vec{v}^{\,\text{tot}}(\vec{q},t)\right]. \tag{99}
$$

We will discuss this tensor in more detail in Sect. 2.5.

Finally, we insert Eq. (99) for $\underline{\underline{p}}^{\text{tot}}(\vec{q},t)$ into Eq. (98) and get the MPQCE for the total ensemble of particles:

$$
\rho_m^{\text{tot}}(\vec{q},t)\left[\frac{\partial}{\partial t} + \left(\vec{v}^{\,\text{tot}}(\vec{q},t)\nabla\right)\right]\vec{v}^{\,\text{tot}}(\vec{q},t) = \vec{f}^{\,\text{tot}}(\vec{q},t) - \nabla\underline{\underline{p}}^{\text{tot}}(\vec{q},t). \tag{100}
$$

As the next issue, we investigate the properties of the pressure tensors $\underline{\underline{p}}^{\text{A}}(\vec{q},t)$, $\underline{\underline{p}}^{\text{tot}}(\vec{q},t)$.

2.5. *Pressure tensor*

We define the pressure tensor $\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ for the sort of particle A as:

$$\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t) := N(\mathrm{A}) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D\; \times \\ \left[m_{\mathrm{A}} \left(\vec{u}_1^{\mathrm{A}} \otimes \vec{u}_1^{\mathrm{A}} \right) - \frac{\hbar^2}{4m_{\mathrm{A}}} \left(\nabla_1^{\mathrm{A}} \otimes \nabla_1^{\mathrm{A}} \right) \ln D \right], \tag{101}$$

so that its components are given by:

$$p_{\alpha\beta}^{\mathrm{A}}(\vec{q},t) = N(\mathrm{A}) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D \left(m_{\mathrm{A}} u_{1\alpha}^{\mathrm{A}} u_{1\beta}^{\mathrm{A}} - \frac{\hbar^2}{4m_{\mathrm{A}}} \frac{\partial^2 \ln D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\beta}^{\mathrm{A}}} \right). \tag{102}$$

Moreover, we define the pressure tensor $\underline{\underline{p}}^{\mathrm{tot}}(\vec{q},t)$ for the total particle ensemble as:

$$\underline{\underline{p}}^{\mathrm{tot}}(\vec{q},t) := \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A}) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D\; \times \\ \left[m_{\mathrm{A}} \left(\vec{\mathrm{u}}_1^{\mathrm{A}} \otimes \vec{\mathrm{u}}_1^{\mathrm{A}} \right) - \frac{\hbar^2}{4m_{\mathrm{A}}} \left(\nabla_1^{\mathrm{A}} \otimes \nabla_1^{\mathrm{A}} \right) \ln D \right], \tag{103}$$

and we can write its components as follows:

$$p_{\alpha\beta}^{\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A}) \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D \left(m_{\mathrm{A}} \mathrm{u}_{1\alpha}^{\mathrm{A}} \mathrm{u}_{1\beta}^{\mathrm{A}} - \frac{\hbar^2}{4m_{\mathrm{A}}} \frac{\partial^2 \ln D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\beta}^{\mathrm{A}}} \right). \tag{104}$$

At the end of this subsection we will prove that the definition in Eq. (101) for $\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ is equivalent to Eq. (89), and that the definition in Eq. (103) for $\underline{\underline{p}}^{\mathrm{tot}}(\vec{q},t)$ is equivalent to Eq. (99).

Before we do that, we will first discuss that we can split both the tensor components $p_{\alpha\beta}^{\mathrm{A}}(\vec{q},t)$ and $p_{\alpha\beta}^{\mathrm{tot}}(\vec{q},t)$ into a classical part and a quantum part in a similar manner to the tensor components $\Pi_{\alpha\beta}^{\mathrm{A}}(\vec{q},t)$ and $\Pi_{\alpha\beta}^{\mathrm{tot}}(\vec{q},t)$—we mention here that splitting the pressure tensor components into classical and quantum parts was already described by Wong (Ref. [28]):

$$p_{\alpha\beta}^{\mathrm{A}}(\vec{q},t) = p_{\alpha\beta}^{\mathrm{A,cl}}(\vec{q},t) + p_{\alpha\beta}^{\mathrm{A,qu}}(\vec{q},t), \tag{105}$$

$$p_{\alpha\beta}^{\mathrm{A,cl}}(\vec{q},t) = N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D\; u_{1\alpha}^{\mathrm{A}} u_{1\beta}^{\mathrm{A}}, \tag{106}$$

$$p_{\alpha\beta}^{\mathrm{A,qu}}(\vec{q},t) = -\,\hbar^2 \frac{N(\mathrm{A})}{4m_{\mathrm{A}}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D \frac{\partial^2 \ln D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\beta}^{\mathrm{A}}}, \tag{107}$$

$$p_{\alpha\beta}^{\mathrm{tot}}(\vec{q},t) = p_{\alpha\beta}^{\mathrm{tot,cl}}(\vec{q},t) + p_{\alpha\beta}^{\mathrm{tot,qu}}(\vec{q},t), \tag{108}$$

$$p_{\alpha\beta}^{\mathrm{tot,cl}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D\; \mathrm{u}_{1\alpha}^{\mathrm{A}} \mathrm{u}_{1\beta}^{\mathrm{A}}, \tag{109}$$

$$p_{\alpha\beta}^{\mathrm{tot,qu}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} p_{\alpha\beta}^{\mathrm{A,qu}}(\vec{q},t) \;=\; -\,\hbar^2 \sum_{\mathrm{A}=1}^{N_S} \frac{N(\mathrm{A})}{4m_{\mathrm{A}}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\; D \frac{\partial^2 \ln D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\beta}^{\mathrm{A}}}. \tag{110}$$

Note that

$$p^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t) \neq \sum_{\mathrm{A}=1}^{N_S} p^{\mathrm{A,cl}}_{\alpha\beta}(\vec{q},t) \tag{111}$$

$$\Longrightarrow \quad p^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t) \neq \sum_{\mathrm{A}=1}^{N_S} p^{\mathrm{A}}_{\alpha\beta}(\vec{q},t), \tag{112}$$

because in Eq. (102), components of the velocity $\vec{u}^{\mathrm{A}}_1(\vec{Q},t)$ appear which are defined by the velocity of the (A, 1) particle relative to the mean particle velocity $\vec{v}^{\mathrm{A}}(\vec{q}^{\,\mathrm{A}}_1,t)$ of particles of sort A, while in Eq. (104), components of the velocity $\vec{\mathrm{u}}^{\mathrm{A}}_1(\vec{Q},t)$ appear which are defined by the velocity of the (A, 1) particle relative to the mean particle velocity $\vec{v}^{\,\mathrm{tot}}(\vec{q}^{\,\mathrm{A}}_1,t)$ for the total particle ensemble.

The inequality in Eq. (112) can be related to the fact mentioned above that the MPQCE in Eq. (90) for a certain sort of particle is a non-linear differential equation. So, the sum over this equation for all the different sorts of particles does not yield the MPQCE in Eq. (100) for the total particle ensemble. Thus, it is reasonable that the sum over all sorts of particles for the pressure tensors $p^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ on the right-hand side of Eq. (112) does not yield the pressure tensor $p^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ for the total particle ensemble.

Moreover, we can write the classical pressure tensor $\underline{\underline{p}}^{\mathrm{A,cl}}(\vec{q},t)$ for a specific sort of particle A in a compact tensor notation, where a dyadic product of the relative velocity $\vec{u}^{\mathrm{A}}_1(\vec{Q},t)$ of the (A, 1) particle appears:

$$\underline{\underline{p}}^{\mathrm{A,cl}}(\vec{q},t) = N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\; D\;\left(\vec{u}^{\mathrm{A}}_1 \otimes \vec{u}^{\mathrm{A}}_1\right). \tag{113}$$

In an analogous manner, the classical pressure tensor $\underline{\underline{p}}^{\mathrm{tot,cl}}(\vec{q},t)$ for the total particle ensemble is related to dyadic products $\vec{\mathrm{u}}^{\mathrm{A}}_1 \otimes \vec{\mathrm{u}}^{\mathrm{A}}_1$ for all sorts of particles $\mathrm{A} \in \{1,\dots,N_S\}$:

$$\underline{\underline{p}}^{\mathrm{tot,cl}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\; D\;\left(\vec{\mathrm{u}}^{\mathrm{A}}_1 \otimes \vec{\mathrm{u}}^{\mathrm{A}}_1\right). \tag{114}$$

This relation of the classical pressure tensors $\underline{\underline{p}}^{\mathrm{A,cl}}(\vec{q},t)$, $\underline{\underline{p}}^{\mathrm{tot,cl}}(\vec{q},t)$ to dyadic products of relative particle velocities is an analog to the calculation of the pressure tensor $\underline{\underline{p}}$ in classical hydrodynamics (Ref. [48], p. 32; Ref. [49], p. 21). So, this is the motivation to call $\underline{\underline{p}}^{\mathrm{A,cl}}(\vec{q},t)$ and $\underline{\underline{p}}^{\mathrm{tot,cl}}(\vec{q},t)$ classical tensors.

As a remark, we note that for the special case of a one-particle system, the associated classical pressure tensor $\underline{\underline{p}}^{\mathrm{cl}}$ vanishes. The reason for this is that for this system, the mean particle velocity $\vec{v}$ and the velocity $\vec{w}$ of the single particle are obviously the same, so the relative velocity $\vec{u}$ of this particle vanishes. Since the classical pressure tensor $\underline{\underline{p}}^{\mathrm{cl}}$ depends on the dyadic product $\vec{u} \otimes \vec{u}$, the classical pressure tensor $\underline{\underline{p}}^{\mathrm{cl}}$ thus vanishes too. Therefore, the classical pressure tensor does not appear in the analysis of one-particle systems in Refs. [13,16–18], or in Ref. [42], pp. 56f. Please note that for a one-particle system the classical momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{cl}}$ does not vanish generally because the particle velocity $\vec{w}$ does not vanish for some one-particle systems (for such a case, see the analysis in Chapter 13 of Ref. [42]).

Now we turn our focus back to many-particle systems with different sorts of particles. For these systems, both the quantum pressure tensor elements $p^{\mathrm{A,qu}}_{\alpha\beta}(\vec{q},t)$ for a certain sort of particle A and the quantum pressure tensor elements $p^{\text{tot,qu}}_{\alpha\beta}(\vec{q},t)$ for the total particle ensemble are just equal to the corresponding quantum momentum flow density tensor elements:

$$p^{\text{A,qu}}_{\alpha\beta}(\vec{q},t) = \Pi^{\text{A,qu}}_{\alpha\beta}(\vec{q},t), \tag{115}$$

$$p^{\text{tot,qu}}_{\alpha\beta}(\vec{q},t) = \Pi^{\text{tot,qu}}_{\alpha\beta}(\vec{q},t), \tag{116}$$

so that we can write, for the corresponding tensors,

$$\underline{\underline{p}}^{\text{A,qu}}(\vec{q},t) = \underline{\underline{\Pi}}^{\text{A,qu}}(\vec{q},t) = -\hbar^2 \frac{N(\text{A})}{4m_\text{A}} \int \text{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\text{A}}_1)\; D\; \left(\nabla^\text{A}_1 \otimes \nabla^\text{A}_1\right) \ln D, \tag{117}$$

$$\underline{\underline{p}}^{\text{tot,qu}}(\vec{q},t) = \underline{\underline{\Pi}}^{\text{tot,qu}}(\vec{q},t) = -\hbar^2 \sum_{\text{A}=1}^{N_S} \frac{N(\text{A})}{4m_\text{A}} \int \text{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\text{A}}_1)\; D\; \left(\nabla^\text{A}_1 \otimes \nabla^\text{A}_1\right) \ln D. \tag{118}$$

Thus, like the quantum momentum flow density tensors $\underline{\underline{\Pi}}^{\text{A,qu}}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{\text{tot,qu}}(\vec{q},t)$, both the quantum pressure tensor $\underline{\underline{p}}^{\text{A,qu}}(\vec{q},t)$ specific to a given sort A of particles and the quantum pressure tensor $\underline{\underline{p}}^{\text{tot,qu}}(\vec{q},t)$ for the total particle ensemble are related only to properties of $D(\vec{Q},t)$, and they vanish in the limit $\hbar \to 0$. Now it becomes clear why we named $\underline{\underline{p}}^{\text{A,qu}}(\vec{q},t)$ and $\underline{\underline{p}}^{\text{tot,qu}}(\vec{q},t)$ quantum tensors.

To end this section, we prove here that the definition in Eq. (101) for $\underline{\underline{p}}^{\text{A}}(\vec{q},t)$ is equivalent to Eq. (89), and the definition in Eq. (103) for $\underline{\underline{p}}^{\text{tot}}(\vec{q},t)$ is equivalent to Eq. (99). In order to prove the equivalence of Eqs. (101) and (89), we show that the quantity $p^{\text{A,cl}}_{\alpha\beta}(\vec{q},t)$ can be expressed in the following way by applying Eqs. (13), (30), (31), (73), and (106):

$$\begin{aligned}
p^{\text{A,cl}}_{\alpha\beta}(\vec{q},t) &= N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\text{A}}_1)\; D(\vec{Q},t)\; u^\text{A}_{1\alpha}(\vec{Q},t)\; u^\text{A}_{1\beta}(\vec{Q},t) \\
&= N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\text{A}}_1)\; D(\vec{Q},t)\; \times \\
&\quad \left[w^\text{A}_{1\alpha}(\vec{Q},t) - v^\text{A}_\alpha(\vec{q}^{\,\text{A}}_1,t)\right] \left[w^\text{A}_{1\beta}(\vec{Q},t) - v^\text{A}_\beta(\vec{q}^{\,\text{A}}_1,t)\right] \\
&= \underbrace{N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}^\text{A}_1\; D(\vec{Q}^\text{A}_1(\vec{q}),t)\; w^\text{A}_{1\alpha}(\vec{Q}^\text{A}_1(\vec{q}),t)\; w^\text{A}_{1\beta}(\vec{Q}^\text{A}_1(\vec{q}),t)}_{=\Pi^{\text{A,cl}}_{\alpha\beta}(\vec{q},t)} \\
&\quad - v^\text{A}_\alpha(\vec{q},t)\; \underbrace{N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}^\text{A}_1\; D(\vec{Q}^\text{A}_1(\vec{q}),t)\; w^\text{A}_{1\beta}(\vec{Q}^\text{A}_1(\vec{q}),t)}_{=j^\text{A}_{m,\beta}(\vec{q},t)\,=\,\rho^\text{A}_m(\vec{q},t)\; v^\text{A}_\beta(\vec{q},t)} \\
&\quad - v^\text{A}_\beta(\vec{q},t)\; \underbrace{N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}^\text{A}_1\; D(\vec{Q}^\text{A}_1(\vec{q}),t)\; w^\text{A}_{1\alpha}(\vec{Q}^\text{A}_1(\vec{q}),t)}_{=j^\text{A}_{m,\alpha}(\vec{q},t)\,=\,\rho^\text{A}_m(\vec{q},t)\; v^\text{A}_\alpha(\vec{q},t)} \\
&\quad + v^\text{A}_\alpha(\vec{q},t)\; v^\text{A}_\beta(\vec{q},t)\; \underbrace{N(\text{A})\, m_\text{A} \int \text{d}\vec{Q}^\text{A}_1\; D(\vec{Q}^\text{A}_1(\vec{q}),t)}_{=\rho^\text{A}_m(\vec{q},t)} \\
&= \Pi^{\text{A,cl}}_{\alpha\beta}(\vec{q},t) - \rho^\text{A}_m(\vec{q},t)\; v^\text{A}_\alpha(\vec{q},t)\; v^\text{A}_\beta(\vec{q},t).
\end{aligned} \tag{119}$$

Then, we find a formula that relates the pressure tensor elements $p^\text{A}_{\alpha\beta}(\vec{q},t)$ for the sort of particle A with the corresponding momentum flow density tensor elements $\Pi^\text{A}_{\alpha\beta}(\vec{q},t)$ by adding Eq. (115)

and Eq. (119):

$$p^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) = \Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) - \rho^{\mathrm{A}}_{m}(\vec{q},t)\; v^{\mathrm{A}}_{\alpha}(\vec{q},t)\; v^{\mathrm{A}}_{\beta}(\vec{q},t). \tag{120}$$

One can find similar equations in classical hydrodynamics (Ref. [5], pp. 11 and 44). Rewriting the equation above as an equation for tensors instead of their components, we find just Eq. (89)—so we have shown the equivalence of Eqs. (89) and (101).

Finally, it remains to show that Eqs. (99) and (103) are equivalent equations for the calculation of $\underline{\underline{p}}^{\mathrm{tot}}(\vec{q},t)$. For this derivation, the quantity $p^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t)$ is transformed by Eqs. (12), (29), (35), (76), and (109) analogously to how Eq. (119) was derived:

$$\begin{aligned}
p^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t) &= \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\; D(\vec{Q},t)\; \mathrm{u}^{\mathrm{A}}_{1\alpha}(\vec{Q},t)\; \mathrm{u}^{\mathrm{A}}_{1\beta}(\vec{Q},t) \\
&= \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\; D(\vec{Q},t)\;\times \\
&\quad \left[w^{\mathrm{A}}_{1\alpha}(\vec{Q},t) - v^{\mathrm{tot}}_{\alpha}(\vec{q}^{\,\mathrm{A}}_1,t)\right]\left[w^{\mathrm{A}}_{1\beta}(\vec{Q},t) - v^{\mathrm{tot}}_{\beta}(\vec{q}^{\,\mathrm{A}}_1,t)\right] \\
&= \underbrace{\sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}^{\mathrm{A}}_1\; D(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)\; w^{\mathrm{A}}_{1\alpha}(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)\; w^{\mathrm{A}}_{1\beta}(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)}_{=\,\Pi^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t)} \\
&\quad -\; v^{\mathrm{tot}}_{\alpha}(\vec{q},t)\; \underbrace{\sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}^{\mathrm{A}}_1\; D(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)\; w^{\mathrm{A}}_{1\beta}(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)}_{=\,j^{\mathrm{tot}}_{m,\beta}(\vec{q},t)\,=\,\rho^{\mathrm{tot}}_{m}(\vec{q},t)\; v^{\mathrm{tot}}_{\beta}(\vec{q},t)} \\
&\quad -\; v^{\mathrm{tot}}_{\beta}(\vec{q},t)\; \underbrace{\sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}^{\mathrm{A}}_1\; D(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)\; w^{\mathrm{A}}_{1\alpha}(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)}_{=\,j^{\mathrm{tot}}_{m,\alpha}(\vec{q},t)\,=\,\rho^{\mathrm{tot}}_{m}(\vec{q},t)\; v^{\mathrm{tot}}_{\alpha}(\vec{q},t)} \\
&\quad +\; v^{\mathrm{tot}}_{\alpha}(\vec{q},t)\; v^{\mathrm{tot}}_{\beta}(\vec{q},t)\; \underbrace{\sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}^{\mathrm{A}}_1\; D(\vec{Q}^{\mathrm{A}}_1(\vec{q}),t)}_{=\,\rho^{\mathrm{tot}}_{m}(\vec{q},t)} \\
&= \Pi^{\mathrm{tot,cl}}_{\alpha\beta}(\vec{q},t) - \rho^{\mathrm{tot}}_{m}(\vec{q},t)\; v^{\mathrm{tot}}_{\alpha}(\vec{q},t)\; v^{\mathrm{tot}}_{\beta}(\vec{q},t).
\end{aligned} \tag{121}$$

Summing Eqs. (116) and (121), we obtain a formula that relates the tensor elements $p^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ and $\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ to each other:

$$p^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t) = \Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t) - \rho^{\mathrm{tot}}_{m}(\vec{q},t)\; v^{\mathrm{tot}}_{\alpha}(\vec{q},t)\; v^{\mathrm{tot}}_{\beta}(\vec{q},t). \tag{122}$$

By writing the equation above in a representation with tensors instead of tensor components, we find Eq. (99). So, the proof of the equivalence of Eqs. (99) and (103) is provided.

2.6. External fields

In this subsection we now briefly discuss which basic formulas and main results of the derivations above change if external electric and magnetic fields $\vec{\mathcal{E}}(\vec{q},t)$, $\vec{\mathcal{B}}(\vec{q},t)$ are present. Here, we mention that the following results are similar to the results in Ref. [31], where analogous equations for MPQHD were similarly derived; however, in Ref. [31], first, the presence of different sorts was not discussed, and second, external fields were taken into account. These fields are described by a vector potential $\vec{\mathcal{A}}(\vec{q},t)$ and a scalar potential $\Phi(\vec{q},t)$ by

$$\vec{\mathcal{B}}(\vec{q},t) = \nabla \times \vec{\mathcal{A}}(\vec{q},t), \tag{123}$$

$$\vec{\mathcal{E}}(\vec{q},t) = -\nabla\Phi(\vec{q},t) - \frac{\partial \vec{\mathcal{A}}(\vec{q},t)}{\partial t}. \tag{124}$$

Moreover, we introduce the kinematic momentum operator $\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}}$; it is given by

$$\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}} = \hat{\vec{p}}_i^{\mathrm{A}} - e_{\mathrm{A}}\vec{\mathcal{A}}(\vec{q}_i^{\mathrm{A}},t). \tag{125}$$

Our analysis above without external fields held $\vec{\mathcal{A}}(\vec{q},t) = \vec{0}$, so there was no need to distinguish between the kinematic momentum operator $\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}}$ and the canonical momentum operator $\hat{\vec{p}}_i^{\mathrm{A}}$. But now we analyze situations where, in general, this is not true anymore, and we have to distinguish these operators. As a rule, in all the equations we previously derived for the field-free case, where the canonical momentum operator $\hat{\vec{p}}_i^{\mathrm{A}}$ appears, it has to be substituted in these equations by the kinematic momentum operator $\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}}$ for the presence of external fields.

Now, the Hamilton operator has this time-dependent form instead of Eq. (7):

$$\hat{H}(\vec{Q},t) = \sum_{\mathrm{A}=1}^{N_S}\sum_{i=1}^{N(\mathrm{A})}\left[\frac{(\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}})^2}{2m_{\mathrm{A}}} + e_{\mathrm{A}}\Phi(\vec{q}_i^{\mathrm{A}},t)\right] + \frac{1}{2}\sum_{\mathrm{A}=1}^{N_S}\sum_{i=1}^{N(\mathrm{A})}\sum_{\mathrm{B}=1}^{N_S}\sum_{j=1}^{N(\mathrm{B})} V_{ij}^{\mathrm{AB}}. \tag{126}$$

For the total particle mass current density $\vec{j}_m^{\mathrm{tot}}(\vec{q},t)$, we find instead of Eqs. (15) and (17):

$$\vec{j}_m^{\mathrm{tot}}(\vec{q},t) = \sum_{\mathrm{A}=1}^{N_S}\sum_{i=1}^{N(\mathrm{A})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_i^{\mathrm{A}})\;\Re\left[\Psi^*(\vec{Q},t)\;\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}}\;\Psi(\vec{Q},t)\right] \tag{127}$$

$$= \sum_{\mathrm{A}=1}^{N_S} N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\mathrm{A}})\;\Re\left[\Psi^*(\vec{Q},t)\;\hat{\vec{\mathcal{D}}}_1^{\mathrm{A}}\;\Psi(\vec{Q},t)\right], \tag{128}$$

so the particle mass current density $\vec{j}_m^{\mathrm{A}}(\vec{q},t)$ for the sort of particle A is now described by

$$\vec{j}_m^{\mathrm{A}}(\vec{q},t) = \sum_{i=1}^{N(\mathrm{A})}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_i^{\mathrm{A}})\;\Re\left[\Psi^*(\vec{Q},t)\;\hat{\vec{\mathcal{D}}}_i^{\mathrm{A}}\;\Psi(\vec{Q},t)\right] \tag{129}$$

$$= N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\mathrm{A}})\;\Re\left[\Psi^*(\vec{Q},t)\;\hat{\vec{\mathcal{D}}}_1^{\mathrm{A}}\;\Psi(\vec{Q},t)\right] \tag{130}$$

instead of Eqs. (18) and (19).

Moreover, the definition of the velocity $\vec{w}_i^{\mathrm{A}}(\vec{Q},t)$ for the (A, i) particle shown in Eq. (26) changes:

$$\vec{w}_i^{\mathrm{A}}(\vec{Q},t) = \frac{1}{m_{\mathrm{A}}}\left(\nabla_i^{\mathrm{A}} S(\vec{Q},t) - e_{\mathrm{A}}\vec{\mathcal{A}}(\vec{q}_i^{\mathrm{A}},t)\right). \tag{131}$$

While the rotation of the velocity $\vec{w}_i^{\mathrm{A}}(\vec{Q},t)$ described by Eq. (26) always vanishes, this is not true anymore for the more general Eq. (131) for $\vec{w}_i^{\mathrm{A}}(\vec{Q},t)$:

As a consequence of Eqs. (123) and (131), we find that

$$\nabla_i^{\mathrm{A}} \times \vec{w}_i^{\mathrm{A}}(\vec{Q},t) = -\frac{e_{\mathrm{A}}}{m_{\mathrm{A}}}\vec{\mathcal{B}}(\vec{q},t). \tag{132}$$

In addition, we note that the old formulas in Eqs. (29) and (30) for $\vec{j}_m^{\mathrm{tot}}(\vec{q},t)$ or $\vec{j}_m^{\mathrm{A}}(\vec{q},t)$, respectively, do not change explicitly for the case that external fields are present. However, an implicit change occurs due to the changed definition for the velocity $\vec{w}_i^{\mathrm{A}}(\vec{Q},t)$. Applying the same arguments, Eq. (23) for $\vec{v}^{\mathrm{A}}(\vec{q},t)$, Eq. (31) for $\vec{u}_i^{\mathrm{A}}(\vec{Q},t)$, Eq. (33) for $\vec{v}^{\,\mathrm{tot}}(\vec{q},t)$, and Eq. (35) for $\vec{\mathrm{u}}_i^{\mathrm{A}}(\vec{Q},t)$ do not change explicitly, but they do change implicitly for the presence of external fields.

Moreover, the force density $\vec{f}^{\,\mathrm{A}}(\vec{q},t)$ for the particles of sort A is now described by the following equation, which replaces Eq. (49):

$$\begin{aligned}\vec{f}^{\,\mathrm{A}}(\vec{q},t) = &- N(\mathrm{A})\left[\sum_{\mathrm{B}=1}^{N_S}(N(\mathrm{B})-\delta_{\mathrm{AB}})\int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t)\nabla V^{\mathrm{AB}}(|\vec{q}-\vec{q}^{\,\mathrm{B}}_{N(\mathrm{B})}|)\right] \\ &+ \frac{e_{\mathrm{A}}}{m_{\mathrm{A}}}\rho_m^{\mathrm{A}}(\vec{q},t)\left[\vec{\mathcal{E}}(\vec{q},t)+\vec{v}^{\mathrm{A}}(\vec{q},t)\times\vec{\mathcal{B}}(\vec{q},t)\right].\end{aligned} \tag{133}$$

In the second line of Eq. (133), extra terms relative to Eq. (49) appear because of the external fields. We did not derive Eq. (133) here in detail, but the extra field terms in this equation are intuitively clear.

So, the force density $\vec{f}^{\,\mathrm{tot}}(\vec{q},t)$ for all particles is given for the presence of external fields by

$$\begin{aligned}\vec{f}^{\,\mathrm{tot}}(\vec{q},t) = -\sum_{\mathrm{A}=1}^{N_S}\Bigg\{&N(\mathrm{A})\left[\sum_{\mathrm{B}=1}^{N_S}(N(\mathrm{B})-\delta_{\mathrm{AB}})\int \mathrm{d}\vec{Q}_1^{\mathrm{A}}\; D(\vec{Q}_1^{\mathrm{A}}(\vec{q}),t)\nabla V^{\mathrm{AB}}(|\vec{q}-\vec{q}^{\,\mathrm{B}}_{N(\mathrm{B})}|)\right] \\ &+ \frac{e_{\mathrm{A}}}{m_{\mathrm{A}}}\rho_m^{\mathrm{A}}(\vec{q},t)\left[\vec{\mathcal{E}}(\vec{q},t)+\vec{v}^{\mathrm{A}}(\vec{q},t)\times\vec{\mathcal{B}}(\vec{q},t)\right]\Bigg\},\end{aligned} \tag{134}$$

which replaces Eq. (51).

In addition, in the old calculations we found two different representations for the momentum flow density tensor elements $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ of sort A. The first one is Eq. (64), which contains components of the canonical momentum flow operator $\hat{\vec{p}}_1^{\mathrm{A}}$. For the presence of external fields, these components must be exchanged because of the rule mentioned above by the components of the corresponding kinematic momentum operator $\hat{\vec{\mathcal{D}}}_1^{\mathrm{A}}$:

$$\begin{aligned}\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t) = N(\mathrm{A})\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\;\frac{1}{4m_{\mathrm{A}}} \\ \times\left[\Psi^*\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\beta}\hat{\mathcal{D}}^{\mathrm{A}}_{1\alpha}\Psi\right)+\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\beta}\Psi\right)^*\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\alpha}\Psi\right)+\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\alpha}\Psi\right)^*\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\beta}\Psi\right)+\left(\hat{\mathcal{D}}^{\mathrm{A}}_{1\beta}\hat{\mathcal{D}}^{\mathrm{A}}_{1\alpha}\Psi\right)^*\Psi\right].\end{aligned} \tag{135}$$

The second one is Eq. (69), which contains components of the vector $\vec{w}_1^{\mathrm{A}}(\vec{Q},t)$. This representation for the tensor elements $\Pi^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ does not change explicitly, but it changes implicitly because for the presence of external fields, the new formula in Eq. (131) holds for the vector $\vec{w}_1^{\mathrm{A}}(\vec{Q},t)$. Applying an analogous argument, it can be found that the formula in Eq. (71) for the momentum flow density tensor elements $\Pi^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ for the total particle ensemble does not change explicitly but implicitly, too.

It can be found for the pressure tensor elements $p^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ and $p^{\mathrm{tot}}_{\alpha\beta}(\vec{q},t)$ that the corresponding Eqs. (102) and (104) remain valid explicitly. However, implicit changes occur due to the components of the velocities $\vec{u}^{\mathrm{A}}_1(\vec{Q},t)$ and $\vec{\mathrm{u}}^{\mathrm{A}}_1(\vec{Q},t)$ appearing in Eq. (102) or Eq. (104), respectively.

Taking all these changes into account for the different quantities discussed above, we eventually find that both for a certain sort of particle A and the total particle ensemble the corresponding MPCEs, MPEEMs, and MPQCEs given in Eqs. (40), (41), (62), (85), (90), and (100) remain valid explicitly for the presence of external fields.

For all the following considerations we assume that no external fields are present.

3. Transformations of the $\underline{\underline{\Pi}}$ and $\underline{\underline{p}}$ tensors

The following analysis is done for quantities for a particular sort of particle denoted by a corresponding index A. It can be made in an analogous way for the corresponding quantities for the total particle ensemble denoted with the index tot. Since we focus in our following analysis on quantities for a particular sort of particle A, we will only indicate by the index A quantities that are related to this sort of particle, but we will not mention this explicitly from now on.

3.1. Kuzmenkov tensors $\underline{\underline{\Pi}}^{K\mathrm{A}}$ and $\underline{\underline{p}}^{K\mathrm{A}}$

In the calculations above we found the formula in Eq. (69) for the elements of the momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$, and the formula in Eq. (102) for the elements of the pressure tensor $\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$. Since these equations are similar to results stated in Ref. [31], from now on we call these tensors, and their corresponding quantum parts and classical parts, Kuzmenkov tensors and denote them with a superscript K.

Due to Eqs. (78) and (113), the classical Kuzmenkov tensors $\underline{\underline{\Pi}}^{K\mathrm{A,cl}}(\vec{q},t)$ and $\underline{\underline{p}}^{K\mathrm{A,cl}}(\vec{q},t)$ are related to dyadic products $\vec{w}^{\mathrm{A}}_1 \otimes \vec{w}^{\mathrm{A}}_1$ or $\vec{u}^{\mathrm{A}}_1 \otimes \vec{u}^{\mathrm{A}}_1$, respectively. So, as mentioned above, these tensors are related to the momentum flow density tensor $\underline{\underline{\Pi}}$ or to the pressure tensor $\underline{\underline{p}}$, respectively, in classical hydrodynamics, and their interpretation is clear.

However, a clear interpretation for the quantum quantities $\underline{\underline{\Pi}}^{K\mathrm{A,qu}}(\vec{q},t)$, $\underline{\underline{p}}^{K\mathrm{A,qu}}(\vec{q},t)$ is missing except for the aspect that they are related to quantum effects. This problem occurs because the term $D\left(\nabla^{\mathrm{A}}_1 \otimes \nabla^{\mathrm{A}}_1\right)\ln D$ appearing in Eq. (117) for these quantities is difficult to understand. In order to close this gap, an alternative to the Kuzmenkov versions $\underline{\underline{\Pi}}^{K\mathrm{A}}(\vec{q},t)$ and $\underline{\underline{p}}^{K\mathrm{A}}(\vec{q},t)$ of the momentum flow density tensor and the pressure tensor is analyzed in Sect. 3.2.

3.2. Wyatt tensors $\underline{\underline{\Pi}}^{W\mathrm{A}}$ and $\underline{\underline{p}}^{W\mathrm{A}}$

The formula (1.57) in R. E. Wyatt's book (Ref. [42], p. 31) implies that the momentum flow density tensor $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$ can be calculated in the following manner (here, $\underline{1}$ is the unit matrix):

$$\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q},t) = \underline{1}P_{\mathrm{A}} + \sum_{i=1}^{N(\mathrm{A})} m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\mathrm{A}}_i)\ D\left[\left(\vec{w}^{\mathrm{A}}_i \otimes \vec{w}^{\mathrm{A}}_i\right) + \left(\vec{d}^{\mathrm{A}}_i \otimes \vec{d}^{\mathrm{A}}_i\right)\right], \tag{136}$$

so that its elements are given for Cartesian coordinates by:

$$\Pi^{W\mathrm{A}}_{\alpha\beta}(\vec{q},t) = P_{\mathrm{A}}\delta_{\alpha\beta} + \sum_{i=1}^{N(\mathrm{A})} m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q}-\vec{q}^{\mathrm{A}}_i)\ D\ \left(w^{\mathrm{A}}_{i\alpha}w^{\mathrm{A}}_{i\beta} + d^{\mathrm{A}}_{i\alpha}d^{\mathrm{A}}_{i\beta}\right). \tag{137}$$

The extra upper superscript W in the equations above for the tensor $\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q},t)$ and its elements $\Pi^{W\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ refers to the fact that this is a version of the tensor $\underline{\underline{\Pi}}^{\mathrm{A}}(\vec{q},t)$ related to Ref. [42].

The quantity P_A appearing in Eqs. (136) and (137) is the scalar quantum pressure given by:

$$P_\mathrm{A}(\vec{q},t) = -\sum_{i=1}^{N(\mathrm{A})} \frac{\hbar^2}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_i^{\,\mathrm{A}})\, \Delta_i^\mathrm{A} D. \tag{138}$$

The naming of the scalar quantum pressure comes from the dependence of $P_\mathrm{A}(\vec{q},t)$ on the probability density $D(\vec{Q},t)$, which is a pure quantum density.

In addition, in Eq. (136) the dyadic product of a vector $\vec{d}_i^{\,\mathrm{A}}$ appears; this vector is defined by

$$\vec{d}_i^{\,\mathrm{A}}(\vec{Q},t) = -\frac{\hbar}{2m_\mathrm{A}} \frac{\nabla_i^\mathrm{A} D}{D}. \tag{139}$$

This vector $\vec{d}_i^{\,\mathrm{A}}(\vec{Q},t)$ is named the osmotic velocity of the (A, i) particle, corresponding to the nomenclature in Ref. [42], p. 327. It is the quantum analog of the particle velocity $\vec{w}_i^{\,\mathrm{A}}(\vec{Q},t)$, and it is related to the shape of $D(\vec{Q},t)$.

It can be shown in a straightforward calculation that the rotation of the osmotic velocity $\vec{d}_i^{\,\mathrm{A}}(\vec{Q},t)$ relative to the coordinate $\vec{q}_i^{\,\mathrm{A}}$ vanishes:

$$\begin{aligned}
\nabla_i^\mathrm{A} \times \vec{d}_i^{\,\mathrm{A}}(\vec{Q},t) &= -\frac{\hbar}{2m_\mathrm{A}} \nabla_i^\mathrm{A} \times \left(\frac{1}{D}\nabla_i^\mathrm{A} D\right) \\
&= -\frac{\hbar}{2m_\mathrm{A}} \left\{ \frac{1}{D} \underbrace{\nabla_i^\mathrm{A} \times (\nabla_i^\mathrm{A} D)}_{=\vec{0}} + \left[\nabla_i^\mathrm{A}\left(\frac{1}{D}\right)\right] \times (\nabla_i^\mathrm{A} D) \right\} \\
&= \frac{\hbar}{2m_\mathrm{A}} \frac{1}{D^2} \underbrace{\left[(\nabla_i^\mathrm{A} D) \times (\nabla_i^\mathrm{A} D)\right]}_{=\vec{0}}.
\end{aligned} \tag{140}$$

Due to the indistinguishability of the particles of sort A, we can also write Eqs. (136), (137), and (138) in the form

$$\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q},t) = \underline{\underline{1}} P_\mathrm{A} + N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\, D \left[\left(\vec{w}_1^{\,\mathrm{A}} \otimes \vec{w}_1^{\,\mathrm{A}}\right) + \left(\vec{d}_1^{\,\mathrm{A}} \otimes \vec{d}_1^{\,\mathrm{A}}\right) \right], \tag{141}$$

$$\Pi^{W\mathrm{A}}_{\alpha\beta}(\vec{q},t) = P_\mathrm{A}\delta_{\alpha\beta} + N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\, D \left(w^\mathrm{A}_{1\alpha} w^\mathrm{A}_{1\beta} + d^\mathrm{A}_{1\alpha} d^\mathrm{A}_{1\beta} \right), \tag{142}$$

$$P_\mathrm{A}(\vec{q},t) = -N(\mathrm{A}) \frac{\hbar^2}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q}-\vec{q}_1^{\,\mathrm{A}})\, \Delta_1^\mathrm{A} D. \tag{143}$$

In order to achieve a better understanding of the different meanings of the particle velocities $\vec{d}_i^{\,\mathrm{A}}(\vec{Q},t)$ and $\vec{w}_i^{\,\mathrm{A}}(\vec{Q},t)$, we calculate, as a small excursion, the velocities w and d for a one-dimensional free Gaussian wave packet for a single particle at the start time $t = 0$. In the literature (Refs. [13,21,22], and Ref. [42], p. 327), this system is popular for the explanation of hydrodynamical quantities. The wave function $\Psi(x, t = 0)$ of this Gaussian wave packet is given by:

$$\Psi(x,0) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{4}} e^{-x^2/(4\sigma^2)} e^{ik_0 x}. \tag{144}$$

Here, σ is related to the width of the wave packet and k_0 is a space- and time-independent wave number. Then, we find:

$$S(x, 0) = \hbar k_0 x, \tag{145}$$

$$D(x, 0) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}} e^{-x^2/(2\sigma^2)}, \tag{146}$$

and the velocities w and d are given by:

$$w(x, 0) = \frac{1}{m}\frac{\partial S}{\partial x} = \frac{\hbar k_0}{m}, \tag{147}$$

$$d(x, 0) = -\frac{\hbar}{2m}\frac{1}{D}\frac{\partial D}{\partial x} = \frac{\hbar}{2m\sigma^2}x. \tag{148}$$

Thus, at $t = 0$, the whole wave packet $\Psi(x, 0)$ moves like a classical particle with a corresponding velocity $w = \hbar k_0/m$, independent of the position x.

As a supplement to this result, it can be shown in a straightforward calculation that the expectation value $\langle\hat{p}\rangle$ of the momentum operator $\hat{p} = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$ for the wave function $\Psi(x, 0)$ is given by

$$\langle\hat{p}\rangle = \langle\Psi(x, 0)\,|\,\hat{p}\,|\,\Psi(x, 0)\rangle = \hbar k_0 = mw. \tag{149}$$

Moreover, the wave packet disperses due to the shape of $D(x, 0)$, and this dispersion can be explained with additional movements of local parts of the wave packet $\Psi(x, 0)$. These dispersion movements vary depending on what part of the wave packet is considered, and they are described by the osmotic velocity $d(x, 0)$. In particular, $d(x, 0)$ is proportional to the position x, so for $x > 0$, this velocity is positive and is related to a forward movement of the front wave packet shoulder; for $x < 0$, it is negative and is related to a rear movement of the backward wave packet shoulder (for this dispersion discussion see also Ref. [13] and Ref. [42], p. 327).

Resuming our general analysis, as can be realized from Eqs. (82) and (101), one can get the pressure tensor by substituting the particle velocities $\vec{w}_1^{\mathrm{A}}(\vec{Q}, t)$ in the equation for the momentum flow density tensor by the corresponding relative velocities $\vec{u}_1^{\mathrm{A}}(\vec{Q}, t)$. So, using Eq. (141) for $\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t)$ as a starting point, we get a "Wyatt version" $\underline{\underline{p}}^{W\mathrm{A}}(\vec{q}, t)$ of the pressure tensor. This tensor and its elements are:

$$\underline{\underline{p}}^{W\mathrm{A}}(\vec{q}, t) = \underline{\underline{1}}P_{\mathrm{A}} + N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\mathrm{A}})\, D\left[\left(\vec{u}_1^{\mathrm{A}} \otimes \vec{u}_1^{\mathrm{A}}\right) + \left(\vec{d}_1^{\mathrm{A}} \otimes \vec{d}_1^{\mathrm{A}}\right)\right], \tag{150}$$

$$p_{\alpha\beta}^{W\mathrm{A}}(\vec{q}, t) = P_{\mathrm{A}}\delta_{\alpha\beta} + N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\mathrm{A}})\; D\;\left(u_{1\alpha}^{\mathrm{A}} u_{1\beta}^{\mathrm{A}} + d_{1\alpha}^{\mathrm{A}} d_{1\beta}^{\mathrm{A}}\right). \tag{151}$$

So, due to Eqs. (78), (113), (141), and (150), we can split each of the Wyatt tensors $\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t)$ and $\underline{\underline{p}}^{W\mathrm{A}}(\vec{q}, t)$ into a classical part and a quantum part in the following form:

$$\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t) = \underline{\underline{\Pi}}^{W\mathrm{A,cl}}(\vec{q}, t) \;+\; \underline{\underline{\Pi}}^{W\mathrm{A,qu}}(\vec{q}, t), \tag{152}$$

$$\underline{\underline{\Pi}}^{W\mathrm{A,cl}}(\vec{q}, t) = \underline{\underline{\Pi}}^{K\mathrm{A,cl}}(\vec{q}, t) \;=\; N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\mathrm{A}})\; D\left(\vec{w}_1^{\mathrm{A}} \otimes \vec{w}_1^{\mathrm{A}}\right), \tag{153}$$

$$\underline{\underline{\Pi}}^{WA,qu}(\vec{q},t) = \underline{\underline{1}}P_A + N(A)\, m_A \int d\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\,A})\, D\left(\vec{d}_1^{\,A} \otimes \vec{d}_1^{\,A}\right), \tag{154}$$

$$\underline{\underline{p}}^{WA}(\vec{q},t) = \underline{\underline{p}}^{WA,cl}(\vec{q},t) \;+\; \underline{\underline{p}}^{WA,qu}(\vec{q},t), \tag{155}$$

$$\underline{\underline{p}}^{WA,cl}(\vec{q},t) = \underline{\underline{p}}^{KA,cl}(\vec{q},t) \;=\; N(A)\, m_A \int d\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\,A})\, D\left(\vec{u}_1^{\,A} \otimes \vec{u}_1^{\,A}\right), \tag{156}$$

$$\underline{\underline{p}}^{WA,qu}(\vec{q},t) = \underline{\underline{\Pi}}^{WA,qu}(\vec{q},t) \;=\; \underline{\underline{1}}P_A + N(A)\, m_A \int d\vec{Q}\; \delta(\vec{q} - \vec{q}_1^{\,A})\, D\left(\vec{d}_1^{\,A} \otimes \vec{d}_1^{\,A}\right). \tag{157}$$

From these equations we realize that for the Wyatt tensors $\underline{\underline{\Pi}}^{WA}(\vec{q},t)$ and $\underline{\underline{p}}^{WA}(\vec{q},t)$, their quantum parts are related to dyadic products $\vec{d}_1^{\,A}\otimes\vec{d}_1^{\,A}$ of the osmotic velocity $\vec{d}_1^{\,A}(\vec{Q},t)$ and to the scalar quantum pressure $P_A(\vec{q},t)$. So, the advantage of the Wyatt tensor versions $\underline{\underline{\Pi}}^{WA}(\vec{q},t)$ and $\underline{\underline{p}}^{WA}(\vec{q},t)$ relative to the corresponding Kuzmenkov tensors is that their quantum parts $\underline{\underline{\Pi}}^{WA,qu}(\vec{q},t)$ and $\underline{\underline{p}}^{WA,qu}(\vec{q},t)$, which are identical, are more straightforward to interpret.

Now, it remains to show that the Wyatt tensors $\underline{\underline{\Pi}}^{WA}(\vec{q},t)$ and $\underline{\underline{p}}^{WA}(\vec{q},t)$ are physically equivalent to the corresponding Kuzmenkov tensors $\underline{\underline{\Pi}}^{KA}(\vec{q},t)$ or $\underline{\underline{p}}^{KA}(\vec{q},t)$, respectively. First, we explain this proof for the pressure tensors $\underline{\underline{p}}^{WA}(\vec{q},t)$ and $\underline{\underline{p}}^{KA}(\vec{q},t)$.

As will be shown below, the Wyatt pressure tensor $\underline{\underline{p}}^{WA}(\vec{q},t)$ is in general not equal to the Kuzmenkov pressure tensor $\underline{\underline{p}}^{KA}(\vec{q},t)$:

$$\underline{\underline{p}}^{WA}(\vec{q},t) \neq \underline{\underline{p}}^{KA}(\vec{q},t). \tag{158}$$

However, it will also be shown below that

$$\nabla\underline{\underline{p}}^{WA}(\vec{q},t) = \nabla\underline{\underline{p}}^{KA}(\vec{q},t) \tag{159}$$

holds, so that both tensors lead to an equivalent input in the MPQCE in Eq. (90)—this is the property that makes them physically equivalent.

So, as a general statement, for a pressure tensor $\underline{\underline{p}}(\vec{q},t)$ only its divergence $\nabla\underline{\underline{p}}(\vec{q},t)$ is physically important, and in this sense it behaves like a scalar potential $\phi(\vec{q},t)$ for which only the gradient $\nabla\phi(\vec{q},t)$ is physically important. Note here that both $\nabla\underline{\underline{p}}(\vec{q},t)$ and $\nabla\phi(\vec{q},t)$ are vectors. Thus, for pressure tensors $\underline{\underline{p}}(\vec{q},t)$ and for the scalar potential $\phi(\vec{q},t)$ mentioned above, we can apply both transformations that keep $\nabla\underline{\underline{p}}(\vec{q},t)$ or $\nabla\phi(\vec{q},t)$, respectively, constant. For the scalar potential $\nabla\phi(\vec{q},t)$, the only degree of freedom for such a transformation is an additive constant independent of the position $\vec{q}$. However, since in Cartesian coordinates the divergence of the tensor $\nabla\underline{\underline{p}}(\vec{q},t)$ is calculated by

$$\nabla\underline{\underline{p}}(\vec{q},t) = \begin{pmatrix} \frac{\partial p_{xx}}{\partial x} + \frac{\partial p_{yx}}{\partial y} + \frac{\partial p_{zx}}{\partial z} \\ \frac{\partial p_{xy}}{\partial x} + \frac{\partial p_{yy}}{\partial y} + \frac{\partial p_{zy}}{\partial z} \\ \frac{\partial p_{xz}}{\partial x} + \frac{\partial p_{yz}}{\partial y} + \frac{\partial p_{zz}}{\partial z} \end{pmatrix}, \tag{160}$$

there are transformations for the different pressure tensor elements $p_{\alpha\beta}(\vec{q},t)$ that make the coordinate derivatives of these tensor elements vary but keep $\nabla\underline{\underline{p}}(\vec{q},t)$ constant (e.g. $p_{xy} \rightarrow p_{xy} + Cx$ and $p_{yy} \rightarrow p_{yy} - Cy$, all other $p_{\alpha\beta}$ remaining unmodified).

In this sense, we can understand the definition in Eq. (151) for the Wyatt pressure tensor $\underline{\underline{p}}^{WA}(\vec{q},t)$ as a tensor version where the physical interpretation of all quantities appearing in this definition are clear. But because of the transformation freedom for the pressure tensor elements $p^{\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ explained above, there are other versions for the pressure tensor $\underline{\underline{p}}^{\mathrm{A}}(\vec{q},t)$ where this physical interpretation is not so clear—the Kuzmenkov pressure tensor $\underline{\underline{p}}^{K\mathrm{A}}(\vec{q},t)$ is one of these other versions.

At this point, we notice that it was already mentioned in Refs. [23,28] that there exist several versions of the pressure tensor $\underline{\underline{p}}(\vec{q},t)$. In addition, Sonego discussed in Ref. [13] the reason mentioned above for the ambiguity of the pressure tensor $\underline{\underline{p}}(\vec{q},t)$. In contrast to our discussion, Sonego restricts the allowed transformations of this tensor to transformations that keep a pressure tensor with symmetric matrix elements $[p_{\alpha\beta}(\vec{q},t) = p_{\beta\alpha}(\vec{q},t)]$ symmetric, but we think that this condition is not mandatory because only the conservation of the tensor divergence $\nabla\underline{\underline{p}}(\vec{q},t)$ is required physically. Moreover, in the same reference, Sonego presented two versions of the pressure tensor, which we would call in our nomenclature the Kuzmenkov pressure tensor $\underline{\underline{p}}^{K}(\vec{q},t)$ and the Wyatt pressure tensor $\underline{\underline{p}}^{W}(\vec{q},t)$. But in contrast to our work, Sonego prefers using the Kuzmenkov pressure tensor $\underline{\underline{p}}^{K}(\vec{q},t)$ to using the Wyatt pressure tensor $\underline{\underline{p}}^{W}(\vec{q},t)$. His reason for this is that he uses a function called the Wigner function to describe the system in the phase space, which yields as a result the Kuzmenkov pressure tensor $\underline{\underline{p}}^{K}(\vec{q},t)$. However, Sonego himself stated that "we do not claim at all that the Wigner function is the correct phase space distribution, nor that such a distribution exists" (Ref. [13], p. 1166). In this sense, we think that it is still reasonable to prefer the Wyatt pressure tensor $\underline{\underline{p}}^{W}(\vec{q},t)$.

We now finish our discussion about the ambiguity of the pressure tensor $\underline{\underline{p}}(\vec{q},t)$ with the remark that similar ambiguities of quantities also appear in other fields of physics. One example for this context is the energy–momentum tensor $\underline{\underline{T}}(\vec{q},t)$ in relativistic physics, which has to fulfill the condition that its four-divergence vanishes, but this condition does not determine the tensor uniquely—a discussion about this context can be found in Ref. [53]. Another example is the gauge ambiguity of the vector potential $\vec{\mathcal{A}}(\vec{q},t)$ and the scalar potential $\Phi(\vec{q},t)$ in electrodynamics:

There is the Lorenz gauge

$$\nabla\vec{\mathcal{A}}(\vec{q},t) + \frac{1}{c^2}\frac{\partial}{\partial t}\Phi(\vec{q},t) = 0, \tag{161}$$

which has the advantage that the description of electrodynamics in relativistic physics becomes very elegant if one applies this gauge. This elegance is a good reason to prefer the Lorenz gauge to other gauges (Ref. [54], pp. 179–181, 377–380).

Nevertheless, the Lorenz gauge is not the only gauge for $\vec{\mathcal{A}}(\vec{q},t)$ and $\Phi(\vec{q},t)$ that one can find in the literature; there is the Coulomb gauge

$$\nabla\vec{\mathcal{A}}(\vec{q},t) = 0 \tag{162}$$

as well, where the divergence of the vector potential $\vec{\mathcal{A}}(\vec{q},t)$ vanishes. The Coulomb gauge can be advantageous for applications where no charges are present. For more details, see Ref. [54], pp. 181–183.

In order to now prove Eqs. (158) and (159), we first transform the term $-\frac{\hbar^2}{4m_{\mathrm{A}}}\frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}}$ appearing in Eq. (102) for the matrix elements $p^{K\mathrm{A}}_{\alpha\beta}(\vec{q},t)$ using Eq. (139):

$$-\frac{\hbar^2}{4m_{\mathrm{A}}}\frac{\partial^2 \ln D}{\partial q^{\mathrm{A}}_{1\alpha}\partial q^{\mathrm{A}}_{1\beta}} = -\frac{\hbar^2}{4m_{\mathrm{A}}}\frac{\partial}{\partial q^{\mathrm{A}}_{1\alpha}}\left(\frac{1}{D}\frac{\partial D}{\partial q^{\mathrm{A}}_{1\beta}}\right)$$

$$= \frac{\hbar^2}{4m_\mathrm{A}} \frac{1}{D^2} \frac{\partial D}{\partial q^\mathrm{A}_{1\alpha}} \frac{\partial D}{\partial q^\mathrm{A}_{1\beta}} - \frac{\hbar^2}{4m_\mathrm{A}} \frac{1}{D} \frac{\partial^2 D}{\partial q^\mathrm{A}_{1\alpha} \partial q^\mathrm{A}_{1\beta}}$$

$$= m_\mathrm{A} d^\mathrm{A}_{1\alpha} d^\mathrm{A}_{1\beta} - \frac{\hbar^2}{4m_\mathrm{A}} \frac{1}{D} \frac{\partial^2 D}{\partial q^\mathrm{A}_{1\alpha} \partial q^\mathrm{A}_{1\beta}}. \tag{163}$$

As the next step, we insert the intermediate result in Eq. (163) into Eq. (102) for $p^{K\mathrm{A}}_{\alpha\beta}(\vec{q}, t)$. Now, $p^{K\mathrm{A}}_{\alpha\beta}(\vec{q}, t)$ can be split into the sum

$$p^{K\mathrm{A}}_{\alpha\beta}(\vec{q}, t) = p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t) + p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t), \tag{164}$$

where

$$p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t) = N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\; D\; \left(u^\mathrm{A}_{1\alpha} u^\mathrm{A}_{1\beta} + d^\mathrm{A}_{1\alpha} d^\mathrm{A}_{1\beta}\right), \tag{165}$$

$$p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t) = -N(\mathrm{A}) \frac{\hbar^2}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\; \frac{\partial^2 D}{\partial q^\mathrm{A}_{1\alpha} \partial q^\mathrm{A}_{1\beta}}. \tag{166}$$

Here, we make the following remark. The naming of the terms $p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t)$ and $p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ is not just a simple numbering, but there is a deeper meaning: The term $p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t)$ contains products of two factors being first-order Cartesian coordinate derivatives of $S(\vec{Q}, t)$ or $D(\vec{Q}, t)$, and the term $p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ contains second-order Cartesian coordinate derivatives of $D(\vec{Q}, t)$.

In an analogous manner, we can also split the corresponding Wyatt matrix element $p^{W\mathrm{A}}_{\alpha\beta}(\vec{q}, t)$ into two summands using Eq. (151):

$$p^{W\mathrm{A}}_{\alpha\beta}(\vec{q}, t) = p^{W\mathrm{A},1}_{\alpha\beta}(\vec{q}, t) + p^{W\mathrm{A},2}_{\alpha\beta}(\vec{q}, t). \tag{167}$$

Here, the summands $p^{W\mathrm{A},1}_{\alpha\beta}(\vec{q}, t)$ and $p^{W\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ are given by:

$$p^{W\mathrm{A},1}_{\alpha\beta}(\vec{q}, t) = N(\mathrm{A})\, m_\mathrm{A} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\; D\; \left(u^\mathrm{A}_{1\alpha} u^\mathrm{A}_{1\beta} + d^\mathrm{A}_{1\alpha} d^\mathrm{A}_{1\beta}\right) \;=\; p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t), \tag{168}$$

$$p^{W\mathrm{A},2}_{\alpha\beta}(\vec{q}, t) = P_\mathrm{A}(\vec{q}, t)\; \delta_{\alpha\beta}. \tag{169}$$

So, the summands $p^{W\mathrm{A},1}_{\alpha\beta}(\vec{q}, t)$ and $p^{K\mathrm{A},1}_{\alpha\beta}(\vec{q}, t)$ are equal. But in general, $p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ and $p^{W\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ are not equal; in particular, $p^{W\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ is always diagonal, and $p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)$ is in general non-diagonal.

Thus, first, we have proved the inequality in Eq. (158) that in general $\underline{\underline{p}}^{W\mathrm{A}}(\vec{q}, t)$ and $\underline{\underline{p}}^{K\mathrm{A}}(\vec{q}, t)$ are not equal.

Second, to prove Eq. (159), the remaining task is to show that the following equation is true:

$$\nabla \underline{\underline{p}}^{K\mathrm{A},2}(\vec{q}, t) = \nabla \underline{\underline{p}}^{W\mathrm{A},2}(\vec{q}, t). \tag{170}$$

The proof for this equation can be done with the following straightforward calculation: We analyze the β component of the tensor divergence $\nabla \underline{\underline{p}}^{K\mathrm{A},2}(\vec{q}, t)$ in Cartesian coordinates:

$$\left[\nabla \underline{\underline{p}}^{K\mathrm{A},2}(\vec{q}, t)\right]_\beta = \sum_{\alpha \in K_\mathrm{Ca}} \frac{\partial p^{K\mathrm{A},2}_{\alpha\beta}(\vec{q}, t)}{\partial q_\alpha}$$

$$= \sum_{\alpha \in K_\mathrm{Ca}} \frac{\partial}{\partial q_\alpha} \left[-N(\mathrm{A}) \frac{\hbar^2}{4m_\mathrm{A}} \int \mathrm{d}\vec{Q}\; \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\; \frac{\partial^2 D}{\partial q^\mathrm{A}_{1\alpha} \partial q^\mathrm{A}_{1\beta}}\right]$$

$$= -N(\mathrm{A}) \frac{\hbar^2}{4m_{\mathrm{A}}} \sum_{\alpha \in K_{\mathrm{Ca}}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}_1^{\,\mathrm{A}})\ \frac{\partial}{\partial q_{1\alpha}^{\mathrm{A}}} \frac{\partial^2 D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\beta}^{\mathrm{A}}} \tag{171}$$

$$= -N(\mathrm{A}) \frac{\hbar^2}{4m_{\mathrm{A}}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}_1^{\,\mathrm{A}})\ \frac{\partial}{\partial q_{1\beta}^{\mathrm{A}}} \sum_{\alpha \in K_{\mathrm{Ca}}} \frac{\partial^2 D}{\partial q_{1\alpha}^{\mathrm{A}} \partial q_{1\alpha}^{\mathrm{A}}}$$

$$= \frac{\partial}{\partial q_\beta} \left[-N(\mathrm{A}) \frac{\hbar^2}{4m_{\mathrm{A}}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}_1^{\,\mathrm{A}})\ \triangle_1^{\mathrm{A}} D \right]$$

$$= \frac{\partial}{\partial q_\beta} P_{\mathrm{A}}(\vec{q}, t)$$

$$= \sum_{\alpha \in K_{\mathrm{Ca}}} \frac{\partial}{\partial q_\alpha} \left[P_{\mathrm{A}}(\vec{q}, t)\ \delta_{\alpha\beta} \right] \tag{172}$$

$$= \sum_{\alpha \in K_{\mathrm{Ca}}} \frac{\partial p_{\alpha\beta}^{W\mathrm{A},2}(\vec{q}, t)}{\partial q_\alpha}$$

$$= \left[\nabla \underline{\underline{p}}^{W\mathrm{A},2}(\vec{q}, t) \right]_\beta$$

$$\Longrightarrow \nabla \underline{\underline{p}}^{K\mathrm{A},2}(\vec{q}, t) = \nabla \underline{\underline{p}}^{W\mathrm{A},2}(\vec{q}, t). \tag{173}$$

The crucial steps of the proof shown above occur between Eqs. (171) and (172), where a rearrangement of the spatial derivatives is done. This rearrangement is possible due to the sum $\sum_{\alpha \in K_{\mathrm{Ca}}}$ appearing in both Eqs. (171) and (172) because this sum corresponds to the fact that, in Cartesian coordinates, for each vector component of a tensor divergence there is a sum with three summands, where each of these three summands depends on spatial derivatives of different tensor matrix elements—Eq. (160) is an illustration of this fact. The rearrangement above changes each of the three summands in this sum, but in doing this the value of the total sum remains unchanged.

Finally, with the proof of Eq. (170), we have the evidence that Eq. (159) is true; thus, both the Kuzmenkov pressure tensor $\underline{\underline{p}}^{K\mathrm{A}}(\vec{q}, t)$ and the Wyatt pressure tensor $\underline{\underline{p}}^{W\mathrm{A}}(\vec{q}, t)$ lead to an equivalent input in the MPQCE in Eq. (90), and therefore they are physically equivalent.

It remains to prove that the momentum flow density tensors $\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t)$ and $\underline{\underline{\Pi}}^{K\mathrm{A}}(\vec{q}, t)$ are physically equivalent. Analogously to our analysis for the pressure tensors, we will show below that in general $\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t)$ and $\underline{\underline{\Pi}}^{K\mathrm{A}}(\vec{q}, t)$ are not equal:

$$\underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t) \neq \underline{\underline{\Pi}}^{K\mathrm{A}}(\vec{q}, t). \tag{174}$$

But, we will also show below that these tensors have the property

$$\nabla \underline{\underline{\Pi}}^{W\mathrm{A}}(\vec{q}, t) = \nabla \underline{\underline{\Pi}}^{K\mathrm{A}}(\vec{q}, t). \tag{175}$$

Due to this property, both tensors lead to an equivalent input in the MPEEM in Eq. (62), making these tensors physically equivalent.

The first step to prove Eqs. (174) and (175) is inserting Eq. (163) into Eq. (69) for the Kuzmenkov tensor elements $\Pi_{\alpha\beta}^{K\mathrm{A}}(\vec{q}, t)$, and to split each of them into a term $\Pi_{\alpha\beta}^{K\mathrm{A},1}(\vec{q}, t)$ containing products of two factors being first-order Cartesian derivatives of $S(\vec{Q}, t)$ or $D(\vec{Q}, t)$, and a term $\Pi_{\alpha\beta}^{K\mathrm{A},2}(\vec{q}, t)$

containing products of second-order Cartesian derivatives of $D(\vec{Q}, t)$. Thus, we get:

$$\Pi^{KA}_{\alpha\beta}(\vec{q}, t) = \Pi^{KA,1}_{\alpha\beta}(\vec{q}, t) + \Pi^{KA,2}_{\alpha\beta}(\vec{q}, t), \tag{176}$$

$$\Pi^{KA,1}_{\alpha\beta}(\vec{q}, t) = N(\mathrm{A})\, m_{\mathrm{A}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\ D\ \left(w^{\mathrm{A}}_{1\alpha} w^{\mathrm{A}}_{1\beta} + d^{\mathrm{A}}_{1\alpha} d^{\mathrm{A}}_{1\beta}\right), \tag{177}$$

$$\Pi^{KA,2}_{\alpha\beta}(\vec{q}, t) = -N(\mathrm{A}) \frac{\hbar^2}{4m_{\mathrm{A}}} \int \mathrm{d}\vec{Q}\ \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\ \frac{\partial^2 D}{\partial q^{\mathrm{A}}_{1\alpha} \partial q^{\mathrm{A}}_{1\beta}}\ =\ p^{KA,2}_{\alpha\beta}(\vec{q}, t). \tag{178}$$

An analogous splitting can be done for the Wyatt tensor elements $\Pi^{WA}_{\alpha\beta}(\vec{q}, t)$ given in Eq. (142):

$$\Pi^{WA}_{\alpha\beta}(\vec{q}, t) = \Pi^{WA,1}_{\alpha\beta}(\vec{q}, t) + \Pi^{WA,2}_{\alpha\beta}(\vec{q}, t), \tag{179}$$

$$\Pi^{WA,1}_{\alpha\beta}(\vec{q}, t) = \Pi^{KA,1}_{\alpha\beta}(\vec{q}, t), \tag{180}$$

$$\Pi^{WA,2}_{\alpha\beta}(\vec{q}, t) = P_{\mathrm{A}}(\vec{q}, t)\delta_{\alpha\beta}\ =\ p^{WA,2}_{\alpha\beta}(\vec{q}, t). \tag{181}$$

We realize that the terms $\Pi^{WA,1}_{\alpha\beta}(\vec{q}, t)$ and $\Pi^{KA,1}_{\alpha\beta}(\vec{q}, t)$ are equal, but in general $\Pi^{WA,2}_{\alpha\beta}(\vec{q}, t)$ and $\Pi^{KA,2}_{\alpha\beta}(\vec{q}, t)$ are not equal.

So, the inequality in Eq. (174) is proven—that, in general, $\underline{\underline{\Pi}}^{WA}(\vec{q}, t)$ and $\underline{\underline{\Pi}}^{KA}(\vec{q}, t)$ are not equal.

For the proof of Eq. (175), which we need to show the physical equivalence of the tensors $\underline{\underline{\Pi}}^{WA}(\vec{q}, t)$ and $\underline{\underline{\Pi}}^{KA}(\vec{q}, t)$, it remains to show that

$$\nabla \underline{\underline{\Pi}}^{WA,2}(\vec{q}, t) = \nabla \underline{\underline{\Pi}}^{KA,2}(\vec{q}, t). \tag{182}$$

Therefore, we take into account that $\underline{\underline{\Pi}}^{KA,2}(\vec{q}, t)$ is just equal to $\underline{\underline{p}}^{KA,2}(\vec{q}, t)$, and $\underline{\underline{\Pi}}^{WA,2}(\vec{q}, t)$ is just equal to $\underline{\underline{p}}^{WA,2}(\vec{q}, t)$. As we proved Eq. (170) already, Eq. (182) must also be true. Thus, we proved Eq. (175), and, finally, we showed that the Wyatt and Kuzmenkov momentum flow density tensors $\underline{\underline{\Pi}}^{WA}(\vec{q}, t)$ and $\underline{\underline{\Pi}}^{KA}(\vec{q}, t)$ are physically equivalent.

As an intermediate conclusion, we found that the Wyatt and the Kuzmenkov pressure tensors $\underline{\underline{p}}^{WA}(\vec{q}, t)$, $\underline{\underline{p}}^{KA}(\vec{q}, t)$ are physically equivalent, and the same holds for the Wyatt and Kuzmenkov momentum flow density tensors $\underline{\underline{\Pi}}^{WA}(\vec{q}, t)$, $\underline{\underline{\Pi}}^{KA}(\vec{q}, t)$. Moreover, the quantum parts of the Wyatt tensors are more easily interpreted than the quantum parts of the Kuzmenkov tensors.

3.3. *System with cylindrical symmetry*

As an additional task, we will now show for an example system that the divergence of the Wyatt pressure tensor $\underline{\underline{p}}^{WA}(\vec{q}, t)$ is more easily calculated than the divergence of the Kuzmenkov pressure tensor $\underline{\underline{p}}^{KA}(\vec{q}, t)$, so its clearer interpretation is not the only advantage of the Wyatt pressure tensor $\underline{\underline{p}}^{WA}(\vec{q}, t)$.

For the analyzed example system with cylindrical symmetry, the use of cylindrical coordinates is advantageous, and it means that we represent the position vector $\vec{q}$ by

$$\vec{q} = q_\rho \vec{e}_\rho + q_\varphi \vec{e}_\varphi + q_z \vec{e}_z, \tag{183}$$

with the cylindrical basis vectors $\vec{e}_\rho$, $\vec{e}_\varphi$, $\vec{e}_z$ instead of the Cartesian representation

$$\vec{q} = q_x \vec{e}_x + q_y \vec{e}_y + q_z \vec{e}_z. \tag{184}$$

Now, we introduce the radius ρ, the phase φ, and the coordinates x, y, and z, depending on q_x, q_y, and q_z by

$$q_x \equiv x = \rho \cos\varphi, \tag{185}$$

$$q_y \equiv y = \rho \sin\varphi, \tag{186}$$

$$q_z \equiv z. \tag{187}$$

We will show how the cylindrical vector components q_ρ, q_φ, and q_z depend on ρ, φ, and z; in particular, we will find that q_φ vanishes.

The transformation between the basis vectors $\vec{e}_\rho$, $\vec{e}_\varphi$, and $\vec{e}_z$ in cylindrical coordinates and the basis vectors in Cartesian coordinates is described by what is called the rotation matrix $\underline{\underline{\Lambda}}(\varphi)$.

This rotation matrix $\underline{\underline{\Lambda}}(\varphi)$ depends on the geometrical orientation of the position vector $\vec{q}$ via the phase φ, and its matrix elements $\Lambda_{\alpha'\alpha}(\varphi)$ have the following form (Ref. [55], p. 231):

$$\begin{pmatrix} \vec{e}_\rho \\ \vec{e}_\varphi \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \Lambda_{\rho x} & \Lambda_{\rho y} & \Lambda_{\rho z} \\ \Lambda_{\varphi x} & \Lambda_{\varphi y} & \Lambda_{\varphi z} \\ \Lambda_{zx} & \Lambda_{zy} & \Lambda_{zz} \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix}. \tag{188}$$

As a notation convention, in the following we write matrix elements of a tensor field $\underline{\underline{T}}(\vec{q})$ or components of a vector field $\vec{b}(\vec{q})$ in Cartesian coordinates as $T_{\alpha\beta}(\vec{q})$ or as $b_\alpha(\vec{q})$, respectively, but in cylindrical coordinates as $T_{\alpha'\beta'}(\vec{q})$ or as $b_{\alpha'}(\vec{q})$, respectively, if it is not explicitly specified what components are meant. Here, the Cartesian indices α, β are elements of the set $K_{\text{Ca}} = \{x, y, z\}$, and the cylindrical indices α', β' are elements of the set $K_{\text{cy}} = \{\rho, \varphi, z\}$.

As a consequence of Eq. (188), vector components $b_\alpha(\vec{q})$ and tensor elements $T_{\alpha\beta}(\vec{q})$ are transformed via (Ref. [56], pp. 4f):

$$b_{\alpha'}(\vec{q}) = \sum_{\alpha \in K_{\text{Ca}}} \Lambda_{\alpha'\alpha}(\varphi)\, b_\alpha(\vec{q}), \tag{189}$$

$$T_{\alpha'\beta'}(\vec{q}) = \sum_{\alpha \in K_{\text{Ca}}} \sum_{\beta \in K_{\text{Ca}}} \Lambda_{\alpha'\alpha}(\varphi)\, \Lambda_{\beta'\beta}(\varphi)\, T_{\alpha\beta}(\vec{q}). \tag{190}$$

Applying Eq. (189), we find for the particular case that the vector field $\vec{b}(\vec{q})$ is the position vector $\vec{q}$ itself:

$$\vec{q} = \rho \vec{e}_\rho + z \vec{e}_z, \tag{191}$$

so $q_\rho \equiv \rho$, and q_φ vanishes. However, for vectors $\vec{b}(\vec{q})$ that are not equal to the position vector $\vec{q}$ itself the component $b_\varphi(\vec{q})$ does not need to vanish.

For the coordinate transformation of the tensor elements $p^{KA}_{\alpha\beta}(\vec{q}, t)$ and $p^{WA}_{\alpha\beta}(\vec{q}, t)$, we take into account the cylindrical symmetry of the system mentioned above. Because of this symmetry, we assume that the wave function Ψ describing this system has the following properties:

The wave function describes a system for N_S different sorts of particles, like in our previous analysis, so $\Psi = \Psi(\vec{Q}, t)$. Moreover, as an additional symmetry property, we assume that the wave function $\Psi(\vec{Q}, t)$ does not depend on the polar angles $\varphi_{i\text{A}}$ of all the (A, i) particles for a certain sort of particle A.

An example of a system with such a wave function is an H_2^+ molecule in its electronic and rotational ground state, because for fixed nuclei we can choose the coordinate system in such a manner that the wave function is independent of the polar angle φ_e of the electron.

Thus, for the $S(\vec{Q},t)$ and $D(\vec{Q},t)$ functions related to a wave function $\Psi(\vec{Q},t)$ of such a system it holds that the following equations are true for any natural number $n = 1,2,\ldots$ and any particle index $i = 1,2,\ldots,N(\mathrm{A})$:

$$\frac{\partial^n S}{\partial \varphi_{i\mathrm{A}}^n} = 0, \tag{192}$$

$$\frac{\partial^n D}{\partial \varphi_{i\mathrm{A}}^n} = 0. \tag{193}$$

Moreover, using Eqs. (102) and (151) it can be easily realized that the matrices for $\underline{\underline{p}}^{X\mathrm{A}}(\vec{q},t)$, where X stands for both the Kuzmenkov and the Wyatt pressure tensors, are symmetric for Cartesian coordinates:

$$p_{\alpha\beta}^{X\mathrm{A}}(\vec{q},t) = p_{\beta\alpha}^{X\mathrm{A}}(\vec{q},t). \tag{194}$$

Regarding this symmetry $p_{\alpha\beta}^{X\mathrm{A}}(\vec{q},t) = p_{\beta\alpha}^{X\mathrm{A}}(\vec{q},t)$ for Cartesian coordinates, we can prove using Eq. (190) for matrix element transformations that this symmetry is true for cylindrical coordinates, too:

$$\begin{aligned} p_{\beta'\alpha'}^{X\mathrm{A}}(\vec{q},t) &= \sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}} \Lambda_{\beta'\alpha}(\varphi)\,\Lambda_{\alpha'\beta}(\varphi)\,p_{\alpha\beta}^{X\mathrm{A}}(\vec{q},t) \\ &\underset{\text{Commutate }\alpha,\beta}{=} \sum_{\beta\in K_{\mathrm{Ca}}}\sum_{\alpha\in K_{\mathrm{Ca}}} \Lambda_{\alpha'\alpha}(\varphi)\,\Lambda_{\beta'\beta}(\varphi)\,\underbrace{p_{\beta\alpha}^{X\mathrm{A}}}_{=p_{\alpha\beta}^{X\mathrm{A}}}(\vec{q},t) \\ &= p_{\alpha'\beta'}^{X\mathrm{A}}(\vec{q},t)\ \Box. \end{aligned} \tag{195}$$

For the following analysis, it is advantageous to split the pressure tensor elements $p_{\alpha\beta}^{X\mathrm{A}}(\vec{q},t)$ into two parts $p_{\alpha\beta}^{X\mathrm{A},1}(\vec{q},t)$ and $p_{\alpha\beta}^{X\mathrm{A},2}(\vec{q},t)$, analogously to the discussions above. Then, we transform each part separately into corresponding cylindrical coordinate matrix elements $p_{\alpha'\beta'}^{X\mathrm{A},1}(\vec{q},t)$ or $p_{\alpha'\beta'}^{X\mathrm{A},2}(\vec{q},t)$, respectively.

Because of Eqs. (165), (166), (168), and (169), the Cartesian coordinate matrix elements $p_{\alpha\beta}^{X\mathrm{A},1}(\vec{q},t)$ and $p_{\alpha\beta}^{X\mathrm{A},2}(\vec{q},t)$ are symmetric:

$$p_{\beta\alpha}^{X\mathrm{A},1}(\vec{q},t) = p_{\alpha\beta}^{X\mathrm{A},1}(\vec{q},t), \tag{196}$$

$$p_{\beta\alpha}^{X\mathrm{A},2}(\vec{q},t) = p_{\alpha\beta}^{X\mathrm{A},2}(\vec{q},t). \tag{197}$$

We find that the cylindrical coordinate matrix elements $p_{\alpha'\beta'}^{X\mathrm{A},1}(\vec{q},t)$ and $p_{\alpha'\beta'}^{X\mathrm{A},2}(\vec{q},t)$ are symmetric, too, by applying a calculation similar to the derivation of Eq. (195):

$$p_{\beta'\alpha'}^{X\mathrm{A},1}(\vec{q},t) = p_{\alpha'\beta'}^{X\mathrm{A},1}(\vec{q},t), \tag{198}$$

$$p_{\beta'\alpha'}^{X\mathrm{A},2}(\vec{q},t) = p_{\alpha'\beta'}^{X\mathrm{A},2}(\vec{q},t). \tag{199}$$

Now, we note the following four points to make the transformations $p_{\alpha\beta}^{X\mathrm{A},1}(\vec{q},t) \to p_{\alpha'\beta'}^{X\mathrm{A},1}(\vec{q},t)$ and $p_{\alpha\beta}^{X\mathrm{A},2}(\vec{q},t) \to p_{\alpha'\beta'}^{X\mathrm{A},2}(\vec{q},t)$:

First, for the calculation of the matrix elements $p^{XA,1}_{\alpha'\beta'}(\vec{q},t)$ and $p^{XA,2}_{\alpha'\beta'}(\vec{q},t)$, one has to evaluate the tensor transformation law in Eq. (190), which leads to sums over corresponding Cartesian matrix elements $p^{XA,1}_{\alpha\beta}(\vec{q},t)$ or $p^{XA,2}_{\alpha\beta}(\vec{q},t)$:

$$p^{XA,1}_{\alpha'\beta'}(\vec{q},t) = \sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}} \Lambda_{\alpha'\alpha}(\varphi)\,\Lambda_{\beta'\beta}(\varphi)\,p^{XA,1}_{\alpha\beta}(\vec{q},t), \tag{200}$$

$$p^{XA,2}_{\alpha'\beta'}(\vec{q},t) = \sum_{\alpha\in K_{\mathrm{Ca}}}\sum_{\beta\in K_{\mathrm{Ca}}} \Lambda_{\alpha'\alpha}(\varphi)\,\Lambda_{\beta'\beta}(\varphi)\,p^{XA,2}_{\alpha\beta}(\vec{q},t). \tag{201}$$

Second, the Cartesian matrix elements $p^{XA,1}_{\alpha\beta}(\vec{q},t)$ depend on the Cartesian vector components $u^{\mathrm{A}}_{1\alpha}(\vec{Q},t)$, $d^{\mathrm{A}}_{1\alpha}(\vec{Q},t)$ [see Eq. (168)]. So, when one calculates the matrix elements $p^{XA,1}_{\alpha'\beta'}(\vec{q},t)$ using Eq. (200), one has to transform the Cartesian vector components $u^{\mathrm{A}}_{1\alpha}(\vec{Q},t)$, $d^{\mathrm{A}}_{1\alpha}(\vec{Q},t)$ using Eq. (189) into the vector components $u^{\mathrm{A}}_{1\alpha'}(\vec{Q},t)$, $d^{\mathrm{A}}_{1\alpha'}(\vec{Q},t)$ for each of the Cartesian matrix elements $p^{XA,1}_{\alpha\beta}(\vec{q},t)$, which appear on the right-hand side of Eq. (200). These velocity components $u^{\mathrm{A}}_{1\alpha'}(\vec{Q},t)$ and $d^{\mathrm{A}}_{1\alpha'}(\vec{Q},t)$ can be calculated from the quantities $S(\vec{Q},t)$ and $D(\vec{Q},t)$ by using Eqs. (13), (23), (26), (30), (31), and (139). We note in this calculation that the divergence $\nabla^{\mathrm{A}}_i S(\vec{Q},t)$ appears in Eq. (26), and that the divergence $\nabla^{\mathrm{A}}_i D(\vec{Q},t)$ appears in Eq. (139)—we calculate these divergences in cylindrical coordinates by applying that the divergence of any scalar function $\Phi(\vec{Q},t)$ related to the coordinate $\vec{q}^{\,\mathrm{A}}_i$ is given in cylindrical coordinates by:

$$\nabla^{\mathrm{A}}_i \Phi(\vec{Q},t) = \frac{\partial\Phi}{\partial\rho_{i\mathrm{A}}}\vec{e}_\rho + \frac{1}{\rho_{i\mathrm{A}}}\frac{\partial\Phi}{\partial\varphi_{i\mathrm{A}}}\vec{e}_\varphi + \frac{\partial\Phi}{\partial z_{i\mathrm{A}}}\vec{e}_z. \tag{202}$$

Third, the Cartesian coordinate derivatives $\frac{\partial}{\partial q^{\mathrm{A}}_{1x}} \equiv \frac{\partial}{\partial x_{1\mathrm{A}}}$ and $\frac{\partial}{\partial q^{\mathrm{A}}_{1y}} \equiv \frac{\partial}{\partial y_{1\mathrm{A}}}$ are present in Eq. (166) for all of the Cartesian matrix elements $p^{KA,2}_{\alpha\beta}(\vec{q},t)$ (besides the zz element). Thus, when one calculates the matrix elements $p^{KA,2}_{\alpha'\beta'}(\vec{q},t)$, one has to transform the Cartesian coordinate derivatives $\frac{\partial}{\partial q^{\mathrm{A}}_{1x}} \equiv \frac{\partial}{\partial x_{1\mathrm{A}}}$ and $\frac{\partial}{\partial q^{\mathrm{A}}_{1y}} \equiv \frac{\partial}{\partial y_{1\mathrm{A}}}$ for the Cartesian matrix elements $p^{KA,2}_{\alpha\beta}(\vec{q},t)$, which appear on the right-hand side of Eq. (201) for $X = K$. Hereby, one has to regard:

$$\frac{\partial}{\partial x_{1\mathrm{A}}} = \underbrace{\frac{\partial\rho_{1\mathrm{A}}}{\partial x_{1\mathrm{A}}}}_{=\cos\varphi_{1\mathrm{A}}}\frac{\partial}{\partial\rho_{1\mathrm{A}}} + \underbrace{\frac{\partial\varphi_{1\mathrm{A}}}{\partial x_{1\mathrm{A}}}}_{=-\frac{\sin\varphi_{1\mathrm{A}}}{\rho_{1\mathrm{A}}}}\frac{\partial}{\partial\varphi_{1\mathrm{A}}} = \cos\varphi_{1\mathrm{A}}\frac{\partial}{\partial\rho_{1\mathrm{A}}} - \frac{\sin\varphi_{1\mathrm{A}}}{\rho_{1\mathrm{A}}}\frac{\partial}{\partial\varphi_{1\mathrm{A}}}, \tag{203}$$

$$\frac{\partial}{\partial y_{1\mathrm{A}}} = \underbrace{\frac{\partial\rho_{1\mathrm{A}}}{\partial y_{1\mathrm{A}}}}_{=\sin\varphi_{1\mathrm{A}}}\frac{\partial}{\partial\rho_{1\mathrm{A}}} + \underbrace{\frac{\partial\varphi_{1\mathrm{A}}}{\partial y_{1\mathrm{A}}}}_{=\frac{\cos\varphi_{1\mathrm{A}}}{\rho_{1\mathrm{A}}}}\frac{\partial}{\partial\varphi_{1\mathrm{A}}} = \sin\varphi_{1\mathrm{A}}\frac{\partial}{\partial\rho_{1\mathrm{A}}} + \frac{\cos\varphi_{1\mathrm{A}}}{\rho_{1\mathrm{A}}}\frac{\partial}{\partial\varphi_{1\mathrm{A}}}. \tag{204}$$

Fourth, one can simplify the transformation calculations by taking into account the symmetry properties in Eqs. (192) and (193) for the $S(\vec{Q},t)$ and $D(\vec{Q},t)$ functions. However, we point out that in spite of these symmetry properties one cannot always omit the derivative relative to the $\varphi_{1\mathrm{A}}$ coordinate in Eqs. (203) and (204)—this is important for the calculation of the matrix element $p^{KA,2}_{\varphi\varphi}(\vec{q},t)$.

Then, we find for the first-order tensor components $p^{XA,1}_{\alpha'\beta'}(\vec{q},t)$:

$$\begin{aligned} p^{KA,1}_{\alpha'\beta'}(\vec{q},t) &= p^{WA,1}_{\alpha'\beta'}(\vec{q},t) \\ &= N(\mathrm{A})\int \mathrm{d}Q\,\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\,D\,m_{\mathrm{A}}\left(u^{\mathrm{A}}_{1\alpha'}u^{\mathrm{A}}_{1\beta'} + d^{\mathrm{A}}_{1\alpha'}d^{\mathrm{A}}_{1\beta'}\right). \end{aligned} \tag{205}$$

That $p^{KA,1}_{\alpha'\beta'}(\vec{q},t)$ and $p^{WA,1}_{\alpha'\beta'}(\vec{q},t)$ are equal is trivial since the corresponding Cartesian matrix elements are equal [see Eq. (168)]. Here, we note that the velocity components $u^{\mathrm{A}}_{1\varphi}$ and $d^{\mathrm{A}}_{1\varphi}$ vanish because of Eq. (202) and the symmetry properties described by Eqs. (192) and (193):

$$w^{\mathrm{A}}_{1\varphi} = \frac{1}{m_{\mathrm{A}}}\frac{1}{\rho_{1\mathrm{A}}}\underbrace{\frac{\partial S}{\partial \varphi_{1\mathrm{A}}}}_{=0} = 0 \implies u^{\mathrm{A}}_{1\varphi} = 0, \tag{206}$$

$$d^{\mathrm{A}}_{1\varphi} = -\frac{\hbar}{2m_{\mathrm{A}}}\frac{1}{D}\frac{1}{\rho_{1\mathrm{A}}}\underbrace{\frac{\partial D}{\partial \varphi_{1\mathrm{A}}}}_{=0} = 0. \tag{207}$$

Therefore, any tensor element $p^{XA,1}_{\alpha'\beta'}(\vec{q},t)$ vanishes where α' or β' is φ.

Moreover, the calculation of the Kuzmenkov second-order tensor elements $p^{KA,2}_{\alpha'\beta'}(\vec{q},t)$ yields these results:

For the $\rho\rho$ matrix element:

$$p^{KA,2}_{\rho\rho}(\vec{q},t) = -N(\mathrm{A})\frac{\hbar^2}{4m_{\mathrm{A}}}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\,\frac{\partial^2 D}{\partial \rho^2_{1\mathrm{A}}}. \tag{208}$$

For the $\rho\varphi$ matrix element:

$$p^{KA,2}_{\rho\varphi} = 0. \tag{209}$$

For the ρz matrix element:

$$p^{KA,2}_{\rho z}(\vec{q},t) = -N(\mathrm{A})\frac{\hbar^2}{4m_{\mathrm{A}}}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\,\frac{\partial^2 D}{\partial \rho_{1\mathrm{A}}\partial z_{1\mathrm{A}}}. \tag{210}$$

For the $\varphi\varphi$ matrix element:

$$p^{KA,2}_{\varphi\varphi}(\vec{q},t) = N(\mathrm{A})\frac{\hbar}{2}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\,\frac{D\,d^{\mathrm{A}}_{1\rho}}{\rho_{1\mathrm{A}}}. \tag{211}$$

For the φz matrix element:

$$p^{KA,2}_{\varphi z} = 0. \tag{212}$$

For the zz matrix element:

$$p^{KA,2}_{zz}(\vec{q},t) = -N(\mathrm{A})\frac{\hbar^2}{4m_{\mathrm{A}}}\int \mathrm{d}\vec{Q}\;\delta(\vec{q}-\vec{q}^{\,\mathrm{A}}_1)\,\frac{\partial^2 D}{\partial z^2_{1\mathrm{A}}}. \tag{213}$$

We do not need to state separate results for the remaining $\varphi\rho$, $z\varphi$, and $z\rho$ matrix elements because of the symmetry described by Eq. (199).

As the next step, we find that the transformation of the second-order Wyatt Cartesian matrix elements $p^{WA,2}_{\alpha\beta}(\vec{q},t)$ into the corresponding cylindrical matrix elements $p^{WA,2}_{\alpha'\beta'}(\vec{q},t)$ is trivial: Because of Eq. (169), $\underline{\underline{p}}^{WA,2}(\vec{q},t) = P_{\mathrm{A}}(\vec{q},t)\,\underline{\underline{1}}$ holds. The unity tensor matrix elements—in Cartesian coordinates being equal to the Kronecker symbol—remain equal to this symbol under the transformation into cylindrical coordinates done by Eq. (190):

$$1_{\alpha\beta} = \delta_{\alpha\beta} \implies 1_{\alpha'\beta'} = \delta_{\alpha'\beta'}. \tag{214}$$

Combining this with the context that the scalar quantum pressure $P_{\mathrm{A}}(\vec{q},t)$ does not change in a coordinate transformation yields this result for the matrix elements $p^{W\mathrm{A},2}_{\alpha'\beta'}(\vec{q},t)$:

$$p^{W\mathrm{A},2}_{\alpha'\beta'}(\vec{q},t) = P_{\mathrm{A}}(\vec{q},t)\;\delta_{\alpha'\beta'}. \tag{215}$$

We mention that the quantity $P_{\mathrm{A}}(\vec{q},t)$ does not change itself under a coordinate transformation because it is a scalar field. However, the coordinate transformation from Cartesian to cylindrical coordinates changes how $P_{\mathrm{A}}(\vec{q},t)$ is calculated in the following manner.

We evaluate $P_{\mathrm{A}}(\vec{q},t)$ from the total particle density $D(\vec{Q},t)$ using Eq. (143), where the Laplace operator $\triangle^{\mathrm{A}}_1$ relative to the coordinate $\vec{q}^{\,\mathrm{A}}_1$ appears. So, we have to regard that in cylindrical coordinates this operator is given by:

$$\triangle^{\mathrm{A}}_1 = \frac{\partial^2}{\partial\rho^2_{1\mathrm{A}}} + \frac{1}{\rho_{1\mathrm{A}}}\frac{\partial}{\partial\rho_{1\mathrm{A}}} + \frac{1}{\rho^2_{1\mathrm{A}}}\frac{\partial^2}{\partial\varphi^2_{1\mathrm{A}}} + \frac{\partial^2}{\partial z^2_{1\mathrm{A}}}. \tag{216}$$

After having calculated the first- and second-order cylindrical elements $p^{X\mathrm{A},1}(\vec{q},t)$ and $p^{X\mathrm{A},2}(\vec{q},t)$, we calculate the corresponding tensor divergences. For this objective, the general equation for calculating the divergence of a tensor field $\nabla\underline{\underline{T}}(\vec{q})$ in cylindrical coordinates has to be evaluated (Ref. [57], p. 60):

$$\begin{aligned}\nabla\underline{\underline{T}}(\vec{q}) = {}& \left[\frac{\partial T_{\rho\rho}}{\partial\rho} + \frac{1}{\rho}\left(\frac{\partial T_{\varphi\rho}}{\partial\varphi} + T_{\rho\rho} - T_{\varphi\varphi}\right) + \frac{\partial T_{z\rho}}{\partial z}\right]\vec{e}_\rho \\ &+ \left[\frac{\partial T_{\rho\varphi}}{\partial\rho} + \frac{1}{\rho}\left(\frac{\partial T_{\varphi\varphi}}{\partial\varphi} + T_{\rho\varphi} + T_{\varphi\rho}\right) + \frac{\partial T_{z\varphi}}{\partial z}\right]\vec{e}_\varphi \\ &+ \left[\frac{\partial T_{\rho z}}{\partial\rho} + \frac{1}{\rho}\left(\frac{\partial T_{\varphi z}}{\partial\varphi} + T_{\rho z}\right) + \frac{\partial T_{zz}}{\partial z}\right]\vec{e}_z.\end{aligned} \tag{217}$$

Here, we mention that in Ref. [38] Andreev and Kuzmenkov also analyze QHD in cylindrical coordinates. However, in their approach, they calculate a tensor divergence of the momentum flow density tensor $\nabla\underline{\underline{\Pi}}$ in cylindrical coordinates by applying the ∇ operator on a tensor component set $\{\Pi_{\alpha\rho},\Pi_{\alpha\varphi},\Pi_{\alpha z}\}$ as if these three components were components of a vector with a parameter $\alpha\in K_{\mathrm{cy}}$, and then they treat the result of this calculation as if it were the α component of the tensor divergence $\nabla\underline{\underline{\Pi}}$. Andreev and Kuzmenkov compensate for their error in this approach by introducing in their QHD equations an additional inertia force. But we think that if one applies Eq. (217) for calculating tensor divergences instead, it is not necessary to introduce this inertia force.

Using Eq. (217) and the symmetry $p^{K\mathrm{A},1}_{\beta'\alpha'}(\vec{q},t) = p^{K\mathrm{A},1}_{\alpha'\beta'}(\vec{q},t)$ for calculating the divergence of the first-order tensors $\underline{\underline{p}}^{X\mathrm{A},1}(\vec{q},t)$, we find:

$$\begin{aligned}\nabla\underline{\underline{p}}^{K\mathrm{A},1}(\vec{q},t) &= \nabla\underline{\underline{p}}^{W\mathrm{A},1}(\vec{q},t) \\ &= \left(\frac{\partial p^{W\mathrm{A},1}_{\rho\rho}}{\partial\rho} + \frac{1}{\rho}p^{W\mathrm{A},1}_{\rho\rho} + \frac{\partial p^{W\mathrm{A},1}_{\rho z}}{\partial z}\right)\vec{e}_\rho \\ &\quad + \left(\frac{\partial p^{W\mathrm{A},1}_{\rho z}}{\partial\rho} + \frac{1}{\rho}p^{W\mathrm{A},1}_{\rho z} + \frac{\partial p^{W\mathrm{A},1}_{zz}}{\partial z}\right)\vec{e}_z.\end{aligned} \tag{218}$$

In addition, for the divergence of the second-order Kuzmenkov tensor $\underline{\underline{p}}^{KA,2}(\vec{q},t)$, we find:

$$\nabla\underline{\underline{p}}^{KA,2}(\vec{q},t) = \left[\frac{\partial p_{\rho\rho}^{KA,2}}{\partial\rho} + \frac{1}{\rho}\left(p_{\rho\rho}^{KA,2} - p_{\varphi\varphi}^{KA,2}\right) + \frac{\partial p_{\rho z}^{KA,2}}{\partial z}\right]\vec{e}_\rho + \left(\frac{\partial p_{\rho z}^{KA,2}}{\partial\rho} + \frac{1}{\rho}p_{\rho z}^{KA,2} + \frac{\partial p_{zz}^{KA,2}}{\partial z}\right)\vec{e}_z. \tag{219}$$

When we calculated $\nabla\underline{\underline{p}}^{KA,2}(\vec{q},t)$ using Eq. (217) and $p_{\beta'\alpha'}^{KA,2}(\vec{q},t) = p_{\alpha'\beta'}^{KA,2}(\vec{q},t)$, we regarded that the derivative $\frac{\partial p_{\varphi\varphi}^{KA,2}(\vec{q},t)}{\partial\varphi}$ vanishes because of the symmetry property in Eq. (193). Moreover, for the divergence of the second-order Wyatt tensor $\underline{\underline{p}}^{WA,2}(\vec{q},t)$, we initially find this intermediate result:

$$\nabla\underline{\underline{p}}^{WA,2}(\vec{q},t) = \frac{\partial P_A}{\partial\rho}\vec{e}_\rho + \frac{1}{\rho}\frac{\partial P_A}{\partial\varphi}\vec{e}_\varphi + \frac{\partial P_A}{\partial z}\vec{e}_z. \tag{220}$$

As the next step, we note that the differential operators $\triangle_1^A$ and $\frac{\partial}{\partial\varphi_{1A}}$ commute—this can be proven trivially by Eq. (216) for the Laplace operator $\triangle_1^A$ in cylindrical coordinates. From this context, we conclude that the derivative $\frac{\partial P_A(\vec{q},t)}{\partial\varphi}$ vanishes due to the symmetry property in Eq. (193):

$$\begin{aligned}\frac{\partial P_A(\vec{q},t)}{\partial\varphi} &= -\frac{\partial}{\partial\varphi}N(A)\frac{\hbar^2}{4m_A}\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\triangle_1^A D \\ &= -N(A)\frac{\hbar^2}{4m_A}\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\frac{\partial}{\partial\varphi_{1A}}\triangle_1^A D \\ &= -N(A)\frac{\hbar^2}{4m_A}\int d\vec{Q}\;\delta(\vec{q}-\vec{q}_1^{\,A})\;\triangle_1^A\underbrace{\frac{\partial D}{\partial\varphi_{1A}}}_{=0} \\ &= 0.\end{aligned} \tag{221}$$

Then, we get this simplified result for $\nabla\underline{\underline{p}}^{WA,2}(\vec{q},t)$:

$$\nabla\underline{\underline{p}}^{WA,2}(\vec{q},t) = \frac{\partial P_A}{\partial\rho}\vec{e}_\rho + \frac{\partial P_A}{\partial z}\vec{e}_z. \tag{222}$$

Finally, by adding Eqs. (218) and (219), we find for the divergence of the Kuzmenkov pressure tensor $\nabla\underline{\underline{p}}^{KA}(\vec{q},t)$:

$$\begin{aligned}\nabla\underline{\underline{p}}^{KA}(\vec{q},t) &= \nabla\underline{\underline{p}}^{KA,1}(\vec{q},t) + \nabla\underline{\underline{p}}^{KA,2}(\vec{q},t) \\ &= \left[\frac{\partial p_{\rho\rho}^{WA,1}}{\partial\rho} + \frac{1}{\rho}p_{\rho\rho}^{WA,1} + \frac{\partial p_{\rho z}^{WA,1}}{\partial z}\right. \\ &\quad \left. + \frac{\partial p_{\rho\rho}^{KA,2}}{\partial\rho} + \frac{1}{\rho}\left(p_{\rho\rho}^{KA,2} - p_{\varphi\varphi}^{KA,2}\right) + \frac{\partial p_{\rho z}^{KA,2}}{\partial z}\right]\vec{e}_\rho \\ &\quad + \left(\frac{\partial p_{\rho z}^{WA,1}}{\partial\rho} + \frac{1}{\rho}p_{\rho z}^{WA,1} + \frac{\partial p_{zz}^{WA,1}}{\partial z} + \frac{\partial p_{\rho z}^{KA,2}}{\partial\rho} + \frac{1}{\rho}p_{\rho z}^{KA,2} + \frac{\partial p_{zz}^{KA,2}}{\partial z}\right)\vec{e}_z,\end{aligned} \tag{223}$$

and by adding Eqs. (218) and (222), we find for the divergence of the Wyatt pressure tensor $\nabla \underline{\underline{p}}^{WA}(\vec{q},t)$:

$$\begin{aligned}\nabla \underline{\underline{p}}^{WA}(\vec{q},t) &= \nabla \underline{\underline{p}}^{WA,1}(\vec{q},t) + \nabla \underline{\underline{p}}^{WA,2}(\vec{q},t) \\ &= \left(\frac{\partial p^{WA,1}_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho\rho} + \frac{\partial p^{WA,1}_{\rho z}}{\partial z} + \frac{\partial P_{\mathrm{A}}}{\partial \rho} \right) \vec{e}_\rho \\ &\quad \left(\frac{\partial p^{WA,1}_{\rho z}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho z} + \frac{\partial p^{WA,1}_{zz}}{\partial z} + \frac{\partial P_{\mathrm{A}}}{\partial z} \right) \vec{e}_z. \end{aligned} \tag{224}$$

As a result, both $\nabla \underline{\underline{p}}^{KA}(\vec{q},t)$ and $\nabla \underline{\underline{p}}^{WA}(\vec{q},t)$ have no $\vec{e}_\varphi$ component due to the symmetry properties described by Eqs. (192) and (193). Apart from this identical property of $\nabla \underline{\underline{p}}^{WA}(\vec{q},t)$ and $\nabla \underline{\underline{p}}^{KA}(\vec{q},t)$, for numerical applications—where $\nabla \underline{\underline{p}}^{WA}(\vec{q},t)$ or $\nabla \underline{\underline{p}}^{KA}(\vec{q},t)$, respectively, are input quantities in the MPQCE in Eq. (90)—the use of the Wyatt pressure tensor $\underline{\underline{p}}^{WA}(\vec{q},t)$ is advantageous.

The reason for this is that the evaluation equation in Eq. (222) for the calculation of the second-order part $\underline{\underline{p}}^{WA,2}(\vec{q},t)$ of the Wyatt pressure tensor is more compact and less complicated than the corresponding Eq. (219) for the calculation of the second-order part $\underline{\underline{p}}^{KA,2}(\vec{q},t)$ of the Kuzmenkov pressure tensor. So, the Wyatt pressure tensor is not only easier to interpret physically than the Kuzmenkov pressure tensor, but it is easier to apply numerically, too.

As the last point in this section, we mention that cylindrical coordinate matrix elements for the parts $\underline{\underline{\Pi}}^{XA,1}(\vec{q},t)$ and $\underline{\underline{\Pi}}^{XA,2}(\vec{q},t)$ of the momentum flow density tensor $\underline{\underline{\Pi}}(\vec{q},t)$ can be derived in an analogous manner to the parts $\underline{\underline{p}}^{XA,1}(\vec{q},t)$ and $\underline{\underline{p}}^{XA,2}(\vec{q},t)$ of the pressure tensor $\underline{\underline{p}}(\vec{q},t)$.

By comparing Eqs. (177) and (180) for the Cartesian matrix elements $\Pi^{XA,1}_{\alpha\beta}(\vec{q},t)$ with Eq. (168) for the Cartesian matrix elements $p^{XA,1}_{\alpha\beta}(\vec{q},t)$, it becomes evident that the formula for the cylindrical coordinate matrix elements $\Pi^{XA,1}_{\alpha'\beta'}(\vec{q},t)$ is found by substituting the vector components of the relative velocity $\vec{u}^{\mathrm{A}}_1(\vec{Q},t)$ by the corresponding vector components of the velocity $\vec{w}^{\mathrm{A}}_1(\vec{Q},t)$ in Eq. (205) for the cylindrical coordinate matrix elements $p^{XA,1}_{\alpha'\beta'}(\vec{q},t)$:

$$\begin{aligned}\Pi^{KA,1}_{\alpha'\beta'}(\vec{q},t) &= \Pi^{WA,1}_{\alpha'\beta'}(\vec{q},t) \\ &= N(\mathrm{A}) \int \mathrm{d}Q\, \delta(\vec{q} - \vec{q}^{\,\mathrm{A}}_1)\, D\, m_{\mathrm{A}} \left(w^{\mathrm{A}}_{1\alpha'} w^{\mathrm{A}}_{1\beta'} + d^{\mathrm{A}}_{1\alpha'} d^{\mathrm{A}}_{1\beta'} \right). \end{aligned} \tag{225}$$

In addition, because of Eqs. (178) and (181), it holds that

$$\Pi^{XA,2}_{\alpha\beta}(\vec{q},t) = p^{XA,2}_{\alpha\beta}(\vec{q},t). \tag{226}$$

So, the cylindrical coordinate matrix elements $\Pi^{XA,2}_{\alpha'\beta'}(\vec{q},t)$ are given by

$$\Pi^{XA,2}_{\alpha'\beta'}(\vec{q},t) = p^{XA,2}_{\alpha'\beta'}(\vec{q},t). \tag{227}$$

Thus, to calculate $\Pi^{XA,2}_{\alpha'\beta'}(\vec{q},t)$, we can just use the results we derived above for $p^{XA,2}_{\alpha'\beta'}(\vec{q},t)$. Therefore, the use of the Wyatt momentum flow density tensor $\underline{\underline{\Pi}}^{WA}(\vec{q},t)$ is advantageous compared to the use of the Kuzmenkov momentum flow density tensor $\underline{\underline{\Pi}}^{KA}(\vec{q},t)$ because the second-order part $\underline{\underline{\Pi}}^{WA,2}(\vec{q},t)$ of the Wyatt tensor can be calculated more easily than the corresponding second-order part $\underline{\underline{\Pi}}^{KA,2}(\vec{q},t)$ of the Kuzmenkov tensor.

4. Summary

In this paper, we derived the MPQHD equations in detail for an exact wave function describing an ensemble of several particle sorts. For this task, we first derived the MPCE related to the conservation of mass for each of the particle sorts. One can also derive an MPCE for the total particle ensemble by summing the MPCEs for all the different sorts of particle. Moreover, we derived, for each sort of particle, two different equations of motion. The first of these equations of motion is the MPEEM; it describes the temporal change of the mass flux density of the particles of the analyzed sort, and one can derive the MPEEM by applying the Ehrenfest theorem for the calculation of this temporal change. The second of these equations of motion is the MPQCE; it is closely related to Cauchy's equation of motion, which is well known in classical hydrodynamics and is related to the momentum balance in fluids. The MPEEMs for the different sorts of particle are linear differential equations, so one can get an MPEEM for the total particle ensemble just by adding up the MPEEMs for all the different sorts of particle. The MPQCEs for the different sorts of particle are non-linear, so adding up these equations does not lead to an MPQCE for the total particle ensemble. However, a derivation of an MPQCE for the total particle ensemble is still possible.

In all the MPQCEs, both for a certain sort of particle and for the total particle ensemble, a quantity appears called the divergence of the pressure tensor. Similar to a potential, this pressure tensor is not defined uniquely. For an MPQCE related to a certain sort of particle, the properties of two different versions of this tensor are discussed: The first is named the "Wyatt pressure tensor" because of the form of the momentum flow density tensor, which is another tensor closely connected to the pressure tensor, in Ref. [42], p. 31. The second is named the "Kuzmenkov pressure tensor" because it appears in Ref. [31]. The terms contributing to the Wyatt pressure tensor can be interpreted physically better than the Kuzmenkov pressure tensor. Moreover, we made a coordinate transformation of both tensor versions from Cartesian coordinates to cyclindrical coordinates and calculated the tensor divergence for both versions in cyclindrical coordinates. This calculation can be performed more easily for the Wyatt pressure tensor than for the Kuzmenkov pressure tensor because a certain summand contributing to the Wyatt pressure tensor is just a scalar multiplied by the diagonal unit tensor, while the corresponding summand contributing to the Kuzmenkov pressure tensor is a full tensor with non-diagonal elements.

In addition, in all the MPEEMs, a quantity called the divergence of the momentum flow density tensor appears, and for an MPEEM related to a certain sort of particle we introduce both a Kuzmenkov version and a Wyatt version of this tensor. We analyzed these two versions of the momentum flow density tensor in an analogous manner to the two versions of the pressure tensor mentioned above. The results of the analysis of the Kuzmenkov and the Wyatt momentum flow density tensors are analogous to those for the two corresponding pressure tensors, so the Wyatt momentum flow density tensor is more easily interpreted and applied than the Kuzmenkov momentum flow density tensor.

These results show that the right choice of pressure tensor can simplify quantum hydrodynamic calculations, and researchers doing quantum hydrodynamics should note this point.

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