Many-particle quantum hydrodynamics: exact equations and pressure tensors

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Abstract

In the first part of this paper, the many-particle quantum hydrodynamics (MPQHD) equations for a system containing many particles of different sorts are derived exactly from the many-particle Schrödinger equation. It includes the derivation of the many-particle continuity equations (MPCE), many-particle Ehrenfest equations of motion (MPEEM), and many-particle quantum Cauchy equations (MPQCE) 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 MPQCEs, there appears a quantity called 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 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.

1 Introduction

Quantum hydrodynamics (QHD) is a concept that was developed already 1926 by Madelung [1,2]. He transformed the Schrödinger equation for a single particle into the corresponding QHD equations. It was further developed by Bohm in 1952 [3,4]. The motivation to name this field QHD is that by applying it one finds differential equations with a similar form like well-known differential equations in classical hydrodynamics, like the continuity equation or the Navier-Stokes equation ([5], p. 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 [1,4,6,22]. First ideas for many-particle quantum hydrodynamics (MPQHD) were already discussed by Bohm [3]. In addition, MPQHD was analyzed using the energy-density functional method [23,25], a time-dependent Hartee-Fock ansatz [26,28], and a non-stationary non-linear Schrödinger equation ansatz for quantum plasma physics [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 [31]. Later, the method was further developed by Kuzmenkov and his colleagues to investigate spin effects [32, 33] and Bose-Einstein-Condensates [34]. Moreover, applications of this method were discussed e.g. related to electrons in graphene [35] and plasma effects [36–41]. In particular, in [38] it is briefly mentioned how to apply MPQHD when several sorts of particles are present, and the MPQHD equations stated in [38–41] describe the special case of two particle sorts in a plasma. In [38–40], these two sorts are electrons and a single ion sort, and in [41], these two sorts are electrons and positrons.

In Sec. 2 of this paper, we are aiming at developing further the methods described in [31, 38] by deriving rigorously 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 the 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 Sec. 2 we just briefly mention the effects of external electromagnetic fields. In addition, in our calculations in Sec. 2 we mention a quantity called the pressure tensor. One can find different versions of this pressure tensor in literature [13, 23, 28, 31]; an explanation for this variety can be found in [13]. In Sec. 3 we pick up the pressure tensor version given in [31] and name it the “Kusmenkov pressure tensor”. In addition, the discussion about QHD in [42], p. 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 particles. The MPCEs are equations related to the 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 $A, B, C$ stands for any number in $\{1, 2, \ldots, N_S\}$ which is related to one sort of particles. For brevity, we denote any $A$-th sort of particles also as the sort of particles $A$ or just as the sort $A$. The $N(A)$ particles of any sort $A$ shall be indistinguishable. In particular, each particle of the sort $A$ has the same
mass \( m_A \) and the same charge \( e_A \). In this publication, spin effects were not considered, for a more general analysis with spin effects one would have to consider that each particle of the 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 particles 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 [31], one can find a discussion where the question is analyzed 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 of the cases that the particles are bosons or fermions – but since we will not make a decomposition of the many-particle wave function into its eigenfunctions within the analysis in our paper, all equations in our paper are valid both for bosons and for fermions.

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

\[
\vec{Q} = \left( \vec{q}^1_1, \vec{q}^1_2, \ldots, \vec{q}^1_{N(1)}, \vec{q}^2_1, \ldots, \vec{q}^2_{N(2)}, \ldots, \vec{q}^N_{S1}, \ldots, \vec{q}^N_{SN} \right) \quad (1)
\]

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)

\[
V_{ij}^{AB} = \begin{cases} 
V^{AB}(|\vec{q}^A_i - \vec{q}^B_j|) & \text{for } (i \neq j) \text{ or } (A \neq B) \\
0 & \text{for } (i = j) \text{ and } (A = B)
\end{cases} \quad (2)
\]

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

\[
V_{ij}^{AB} = V_{ji}^{BA}, \quad (3)
\]

\[
\nabla_i V_{ij}^{AB} = -\nabla_j V_{ji}^{BA}, \quad (4)
\]

where \( \nabla_i \) is the Nabla operator relative to the coordinate \( \vec{q}^A_i \). Later, we will explain what happens if external fields are present.

The canonical momentum operator \( \hat{P}^A_i \) relative to the coordinate \( \vec{q}^A_i \) is

\[
\hat{P}^A_i = \frac{\hbar}{i} \nabla_i^A. \quad (5)
\]

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Then, the Schrödinger equation of the system is given by

$$i\hbar \frac{\partial \Psi(\vec{Q}, t)}{\partial t} = \hat{H}(\vec{Q}) \Psi(\vec{Q}, t)$$  \hspace{1cm} (6)$$

with a Hamiltonian

$$\hat{H}(\vec{Q}) = \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \left(\frac{\vec{P}_i^A}{2m_A}\right)^2 + \frac{1}{2} \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \sum_{B=1}^{N(B)} \sum_{j=1}^{N(A)} V_{ij}^{AB}. \hspace{1cm} (7)$$

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

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

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

$$d\vec{Q}_i^A = \frac{d\vec{Q}}{d\vec{q}_i^A}. \hspace{1cm} (9)$$

Note that $d\vec{q}_i^A$ 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

$$D(\vec{Q}, t) = \left| \Psi(\vec{Q}, t) \right|^2. \hspace{1cm} (10)$$

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

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

$$\rho_m^{\text{tot}}(\vec{q}, t) = \sum_{A=1}^{N_S} m_A \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) D(\vec{Q}, t)$$  \hspace{1cm} (11)$$

$$= \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q}_i^A D(\vec{Q}_i^A(\vec{q}), t). \hspace{1cm} (12)$$

Moreover, $\vec{Q}_i^A(\vec{q})$ means that in the particle coordinate set $\vec{Q}$ given by Eqn. (11), the coordinate vector $\vec{q}_i^A$ is set to $\vec{q}$.

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

$$\rho_m^A(\vec{q}, t) = N(A) m_A \int d\vec{Q}_i^A D(\vec{Q}_i^A(\vec{q}), t), \hspace{1cm} (13)$$
and it holds
\[ \rho_{m}^{\text{tot}}(\vec{q}, t) = \sum_{A=1}^{N_S} \rho_{m}^{A}(\vec{q}, t). \] (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 a next quantity, we define the total particle mass current density \( \vec{j}_{m}^{\text{tot}}(\vec{q}, t) \) as:

\[ \vec{j}_{m}^{\text{tot}}(\vec{q}, t) = \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_{i}^{A}) \, \Re \left[ \Psi^{*}(\vec{Q}, t) \, \hat{\vec{p}}_{i}^{A} \, \Psi(\vec{Q}, t) \right]. \] (15)

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

\[ \vec{j}_{m}^{\text{tot}}(\vec{q}, t) = h \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_{i}^{A}) \, \Im \left[ \Psi^{*}(\vec{Q}, t) \, \nabla_{A}^{i} \Psi(\vec{Q}, t) \right]. \] (16)

For the case of a single particle system, Eqn. (17) turns into the definition of the particle current density ([31], p. 144f. and [44], p. 24).

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

\[ \vec{j}_{m}^{A}(\vec{q}, t) = \sum_{i=1}^{N(A)} \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_{i}^{A}) \, \Im \left[ \Psi^{*}(\vec{Q}, t) \, \nabla_{A}^{i} \Psi(\vec{Q}, t) \right], \] (18)

so, it holds

\[ \vec{j}_{m}^{\text{tot}}(\vec{q}, t) = \sum_{A=1}^{N_S} \vec{j}_{m}^{A}(\vec{q}, t). \] (20)

Moreover, we note that because of Eqn. (18), the quantity \( \vec{j}_{m}^{A}(\vec{q}, t) \) can be interpreted as the expectation value of this operator \( \vec{j}_{m}^{A}(\vec{Q}, \vec{q}) \) [31]:

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\[
\hat{\mathbf{j}}^A_m(\vec{Q}, \vec{q}) = \frac{1}{2} \sum_{i=1}^{N(A)} \left[ \delta(\vec{q} - \vec{q}_i^A) \hat{p}_i^A + \hat{p}_i^A \delta(\vec{q} - \vec{q}_i^A) \right], \quad (21)
\]
\[
\vec{j}^A_m(\vec{q}, t) = \int d\vec{Q} \, \Psi^*(\vec{Q}, t) \hat{\mathbf{j}}^A_m(\vec{Q}, \vec{q}) \Psi(\vec{Q}, t). \quad (22)
\]

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

\[
\vec{v}^A(\vec{q}, t) = \frac{\vec{j}^A_m(\vec{q}, t)}{\rho^A_m(\vec{q}, t)} \quad (23)
\]

For all positions \( \vec{q}_0 \), where \( \rho^A_m(\vec{q}_0, t) = 0 \), we define:

\[
\vec{v}^A(\vec{q}_0, t) = \lim_{\vec{q} \to \vec{q}_0} \frac{\vec{j}^A_m(\vec{q}, t)}{\rho^A_m(\vec{q}, t)} \quad (24)
\]

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

\[
\Psi(\vec{Q}, t) = a(\vec{Q}, t) \exp \left[ \frac{iS(\vec{Q}, t)}{\hbar} \right] \quad (25)
\]

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

\[
\vec{w}^A_i(\vec{Q}, t) = \frac{1}{m^A} \nabla^A_i S(\vec{Q}, t). \quad (26)
\]

Note that for the velocity of the \((A, i)\)-th particle, we assigned the letter \( w \), and for the mean particle velocity for particles of the 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 e.g. in \([3]\), p. 2f., 11f., and 44f. As Madelung realized already in 1927 \([2]\) for the case of a single-particle system, the direct consequence of the definition \((26)\) for the velocity \( \vec{w}^A_i(\vec{Q}, t) \) of the \((A, i)\)-th particle is that the rotation of this velocity relative to the coordinate \( \vec{q}_i^A \) vanishes:

\[
\nabla^A_i \times \vec{w}^A_i(\vec{Q}, t) = \vec{0}. \quad (27)
\]

The definition above for \( \vec{w}^A_i(\vec{Q}, t) \) can now be used to do the following transformation of the term \( \Im \left[ \Psi^*(\vec{Q}, t) \nabla^A_i \Psi(\vec{Q}, t) \right] \) appearing in Eqn. \((17)\) for \( \vec{j}_m^\text{tot}(\vec{q}, t) \):
With this transformation, we find the following form for \( \mathbf{j} \):

\[
\mathbf{j} = \begin{bmatrix} \Psi^*(\mathbf{\bar{q}}, t) \nabla^\Lambda \Psi(\mathbf{\bar{q}}, t) \end{bmatrix} = \begin{bmatrix} \frac{a(\mathbf{\bar{q}}, t) \nabla^\Lambda a(\mathbf{\bar{q}}, t)}{\mathbb{R}} + \frac{i}{\hbar} a(\mathbf{\bar{q}}, t)^2 \nabla^\Lambda S(\mathbf{\bar{q}}, t) \end{bmatrix} = \begin{bmatrix} \frac{m_A}{\hbar} D(\mathbf{\bar{q}}, t) \mathbf{\bar{w}}^\Lambda(\mathbf{\bar{q}}, t) \end{bmatrix}.
\]

(28)

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

\[
\mathbf{j}^{tot}_m(\mathbf{q}, t) = \sum_{A=1}^{N_s} N(A) m_A \int \mathbf{\delta} \mathbf{\bar{Q}}_1^\Lambda D(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t) \mathbf{\bar{w}}_1^\Lambda(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t).
\]

(29)

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

\[
\mathbf{j}^A_m(\mathbf{q}, t) = N(A) m_A \int \mathbf{\delta} \mathbf{\bar{Q}}_1^\Lambda D(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t) \mathbf{\bar{w}}_1^\Lambda(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t).
\]

(30)

Eqn. (30) is a logical result for \( \mathbf{j}^A_m(\mathbf{q}, t) \) because it can be explained in the following way: For the situation that the \( (A, 1) \)-particle is located at \( \mathbf{\bar{q}} \) 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 \( D(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t) \mathbf{\bar{w}}_1^\Lambda(\mathbf{\bar{Q}}_1^\Lambda(\mathbf{q}), t) \) over the infinitesimal \( d\mathbf{Q}^\Lambda_1 \) multiplied by \( m_A \). Since the \( N(A) \) particles of the sort \( A \) cannot be distinguished from each other, the flux density \( \mathbf{j}^A_m(\mathbf{q}, t) \) for the \( N(A) \) particles of the sort \( A \) is then just \( N(A) \) times this integral.

As a further quantity, we define the relative velocity \( \mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) \) of the \( (A, i) \)-particle as:

\[
\mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) = \mathbf{\bar{u}}^\Lambda_i(\mathbf{q}, t) - \mathbf{\bar{v}}^\Lambda(\mathbf{q}, t).
\]

(31)

The motivation to name it relative velocity is that \( \mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) \) is the velocity of the \( (A, i) \)-particle relative to \( \mathbf{\bar{v}}^\Lambda(\mathbf{q}, t) \). Moreover, \( \mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) \) has the following property:

The \( (A, i) \)-particle shall be in the position \( \mathbf{q}^\Lambda_i = \mathbf{q} \), so \( \mathbf{Q} = \mathbf{Q}_1^\Lambda(\mathbf{q}) \), and we average \( \mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) \) over all positions which the other particles can occupy. Hereby, we weigh \( \mathbf{\bar{u}}^\Lambda_i(\mathbf{Q}, t) \) with the probability \( D(\mathbf{Q}, t) \) that the positions of all particles are given by \( \mathbf{Q} \). This average for the relative velocity \( \mathbf{\bar{u}}^\Lambda(\mathbf{Q}, t) \) vanishes. In the following calculation, the vanishing of this average is shown, and we use in this calculation Eqns. (33) and (30):

\[
\int d\mathbf{Q} \mathbf{\delta}(\mathbf{\bar{q}} - \mathbf{q}^\Lambda_i) D(\mathbf{Q}, t) \bar{u}^\Lambda_i(\mathbf{Q}, t) = \int d\mathbf{Q}_1^\Lambda D(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) \bar{u}_1^\Lambda(\mathbf{Q}_1^\Lambda(\mathbf{q}), t)
\]

\[
= \int d\mathbf{Q}_1^\Lambda D(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) \bar{u}_1^\Lambda(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) = \int d\mathbf{Q}_1^\Lambda D(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) \left( \bar{u}_1^\Lambda(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) - \bar{v}^\Lambda(\mathbf{q}, t) \right)
\]

\[
= \int d\mathbf{Q}_1^\Lambda D(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) \bar{w}_1^\Lambda(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) - \int d\mathbf{Q}_1^\Lambda D(\mathbf{Q}_1^\Lambda(\mathbf{q}), t) \bar{v}^\Lambda(\mathbf{q}, t)
\]

\[
= \frac{1}{N(A)m_A} \rho^\Lambda_m(\mathbf{q}, t)
\]
\[ \frac{1}{N(A) m_A} \left( \vec{j}^A_m(\vec{q}, t) - \rho^A_m(\vec{q}, t) \vec{v}^A_m(\vec{q}, t) \right) = \vec{0}. \]  

(32)

In this context, we call the relative velocities \( \vec{u}^A_i(\vec{Q}, t) \) also 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 \( \vec{v}^A_m(\vec{q}, t) \) and \( \vec{u}^A_i(\vec{Q}, t) \).

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

\[ \vec{v}^{\text{tot}}(\vec{q}, t) = \frac{\vec{j}^{\text{tot}}_m(\vec{q}, t)}{\rho^{\text{tot}}_m(\vec{q}, t)}, \]

(33)

and for all positions \( \vec{q}_0 \), where \( \rho^{\text{tot}}_m(\vec{q}_0, t) = 0 \), it is:

\[ \vec{v}^{\text{tot}}(\vec{q}_0, t) = \lim_{\vec{q} \to \vec{q}_0} \frac{\vec{j}^{\text{tot}}_m(\vec{q}, t)}{\rho^{\text{tot}}_m(\vec{q}, t)}. \]

(34)

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

\[ \vec{u}^A_i(\vec{Q}, t) := \vec{u}^A_i(\vec{Q}, t) - \vec{v}^{\text{tot}}(\vec{q}^A_i, t). \]

(35)

Note that \( \vec{u}^A_i(\vec{Q}, t) \) is the relative velocity of the \((A, i)\)-particle to \( \vec{v}^{\text{tot}}(\vec{q}^A_i, t) \), while \( \vec{u}^A_i(\vec{Q}, t) \) is the relative velocity of this particle to \( \vec{v}^A(\vec{q}^A_i, t) \). We emphasize that this is an expansion relative to [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 ([43], p. 144f. and [44], p. 24).

Therefore, we calculate the time derivative of \( \rho^A_m(\vec{q}, t) \) by inserting the Schrödinger equation (6) into Eqn. (13):

\[ \frac{\partial \rho^A_m(\vec{q}, t)}{\partial t} = N(A) m_A \int d\vec{Q}_1^A \left( \frac{\partial \Psi^*(\vec{Q}_1^A, t)}{\partial t} \Psi(\vec{Q}_1^A, t) + \Psi^*(\vec{Q}_1^A, t) \frac{\partial \Psi(\vec{Q}_1^A, t)}{\partial t} \right) \]

\[ = \frac{2N(A) m_A}{\hbar} \int d\vec{q} \delta(\vec{q} - \vec{q}^A_i) \Im \left[ \Psi^*(\vec{Q}, t) \dot{H}(\vec{Q}) \Psi(\vec{Q}, t) \right]. \]

(36)

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

\[ \Im \left( \Psi^* \dot{H} \Psi \right) = \Im \left( \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \Psi^* \frac{\hbar^2}{2m_B} \Delta_j^B \Psi + \frac{1}{2} \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \sum_{C=1}^{N_S} \sum_{k=1}^{N(C)} \Psi^* V_{jk BC}^B \Psi \right). \]
\[
\sum_{B=1}^{N_B} \sum_{j=1}^{N(B)} \frac{\hbar^2}{2m_B} \Im \left[ \nabla_j^B (\Psi^\ast \nabla_j^B \Psi) - \left( \nabla_j^B \Psi^\ast \right) (\nabla_j^B \Psi) \right] \in \mathbb{R}
\]

where \( \Delta_j^B \) is the Laplace operator relative to the coordinate \( \vec{q}_j^B \).

As a next step, we insert Eqn. (37) into Eqn. (36), and after that, the summand for the case \( \{B = A, j = 1\} \) is extracted out of the double sum over \( B, j \). We can then transform the integration over the coordinate \( \vec{q}_B \) 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:

\[
\frac{\partial \rho_m^A(\vec{q}, t)}{\partial t} = -\hbar N(A) m_A \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \frac{1}{m_B} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \Im \left[ \nabla_j^B (\Psi^\ast \nabla_j^B \Psi) \right]
\]

Finally, regarding the \( \delta \)-function in Eqn. (38), we can substitute the outer Nabla operator \( \nabla_1^A \) in the imaginary part by a \( \nabla \) operator related to the coordinate \( \vec{q} \) in the following manner:

\[
\frac{\partial \rho_m^A(\vec{q}, t)}{\partial t} = -\nabla \left\{ \hbar N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \Im \left[ \Psi^\ast(\vec{Q}, t) \nabla_1^A \Psi(\vec{Q}, t) \right] \right\}.
\]
We note here that Eqns. (40), (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 \( \vec{J}_m^A(\vec{q}, t) \) for this sort \( A \). We do not regard the indistinguishability of the particles of each sort form the beginning 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 derivation of Eqn. (18) instead of Eqn. (19) and transform it, using Eqn. (5) for the momentum operator:

\[
\frac{\partial j_m^A(\vec{q}, t)}{\partial t} = \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \frac{\partial}{\partial t} \left[ \Psi^*(\vec{Q}, t) \hat{p}_i^A \Psi(\vec{Q}, t) \right] 
\]

\[
= \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \frac{\partial}{\partial t} \left[ h \, \Psi^*(\vec{Q}, t) \nabla_i^A \Psi(\vec{Q}, t) \right]. \tag{42}
\]

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

\[
h \frac{\partial}{\partial t} \Re \left[ \Psi^* \nabla_i^A \Psi \right] = h \Re \left[ \left( \frac{\partial \Psi^*}{\partial t} \right) \nabla_i^A \Psi + \Psi^* \nabla_i^A \left( \frac{\partial \Psi}{\partial t} \right) \right] 
\]

\[
= h \Re \left[ \left( \frac{1}{i\hbar} \hat{H} \Psi \right)^* \nabla_i^A \Psi + \Psi^* \nabla_i^A \left( \frac{1}{i\hbar} \hat{H} \Psi \right) \right] \tag{43}
\]

\[
= \Re \left\{ \left( -\sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \frac{\hbar^2}{2m_B} \left( \Delta_j^B \Psi^* \right) + \frac{1}{2} \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \sum_{C=1}^{N_S} \sum_{k=1}^{N(C)} \Psi^* V_{jk}^{BC} \Psi \right) \right\} (\nabla_i^A \Psi) 
\]

\[
+ \Psi^* \nabla_i^A \left( \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \frac{\hbar^2}{2m_B} \left( \Delta_j^B \Psi \right) - \frac{1}{2} \sum_{B=1}^{N_S} \sum_{j=1}^{N(B)} \sum_{C=1}^{N_S} \sum_{k=1}^{N(C)} V_{jk}^{BC} \Psi \right) \}
\]

\[
= \Re \left\{ \sum_{B,j} \frac{\hbar^2}{2m_B} \left[ \Psi^* \nabla_i^A \left( \Delta_j^B \Psi \right) - \left( \Delta_j^B \Psi^* \right) \nabla_i^A \Psi \right] + \frac{1}{2} \sum_{B,j,k} \Psi^* \left[ V_{jk}^{BC} \nabla_i^A \Psi - \nabla_i^A \left( V_{jk}^{BC} \Psi \right) \right] \right\}
\]
\[
\mathfrak{R} \left\{ \sum_{B,j} \frac{\hbar^2}{2m_B} \sum_{\beta \in K_C} \left[ \Psi^A_i \nabla^A_i \left( \frac{\partial^2 \Psi}{\partial q^B_{j\beta} \partial q^B_{j\beta}} \right) - \left( \frac{\partial^2 \Psi^*}{\partial q^B_{j\beta} \partial q^B_{j\beta}} \right) (\nabla^A_i \Psi) \right] \right\}
- \frac{1}{2} |\Psi|^2 \sum_{B,C,j,k} \nabla^A_i V^B_{jk}
\]

\[
= \mathfrak{R} \left\{ \sum_{B,j} \frac{\hbar^2}{2m_B} \sum_{\beta \in K_C} \left\{ \frac{\partial}{\partial q^B_{j\beta}} \left[ \Psi^A_i \nabla^A_i \left( \frac{\partial \Psi}{\partial q^B_{j\beta}} \right) \right] - \left( \frac{\partial \Psi^*}{\partial q^B_{j\beta}} \right) \nabla^A_i \left( \frac{\partial \Psi}{\partial q^B_{j\beta}} \right) \right\} \right\}
- \frac{1}{2} D \sum_{B,C,j,k} \left( \delta_{ij} \delta_{AB} \nabla^A_i V^B_{ik} + \delta_{ik} \delta_{AC} \nabla^A_i V^B_{ji} \right)
\]

\[
\varphi \left\{ \sum_{B,j} \frac{\hbar^2}{2m_B} \sum_{\beta \in K_C} \frac{\partial}{\partial q^B_{j\beta}} \left[ \Psi^A_i \nabla^A_i \left( \frac{\partial \Psi}{\partial q^B_{j\beta}} \right) - \left( \frac{\partial \Psi^*}{\partial q^B_{j\beta}} \right) (\nabla^A_i \Psi) \right] \right\}
- D \sum_{B,j} \nabla^A_i V^B_{ij}.
\] (44)

With this result, we get the following intermediate result for \( \frac{\partial \tilde{f}^A_i (\tilde{q}, t)}{\partial t} \):

\[
\frac{\partial \tilde{f}^A_i (\tilde{q}, t)}{\partial t} = \sum_{i=1}^{N(A)} \sum_{B=1}^{N_S} \sum_{i=1}^{N(B)} \int d\tilde{Q} \delta(\tilde{q} - \tilde{q}^A_i) \frac{\hbar^2}{2m_B} \times \mathfrak{R} \left\{ \sum_{\beta \in K_C} \frac{\partial}{\partial q^B_{j\beta}} \left[ \Psi^A_i \nabla^A_i \left( \frac{\partial \Psi}{\partial q^B_{j\beta}} \right) - \left( \frac{\partial \Psi^*}{\partial q^B_{j\beta}} \right) (\nabla^A_i \Psi) \right] \right\}
- \sum_{i=1}^{N(A)} \sum_{B=1}^{N_S} \sum_{i=1}^{N(B)} \int d\tilde{Q} \delta(\tilde{q} - \tilde{q}^A_i) D \nabla^A_i V^B_{ij}.
\] (45)

The term in the last line of Eqn. (45) is the force density \( \tilde{f}^A_i (\tilde{q}, t) \) for all particles of the sort A; it is caused by the two-particle potential \( V^A_{ij} \):

\[
\tilde{f}^A_i (\tilde{q}, t) = \sum_{i=1}^{N(A)} \left[ - \sum_{B=1}^{N_S} \sum_{i=1}^{N(B)} \int d\tilde{Q} \delta(\tilde{q} - \tilde{q}^A_i) D(\tilde{Q}, t) \nabla^A_i V^A_{ij} \right].
\] (46)

Please regard that in spite of Eqn. (4) the summands in the triple sum are not antisymmetric relative to a permutation of \( \{A, i\} \leftrightarrow \{B, j\} \) because of the argument \( \tilde{q} - \tilde{q}^A_i \) in the \( \delta \)-function. This is related to the fact that the term in squared brackets in Eqn. (46) is the force density.
for the (A, i)-th particle.

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

\[
\vec{f}^A (\vec{q}, t) = - N(A) \sum_{i=1}^{N(A)} \sum_{B=1, B \neq A}^{N(B)} \sum_{j=1}^{N(B)} \int d\vec{Q} \delta (\vec{q} - \vec{q}_i^A) D(\vec{Q}, t) \nabla_i^A V_{ij}^{AB} \\
- N(A) N(A) \sum_{i=1}^{N(A)} \sum_{j=1}^{N(A)} \int d\vec{Q} \delta (\vec{q} - \vec{q}_i^A) D(\vec{Q}, t) \nabla_i^A V_{ij}^{AA}.
\]  

(47)

The first line in Eqn. (47) is related to the case \( B \neq A \), and the second line in this equation is related to the case \( B = A \).

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

We substitute the sum over \( i \) each in the first line and in the second line of Eqn. (47) by its summand for \( i = 1 \) multiplied by \( N(A) \). Moreover, in the first line, we substitute the sum over \( j \) by its summand for \( j = N(B) \) multiplied by \( N(B) \), and in the second line, we substitute the sum over \( j \) by its summand for \( j = N(A) \) multiplied by \( (N(A) - 1) \). Combining these substitutions with the definition (2) for the potential terms \( V_{ij}^{AB} \) leads to this result:

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

(48)

The reader might wonder why we choose the last summand for \( j = N(A) \) or \( j = N(B) \), respectively, for the substitution of the sums over \( j \) in Eqn. (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 the sort A as representative particles for the consideration of the two-particle interaction between the particles of the sort A since the interaction of a particle with itself is excluded.

Here, the transformation of the second line of Eqn. (47) into the term appearing in the second line of Eqn. (48) can be interpreted in this manner: The (A,1)-particle and the (A, N(A))-particle are chosen as representative particles for the two-particle interaction between the particles of the sort A. This choice is appropriate because for \( N(A) > 1 \), the (A, 1)-particle and the (A, N(A))-particle are different particles. Though, the (A,1)-particle and the (A, N(A))-particle are the same particle for the special case \( N(A) = 1 \), but this case is still evaluated in Eqn. (48) correctly, since for \( N(A) = 1 \), the factor \( (N(A) - 1) \) in
the second line of Eqn. (48) is zero – so we regard rightly that for $N(A) = 1$ the single particle of the sort A cannot interact with other particles of this sort A. This explanation above gives a clear reason why we choose $j = N(A)$ instead of $j = 1$ for the transformation of the term appearing in the second line of Eqn. (47). However, we could have used $j = 1$ for the transformation of the term appearing in the first line of Eqn. (47) because it is related to interactions between particles of different sorts. But there we still used the last summand for $j = N(B)$ because, as a consequence, we can now combine the two lines in Eqn. (48) in this compact final result for $\vec{f}_A(q, t)$:

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

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

$$\vec{f}^{\text{tot}}(q, t) = \sum_{A=1}^{N_S} \vec{f}_A(q, t)$$

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

In [38], a particle ensemble for two sorts of particles, namely electrons and one ion sort, is examined, and hereby, the Coulomb force density for the electrons is shown. Eqn. (49) is a generalization of this result for an arbitrary number $N_S$ of sorts of particles and any two-particle potential which can be described by Eqn. (2). Having discussed the force density term $\vec{f}_A(q, t)$ in the intermediate result (45) for $\frac{\partial \vec{j}_q^A(q,j,	au)}{\partial t}$, we will now analyze the remaining term. Therefore, we define a vector $\vec{x}_j^B(\vec{Q}, A, i, \alpha)$

$$\vec{x}_j^B(\vec{Q}, A, i, \alpha) = \frac{\hbar^2}{2m_B} \Re \left[ \Psi^* \frac{\partial}{\partial q_{1a}} \left( \nabla_j^B \Psi \right) - \nabla_j^B \Psi^* \left( \frac{\partial \Psi}{\partial q_{1a}} \right) \right]$$

(52)

with a $\beta$-component

$$x_{j\beta}^B(\vec{Q}, A, i, \alpha) = \frac{\hbar^2}{2m_B} \Re \left[ \Psi^* \frac{\partial}{\partial q_{1a}} \left( \frac{\partial \Psi}{\partial q_{j\beta}} \right) - \frac{\partial \Psi^*}{\partial q_{j\beta}} \left( \frac{\partial \Psi}{\partial q_{1a}} \right) \right].$$ (53)

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

With the definition (52), the \( \alpha \)-component of \( \frac{\partial A_m(\vec{q}, t)}{\partial t} \) is given by:

\[
\frac{\partial j_m^A(\vec{q}, t)}{\partial t} = f_A^A(\vec{q}, t) + \sum_{i=1}^{N(A)} \sum_{B=1}^{N(B)} N_S \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \times \sum_{B=1}^{N(B)} \sum_{j=1}^{N(S)} \int d\vec{q} \delta(\vec{q} - \vec{q}_j^A) \nabla B_j \vec{x}_j^B(\vec{Q}, A, i, \alpha).
\]

(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 \( \{ A, i \} \) is not equal to the tuple \( \{ B, j \} \), and for the second type, these two tuples are equal. By separating these two summand types, we get:

\[
\frac{\partial j_m^A(\vec{q}, t)}{\partial t} = f_A^A(\vec{q}, t) + \sum_{i=1}^{N(A)} \sum_{B=1}^{N(B)} N_S \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \int d\vec{q} \delta(\vec{q} - \vec{q}_j^A) \nabla B_j \vec{x}_j^B(\vec{Q}, A, i, \alpha).
\]

(55)

In the middle line of the equation above, a volume integral appears over the coordinate \( \vec{q}_j^B \). 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 \( \vec{q}_i^A \) contains the \( \delta \)-function \( \delta(\vec{q} - \vec{q}_i^A) \). This context leads to:

\[
\frac{\partial j_m^A(\vec{q}, t)}{\partial t} = f_A^A(\vec{q}, t) - \sum_{\beta \in K_{Ca}} \frac{\partial}{\partial q_\beta} \left\{ - \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \frac{\hbar^2}{2m_A} \Re \left[ \Psi^* \frac{\partial}{\partial q_{i\alpha}} \left( \frac{\partial \Psi}{\partial q_{i\beta}} \right) - \left( \frac{\partial \Psi^*}{\partial q_{i\alpha}} \right) \left( \frac{\partial \Psi}{\partial q_{i\beta}} \right) \right] \right\} \left\{ \vec{\nu}_j^B \vec{x}_j^B(\vec{Q}, A, i, \alpha) \right\}_{\{B,j\} \neq \{A,i\}}.
\]

(56)

Then, we take into account the indistinguishability of the particles of one sort and find the following result for \( \frac{\partial j_m^A(\vec{q}, t)}{\partial \vec{q}} \):
\[
\frac{\partial j_{m,\alpha}(\vec{q}, t)}{\partial t} = f_{\alpha}(\vec{q}, t) - \sum_{\beta \in K_{\text{Ca}}} \frac{\partial}{\partial q_\beta} \left\{ -N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \frac{\hbar^2}{2m_A} \Re \left[ \Psi^* \frac{\partial}{\partial q_{1\alpha}} \left( \frac{\partial \Psi}{\partial q_{1\beta}} \right) - \left( \frac{\partial \Psi^*}{\partial q_{1\beta}} \right) \left( \frac{\partial \Psi}{\partial q_{1\alpha}} \right) \right] \right\}. \tag{57}
\]

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

\[
\Pi_{\alpha\beta}^A(\vec{q}, t) = -N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \frac{\hbar^2}{2m_A} \Re \left[ \Psi^* \frac{\partial}{\partial q_{1\alpha}} \left( \frac{\partial \Psi}{\partial q_{1\beta}} \right) - \left( \frac{\partial \Psi^*}{\partial q_{1\beta}} \right) \left( \frac{\partial \Psi}{\partial q_{1\alpha}} \right) \right]. \tag{58}
\]

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

\[
\Pi_{\alpha\beta}^A(\vec{q}, t) = \Pi_{\beta\alpha}^A(\vec{q}, t). \tag{59}
\]

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

\[
\frac{\partial j_{m,\alpha}(\vec{q}, t)}{\partial t} = f_{\alpha}(\vec{q}, t) - \sum_{\beta \in K_{\text{Ca}}} \frac{\partial}{\partial q_\beta} \Pi_{\beta\alpha}^A(\vec{q}, t). \tag{60}
\]

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

\[
\nabla T(\vec{q}) = \sum_{\alpha \in K_{\text{Ca}}} \sum_{\beta \in K_{\text{Ca}}} \frac{\partial T_{\alpha\beta}(\vec{q})}{\partial q_\alpha} \epsilon_\beta. \tag{61}
\]

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

\[
\frac{\partial j_{m}^A(\vec{q}, t)}{\partial t} = \vec{f}^A(\vec{q}, t) - \nabla \Pi^A(\vec{q}, t). \tag{62}
\]

Our motivation to name the equation above as the many-particle Ehrenfest equation of motion (MPEEM) is the following: In Eqn. (21), we defined the operator \(\hat{j}_{m}^A(\vec{Q}, \vec{q})\), and we can interpret the quantity \(\hat{j}_{m}^A(\vec{q}, t)\) as the expectation value for it. So, the Ehrenfest theorem (\cite{lapin1953} and \cite{lapin1956}, p. 28ff.) predicates that we can calculate the time derivative of the mass flux density for particles of the sort A by this equation:

\[
\frac{\partial \hat{j}_{m}^A(\vec{q}, t)}{\partial t} = \frac{i}{\hbar} \int d\vec{Q} \Psi^*(\vec{Q}, t) \left[ \hat{H}(\vec{Q}), \hat{j}_{m}^A(\vec{Q}, \vec{q}) \right] \Psi(\vec{Q}, t). \tag{63}
\]
Indeed, by combining Eqs. (42) and (43), one can realize that the equation above is equivalent to our result (62) for \( \frac{\partial \tilde{J}^A_m}{\partial q} \). This concept of applying the Ehrenfest theorem to derive quantum hydrodynamical equations was already discussed by Epstein in [47].

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

\[
\Pi^A_{\alpha\beta}(\vec{q}, t) = N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \times \frac{1}{2m_A} R \left[ \Psi^* (\hat{p}^A_{\alpha_{1\beta}} \hat{p}^A_{1\beta} \Psi) + (\hat{p}^A_{1\beta} \Psi)^* (\hat{p}^A_{1\alpha} \Psi) \right]
\]

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

\[
R \left[ \Psi^* \frac{\partial}{\partial q_{1\alpha}} \left( \frac{\partial \Psi}{\partial q_{1\beta}} \right) \right] = R \left\{ a e^{-iS/\hbar} \frac{\partial}{\partial q_{1\alpha}} \left( a e^{iS/\hbar} \right) \right\}
\]

And the transformation for the second term is:

\[
- R \left[ \left( \frac{\partial \Psi^*}{\partial q_{1\beta}} \right) \left( \frac{\partial \Psi}{\partial q_{1\alpha}} \right) \right] = - R \left[ \left( \frac{\partial (a e^{-iS/\hbar})}{\partial q_{1\beta}} \right) \left( \frac{\partial (a e^{iS/\hbar})}{\partial q_{1\alpha}} \right) \right]
\]
Thus, by inserting Eqns. (65) and (66) into Eqn. (58), we get as an intermediate result for the tensor elements:

\[
\Pi_{\alpha\beta}^A(q, t) = \frac{\mathcal{N}(A)}{N} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \times a^2 \left[ m_A \omega_{1\alpha}^A \omega_{1\beta}^A - \frac{\hbar^2}{2m_A} \left( \frac{1}{a^2} \frac{\partial^2 a}{\partial q_1^{A\alpha} \partial q_1^{A\beta}} - \frac{1}{a^2} \frac{\partial a}{\partial q_1^{A\alpha}} \frac{\partial a}{\partial q_1^{A\beta}} \right) \right].
\]

Regarding \(a^2 = D\), it can be derived that:

\[
\frac{1}{2} \frac{\partial^2 \ln D}{\partial q_1^{A\alpha} \partial q_1^{A\beta}} = \frac{1}{2} \frac{\partial}{\partial q_1^{A\alpha}} \left( \frac{1}{D} \frac{\partial D}{\partial q_1^{A\beta}} \right) = \frac{1}{2} \frac{\partial}{\partial q_1^{A\beta}} \left( \frac{1}{D} \frac{\partial D}{\partial q_1^{A\alpha}} \right) = \frac{1}{a} \frac{\partial}{\partial q_1^{A\alpha}} \left( \frac{1}{a} \frac{\partial a}{\partial q_1^{A\beta}} \right) = \frac{1}{a} \frac{\partial a}{\partial q_1^{A\alpha}} \frac{\partial a}{\partial q_1^{A\beta}}.
\]

So we can write Eqn. (67) in the following form, which is the second way to express \(\Pi_{\alpha\beta}^A(q, t)\):

\[
\Pi_{\alpha\beta}^A(q, t) = \mathcal{N}(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left( m_A \omega_{1\alpha}^A \omega_{1\beta}^A - \frac{\hbar^2}{4m_A} \frac{\partial^2 \ln D}{\partial q_1^{A\alpha} \partial q_1^{A\beta}} \right).
\]

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

\[
\Pi_{\alpha\beta}^{\text{tot}}(q, t) = \sum_{A=1}^{N_S} \Pi_{\alpha\beta}^A(q, t),
\]

Moreover, both the matrix elements \(\Pi_{\alpha\beta}^A(q, t)\) for a particular sort of particles \(A\) and the matrix elements \(\Pi_{\alpha\beta}^{\text{tot}}(q, t)\) for all particles can be split each in a classical part (cl) and a quantum part (qu):

\[
\Pi_{\alpha\beta}^A(q, t) = \Pi_{\alpha\beta}^{A,\text{cl}}(q, t) + \Pi_{\alpha\beta}^{A,\text{qu}}(q, t),
\]

\[
\Pi_{\alpha\beta}^{A,\text{cl}}(q, t) = \mathcal{N}(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D w_{1\alpha}^A w_{1\beta}^A,
\]

\[
\Pi_{\alpha\beta}^{A,\text{qu}}(q, t) = -\frac{\hbar^2}{4m_A} \mathcal{N}(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \frac{\partial^2 \ln D}{\partial q_1^{A\alpha} \partial q_1^{A\beta}}.
\]
\[ \Pi_{\alpha\beta}^{tot}(\vec{q}, t) = \Pi_{\alpha\beta}^{tot, cl}(\vec{q}, t) + \Pi_{\alpha\beta}^{tot, qu}(\vec{q}, t), \]  

(75)

\[ \Pi_{\alpha\beta}^{tot, cl}(\vec{q}, t) = \sum_{A=1}^{N_S} \Pi_{\alpha\beta}^{A, cl}(\vec{q}, t) = \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^\lambda) \ D \ w_{1\alpha}^A w_{1\beta}^A, \]  

(76)

\[ \Pi_{\alpha\beta}^{tot, qu}(\vec{q}, t) = \sum_{A=1}^{N_S} \Pi_{\alpha\beta}^{A, qu}(\vec{q}, t) = -\hbar^2 \sum_{A=1}^{N_S} N(A) \frac{m_A}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^\lambda) \ D \frac{\partial^2 \ln D}{\partial q_{1\alpha} \partial q_{1\beta}}. \]  

(77)

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

\[ \Pi_{\alpha\beta}^{A, cl}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^\lambda) \ D \ (\vec{w}_1^A \otimes \vec{w}_1^A). \]  

(78)

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

\[ \Pi_{\alpha\beta}^{tot, cl}(\vec{q}, t) = \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^\lambda) \ D \ (\vec{w}_1^A \otimes \vec{w}_1^A). \]  

(79)

This relation of the classical tensors \( \Pi_{\alpha\beta}^{A, cl}(\vec{q}, t), \ Pi_{\alpha\beta}^{tot, cl}(\vec{q}, t) \) to dyadic products of particle velocities is an analog to the calculation of the momentum flow density tensor \( \Pi \) in classical hydrodynamics: The equation which is a classical analog to the Ehrenfest equation of motion can be found in [49], p. 32 and [50], p. 21. Viewing this equation, one can realize that in classical hydrodynamics, the momentum flow density tensor \( \Pi \) contains dyadic products of particle velocities. So, this is why we name \( \Pi_{\alpha\beta}^{A, cl}(\vec{q}, t), \ Pi_{\alpha\beta}^{tot, cl}(\vec{q}, t) \) classical tensors.

As a consequence of Eqns. (74), (77), compact forms also exist for the quantum tensors \( \Pi_{\alpha\beta}^{A, qu}(\vec{q}, t) \) and \( \Pi_{\alpha\beta}^{tot, qu}(\vec{q}, t) \):

\[ \Pi_{\alpha\beta}^{A, qu}(\vec{q}, t) = -\hbar^2 \sum_{A=1}^{N_S} N(A) \frac{m_A}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^\lambda) \ D \ (\nabla_1^A \otimes \nabla_1^A) \ln D, \]  

(80)

\[ \Pi_{\alpha\beta}^{tot, qu}(\vec{q}, t) = -\hbar^2 \sum_{A=1}^{N_S} N(A) \frac{m_A}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^\lambda) \ D \ (\nabla_1^A \otimes \nabla_1^A) \ln D. \]  

(81)

The term \( \nabla_1^A \otimes \nabla_1^A \) appearing in the two equations above is a dyadic product of the nabla operator \( \nabla_1^A \) for the \((A,1)\)-particle. In contrast to the classical parts, both the quantum tensor \( \Pi_{\alpha\beta}^{A, qu}(\vec{q}, t) \) for a certain sort of particles \( A \) and the quantum tensor \( \Pi_{\alpha\beta}^{tot, qu}(\vec{q}, t) \) 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 as quantum tensors.
Finally, we can find using Eqns. (72), (75), and (78) – (81) these compact forms for the tensors $\Pi^A(\vec{q}, t)$ and $\Pi^\text{tot}(\vec{q}, t)$:

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

$$\Pi^\text{tot}(\vec{q}, t) = \sum_{A=1}^{N_S} \Pi^A(\vec{q}, t) \quad (83)$$

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

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

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

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

Having derived the MPEEM both for all particles and for each sort of particles, we will now derive the corresponding many-particle quantum Cauchy equations (MPQCE).
2.4 Derivation of the MPQCE

The starting point of the derivation of the MPQCE for particles of the sort A is the corresponding MPEEM (62):

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

$$
\frac{\partial j^A_m(\vec{q}, t)}{\partial t} = \frac{\partial}{\partial t} \left( \rho^A_m \vec{v}^A \right) = \rho^A_m \frac{\partial \vec{v}^A}{\partial t} + \frac{\partial \rho^A_m}{\partial t} \vec{v}^A
$$

$$
= - \left( \nabla j^A_m \right) \vec{v}^A + \rho^A_m \frac{\partial \vec{v}^A}{\partial t}
$$

$$
= - \sum_{\alpha \in K_{Ca}} \vec{e}_\alpha \left[ \nabla \left( j^A_m v^A_\alpha \right) \right] + \sum_{\alpha \in K_{Ca}} \vec{e}_\alpha \left[ j^A_m \left( \nabla v^A_\alpha \right) \right] + \rho^A_m \frac{\partial \vec{v}^A}{\partial t}
$$

$$
= \rho^A_m \left[ \frac{\partial}{\partial t} + (\vec{v}^A \nabla) \right] \vec{v}^A - \nabla \left[ \rho^A_m \left( \vec{v}^A \otimes \vec{v}^A \right) \right] = (\rho^A_m \vec{v}^A \nabla) \vec{v}^A. \quad (86)
$$

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

$$
\frac{\partial j^A_m(\vec{q}, t)}{\partial t} = \rho^A_m \left[ \frac{\partial}{\partial t} + (\vec{v}^A \nabla) \right] \vec{v}^A - \nabla \left[ \rho^A_m \left( \vec{v}^A \otimes \vec{v}^A \right) \right]. \quad (87)
$$

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

$$
\rho^A_m \left[ \frac{\partial}{\partial t} + (\vec{v}^A \nabla) \right] \vec{v}^A = \vec{f}^A - \nabla p^A(\vec{q}, t) = \vec{f}^A - \nabla \left[ \Pi^A - \rho^A_m \left( \vec{v}^A \otimes \vec{v}^A \right) \right]. \quad (88)
$$

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

$$
p^A(\vec{q}, t) = \Pi^A(\vec{q}, t) - \rho^A_m(\vec{q}, t) \left[ \vec{v}^A(\vec{q}, t) \otimes \vec{v}^A(\vec{q}, t) \right]. \quad (89)
$$

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

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

$$
\rho^A_m(\vec{q}, t) \left[ \frac{\partial}{\partial t} + (\vec{v}^A(\vec{q}, t) \nabla) \right] \vec{v}^A(\vec{q}, t) = \vec{f}^A(\vec{q}, t) - \nabla p^A(\vec{q}, t). \quad (90)
$$
Now, we discuss why we name the equation above many-particle quantum Cauchy equation (MPQCE):

In classical hydrodynamics, 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 [51], p. 205, [52]:

\[ \rho_m(\vec{q}, t) \frac{d\vec{v}(\vec{q}, t)}{dt} = \vec{f}(\vec{q}, t) + \nabla \sigma(\vec{q}, t), \]  

(91)

In the equation above, the quantity \( \sigma(\vec{q}, t) \) 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 [51], p. 4-6:

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

(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 \( (\vec{v}(\vec{q}, t) \nabla) \vec{v}(\vec{q}, t) \) 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

\[ \sigma(\vec{q}, t) = -p(\vec{q}, t), \]  

(93)

and insert Eqns. (92) and (93) into Cauchy’s equation of motion (91), we realize that Cauchy’s equation of motion takes indeed the form of the MPQCE (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:

\[ \nabla \sigma(\vec{q}, t) \approx -\nabla P(\vec{q}, t) + \eta \nabla(\vec{v}(\vec{q}, t)) + (\zeta + \frac{\eta}{3}) \nabla(\nabla \vec{v}(\vec{q}, t)), \]  

(94)

where \( P(\vec{q}, t) \) is the scalar pressure, and \( \zeta \) and \( \eta \) are called coefficients of viscosity. So, the Navier-Stokes equation has the following form ([5], p. 44f. and [53]):

\[ \rho_m(\vec{q}, t) \left[ \frac{\partial}{\partial t} + (\vec{v}(\vec{q}, t) \nabla) \right] \vec{v}(\vec{q}, t) = \vec{f}(\vec{q}, t) - \nabla P(\vec{q}, t) + \eta \nabla(\vec{v}(\vec{q}, t)) + (\zeta + \frac{\eta}{3}) \nabla(\nabla \vec{v}(\vec{q}, t)). \]  

(95)

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

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

Here, one realizes a contrast to the derivation of the MPCE and the MPEEM for the total particle ensemble (see Eqsns. (41), (85)), which could be derived by summing up all the corresponding equations for the particular sorts of particles (see Eqns. (40), (62)). This context is related to the point that both the MPCE and the MPEEM for a particular sort of particles 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 Eqn. (90) because the MPQCE for all particles can be derived from the MPEEM (85) for all particles in an analogous manner like the MPQCE (90) specific for a certain sort of particles.

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

$$\frac{\partial \vec{j}^m(\vec{q}, t)}{\partial t} = \frac{\partial}{\partial t} (\rho^m v^m) = \rho^m \frac{\partial v^m}{\partial t} + \rho^m \frac{\partial \vec{v}^m}{\partial t}$$

$$= - \left( \nabla \vec{j}^m \right) \vec{v}^m + \rho^m \frac{\partial \vec{v}^m}{\partial t}$$

$$= - \sum_{\alpha \in K_C_a} \vec{e}_\alpha \left[ v^m_\alpha \left( \nabla \vec{j}^m \right) \right] + \rho^m \frac{\partial \vec{v}^m}{\partial t}$$

$$= - \sum_{\alpha \in K_C_a} \vec{e}_\alpha \left[ \nabla \left( \vec{j}^m v^m_\alpha \right) \right] + \sum_{\alpha \in K_C_a} \vec{e}_\alpha \left[ \vec{j}^m \left( \nabla v^m_\alpha \right) \right] + \rho^m \frac{\partial \vec{v}^m}{\partial t}$$

$$= \rho^m \left[ \frac{\partial}{\partial t} + \left( \vec{v}^m \nabla \right) \right] \vec{v}^m - \sum_{\alpha \in K_C_a} \sum_{\beta \in K_C_a} \vec{e}_\alpha \left[ \frac{\partial}{\partial q_\beta} \left( \rho^m v^m_\alpha v^m_\beta \right) \right]$$

$$= \rho^m \left[ \frac{\partial}{\partial t} + \left( \vec{v}^m \nabla \right) \right] \vec{v}^m - \sum_{\alpha \in K_C_a} \sum_{\beta \in K_C_a} \frac{\partial \left( \rho^m v^m_\alpha v^m_\beta \right)}{\partial q_\alpha} \vec{e}_\beta. \quad (96)$$
Regarding the tensor divergence definition (61), we now write the last term in the equation above as a tensor divergence:

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

(97)

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

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

(98)

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

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

(99)

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

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

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

(100)

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

2.5 Pressure tensor

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

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

(101)

so that its components are given by:

\[
\rho_{\alpha\beta}^{A}(\vec{q},t) = N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \, D \left( m_A u_{1\alpha}^A u_{1\beta}^A - \frac{\hbar^2}{4m_A} \frac{\partial^2 \ln D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A} \right).
\]

(102)
Moreover, we define the pressure tensor $p_{\text{tot}}(\vec{q}, t)$ for the total particle ensemble as:

$$p_{\text{tot}}(\vec{q}, t) := \sum_{A=1}^{N_S} N(A) \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_1^A) \, D \times \left[ m_A (\vec{u}_1^A \otimes \vec{u}_1^A) - \frac{\hbar^2}{4m_A} \left( \nabla_1^A \otimes \nabla_1^A \right) \ln D \right],$$

(103)

and we can write its components as follows:

$$p_{\alpha\beta}^{\text{tot}}(\vec{q}, t) = \sum_{A=1}^{N_S} N(A) \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_1^A) \, D \left( m_A u_{1\alpha}^A u_{1\beta}^A - \frac{\hbar^2}{4m_A} \frac{\partial^2 \ln D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A} \right).$$

(104)

At the end of this Sec. 2.5, we will prove that the definition (101) for $p_{\alpha\beta}(\vec{q}, t)$ is equivalent to Eqn. (89), and that the definition (103) for $p_{\text{tot}}(\vec{q}, t)$ is equivalent to Eqn. (99).

But before we do that, we will first discuss that we can split up both the tensor components $p_{\alpha\beta}(\vec{q}, t)$ and $p_{\text{tot}}^{\alpha\beta}(\vec{q}, t)$ in a classical part and a quantum part in a similar manner like the tensor components $\Pi_{\alpha\beta}(\vec{q}, t)$ and $\Pi_{\text{tot}}^{\alpha\beta}(\vec{q}, t)$. We mention here that a splitting of the pressure tensor components in a classical part and a quantum part was already described by Wong [28]:

$$p_{\alpha\beta}(\vec{q}, t) = p_{\alpha\beta}^{\text{cl}}(\vec{q}, t) + p_{\alpha\beta}^{\text{qu}}(\vec{q}, t),$$

(105)

$$p_{\alpha\beta}^{\text{cl}}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_1^A) \, D \, u_{1\alpha}^A u_{1\beta}^A,$n

(106)

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

(107)

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

(108)

$$p_{\alpha\beta}^{\text{tot,cl}}(\vec{q}, t) = \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_1^A) \, D \, u_{1\alpha}^A u_{1\beta}^A,$n

(109)

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

(110)

Note that

$$p_{\alpha\beta}^{\text{tot,cl}}(\vec{q}, t) \neq \sum_{A=1}^{N_S} p_{\alpha\beta}^{\text{cl}}(\vec{q}, t)$$

(111)

$$p_{\alpha\beta}^{\text{tot}}(\vec{q}, t) \neq \sum_{A=1}^{N_S} p_{\alpha\beta}^{A}(\vec{q}, t),$$

(112)
because in Eqn. (102), components of the velocity $\vec{u}^A_1(\vec{Q}, t)$ appear which are defined by the velocity of the $(A, 1)$-particle relative to the mean particle velocity $\vec{v}^A(\vec{q}^A_1, t)$ of particles of the sort A, while in Eqn. (104), components of the velocity $\vec{u}^A_1(\vec{Q}, t)$ appear which are defined by the velocity of the $(A, 1)$-particle relative to the mean particle velocity $\vec{v}^{\text{tot}}(\vec{q}^A_1, t)$ for the total particle ensemble.

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

Moreover, we can write the classical pressure tensor $p^{A,cl}(\vec{q}, t)$ for a specific sort of particles A in a compact tensor notation, where a dyadic product of the relative velocity $\vec{u}^A_1(\vec{Q}, t)$ of the $(A, 1)$-particle appears:

$$p^{A,cl}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D (\vec{u}^A_1 \otimes \vec{u}^A_1). \quad (113)$$

In an analogous manner, the classical pressure tensor $p^{\text{tot},cl}(\vec{q}, t)$ for the total particle ensemble is related to dyadic products $\vec{u}^A_1 \otimes \vec{u}^A_1$ for all sorts of particles $A \in \{ 1, \ldots, N_S \}$:

$$p^{\text{tot},cl}(\vec{q}, t) = \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D (\vec{u}^A_1 \otimes \vec{u}^A_1). \quad (114)$$

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

As a remark, we note that for the special case of a one-particle system, the associated classical pressure tensor $p^{cl}$ 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 $p^{cl}$ depends on the dyadic product $\vec{u} \otimes \vec{u}$, thus, the classical pressure tensor $p^{cl}$ vanishes, too. Therefore, the classical pressure tensor does not appear in the analysis of one-particle systems in these references [13][16][18], and [32], p. 56f. Please note that for a one-particle system the classical momentum flow density tensor $\Pi^{cl}$ does not vanish generally because the particle velocity $\vec{w}$ does not vanish for some one-particle systems (see for such a case the analysis in chapter 13 of [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 \( p_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) \) for a certain sort of particles \( A \) and the quantum pressure tensor elements \( p_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) \) for the total particle ensemble are just equal to the corresponding quantum momentum-flow density tensor elements:

\[
\begin{align*}
  p_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) & = \Pi_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t), \quad (115) \\
  p_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) & = \Pi_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t), \quad (116)
\end{align*}
\]

so that we can write for the corresponding tensors

\[
\begin{align*}
  p_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) & = \Pi_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) = -\frac{\hbar^2 N(A)}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D(\nabla_1^A \otimes \nabla_1^A) \ln D, \quad (117) \\
  p_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) & = \Pi_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) = -\frac{\hbar^2 N_S}{4m_A} \sum_{A=1}^{N_S} N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D(\nabla_1^A \otimes \nabla_1^A) \ln D. \quad (118)
\end{align*}
\]

Thus, like the quantum momentum-flow density tensors \( \Pi_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) \) and \( \Pi_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) \), both the quantum pressure tensor \( p_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) \) specific for a given sort \( A \) of particles and the quantum pressure tensor \( p_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) \) 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 \( p_{\alpha \beta}^{A,\text{qu}}(\vec{q}, t) \) and \( p_{\alpha \beta}^{\text{tot},\text{qu}}(\vec{q}, t) \) as quantum tensors.

At the end of this chapter, here we prove that the definition (101) for \( p_{\alpha \beta}^{A}(\vec{q}, t) \) is equivalent to Eqn. (89), and the definition (103) for \( p_{\alpha \beta}^{\text{tot}}(\vec{q}, t) \) is equivalent to Eqn. (99).

In order to prove the equivalence of Eqns. (101) and (89), we show that the quantity \( p_{\alpha \beta}^{A,\text{cl}}(\vec{q}, t) \) can be expressed in the following way by applying Eqns. (13), (30), (31), (73), and (106):

\[
\begin{align*}
  p_{\alpha \beta}^{A,\text{cl}}(\vec{q}, t) & = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D(\vec{Q}, t) u_{1\alpha}^A(\vec{Q}, t) v_{1\beta}^A(\vec{Q}, t) \\
  & = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D(\vec{Q}, t) \times \\
  & \left[ u_{1\alpha}^A(\vec{Q}, t) - v_{1\alpha}^A(\vec{q}_1^A, t) \right] \left[ u_{1\beta}^A(\vec{Q}, t) - v_{1\beta}^A(\vec{q}_1^A, t) \right]
\end{align*}
\]
\[
\begin{align*}
&= N(A) m_A \int d\vec{q}_1 \ D(\vec{q}_1, t) \ w_{1\alpha}(\vec{q}_1, t) \ w_{1\beta}(\vec{q}_1, t) \\
&= \Pi_{\alpha\beta}(\vec{q}, t) \\
&- v_\alpha(\vec{q}, t) \ N(A) m_A \int d\vec{q}_1 \ D(\vec{q}_1, t) \ w_{1\alpha}(\vec{q}_1, t) \\
&= j_{m,\alpha}(\vec{q}, t) = \rho_{m}(\vec{q}, t) \ v_\alpha(\vec{q}, t) \\
&- v_\beta(\vec{q}, t) \ N(A) m_A \int d\vec{q}_1 \ D(\vec{q}_1, t) \ w_{1\beta}(\vec{q}_1, t) \\
&= j_{m,\beta}(\vec{q}, t) = \rho_{m}(\vec{q}, t) \ v_\beta(\vec{q}, t) \\
&+ v_\alpha(\vec{q}, t) \ v_\beta(\vec{q}, t) \ N(A) m_A \int d\vec{q}_1 \ D(\vec{q}_1, t) \\
&= \Pi_{\alpha\beta}(\vec{q}, t) - \rho_{m}(\vec{q}, t) \ v_\alpha(\vec{q}, t) \ v_\beta(\vec{q}, t).
\end{align*}
\]

(119)

Then, we find a formula that relates the pressure tensor elements \( p_{\alpha\beta}(\vec{q}, t) \) for the sort of particles \( A \) with the corresponding momentum flow density tensor elements \( \Pi_{\alpha\beta}(\vec{q}, t) \) by adding Eqn. (115) and Eqn. (119):

\[
\begin{align*}
&= \Pi_{\alpha\beta}(\vec{q}, t) - \rho_{m}(\vec{q}, t) \ v_\alpha(\vec{q}, t) \ v_\beta(\vec{q}, t).
\end{align*}
\]

(120)

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

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

\[
\begin{align*}
&= \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \ \delta(\vec{q} - \vec{q}_1) \ D(\vec{Q}, t) \ u_{1\alpha}(\vec{Q}, t) \ u_{1\beta}(\vec{Q}, t) \\
&= \sum_{A=1}^{N_S} N(A) m_A \int d\vec{Q} \ \delta(\vec{q} - \vec{q}_1) \ D(\vec{Q}, t) \times \\
&\left[ u_{1\alpha}(\vec{Q}, t) - v_{\alpha}^{\text{tot}}(\vec{q}_1, t) \right] \left[ u_{1\beta}(\vec{Q}, t) - v_{\beta}^{\text{tot}}(\vec{q}_1, t) \right]
\end{align*}
\]

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Summing up Eqns. (116) and (121), we obtain a formula that relates the tensor elements \( p_{\alpha\beta}^{\text{tot}}(\vec{q}, t) \) and \( \Pi_{\alpha\beta}^{\text{tot,cl}}(\vec{q}, t) \) to each other:

\[
  p_{\alpha\beta}^{\text{tot}}(\vec{q}, t) = \Pi_{\alpha\beta}^{\text{tot,cl}}(\vec{q}, t) - \rho_{m}^{\text{tot}}(\vec{q}, t) v_{\alpha}^{\text{tot}}(\vec{q}, t) v_{\beta}^{\text{tot}}(\vec{q}, t). \tag{122}
\]

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

### 2.6 External fields

In this chapter, it is now briefly discussed which basic formulas and main results of the derivations above change if external electric and magnetic fields \( \vec{E}(\vec{q}, t), \vec{B}(\vec{q}, t) \) are present.

Here, we mention that the following results are similar to the results in [31], where analogous equations for MPQHD were derived like here – but, in [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 \( \vec{A}(\vec{q}, t) \) and a scalar potential \( \Phi(\vec{q}, t) \) by

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

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

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

\[
  \hat{\mathcal{D}}_i^A = \hat{\mathcal{p}}_i - e_A \vec{A}(\vec{q}_i^A, t). \tag{125}
\]
In our analysis above without external fields held $\vec{A}(\vec{q},t) = 0$, so, there was no need to distinguish between the kinematic momentum operator $\hat{\vec{D}}_i^A$ and the canonical momentum operator $\hat{\vec{p}}_i^A$. 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 $\hat{\vec{p}}_i^A$ appears, it has to be substituted in these equations by the kinematic momentum operator $\hat{\vec{D}}_i^A$ for the presence of external fields.

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

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

For the total particle mass current density $\vec{J}^m_{\text{tot}}(\vec{q},t)$, we find instead of Eqns. (15) and (17):

$$\vec{J}^m_{\text{tot}}(\vec{q},t) = \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \Re \left[ \Psi^*(\vec{Q},t) \hat{\vec{D}}_i^A \Psi(\vec{Q},t) \right]$$ (127)

$$\vec{J}^m_{\text{tot}}(\vec{q},t) = \sum_{A=1}^{N_S} \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \Re \left[ \Psi^*(\vec{Q},t) \hat{\vec{D}}_i^A \Psi(\vec{Q},t) \right],$$ (128)

so the particle mass current density $\vec{J}^m_{\text{tot}}(\vec{q},t)$ for the sort of particles A is now described by

$$\vec{J}^m_{\text{tot}}(\vec{q},t) = \sum_{i=1}^{N(A)} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) \Re \left[ \Psi^*(\vec{Q},t) \hat{\vec{D}}_i^A \Psi(\vec{Q},t) \right]$$ (129)

$$\vec{J}^m_{\text{tot}}(\vec{q},t) = \sum_{A=1}^{N_S} \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^A) \Re \left[ \Psi^*(\vec{Q},t) \hat{\vec{D}}_i^A \Psi(\vec{Q},t) \right]$$ (130)

instead by Eqns. (13), (19).

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

$$\vec{w}_i^A(\vec{Q},t) = \frac{1}{m_A} \left( \nabla_i^A \Psi(\vec{Q},t) - e_A \vec{A}(\vec{q}_i^A,t) \right).$$ (131)

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

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

$$\nabla_i^A \times \vec{w}_i^A(\vec{Q},t) = -\frac{e_A}{m_A} \vec{E}(\vec{q},t).$$ (132)

In addition, we note that the old formulas (29) and (30) for $\vec{J}^m_{\text{tot}}(\vec{q},t)$ or $\vec{J}^m_{\text{tot}}(\vec{q},t)$, 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 \( \vec{w}_i^A(\vec{Q}, t) \). Applying the same argumentation, Eqn. (23) for \( \vec{v}_i^A(\vec{q}, t) \), Eqn. (33) for \( \vec{u}_i^A(\vec{Q}, t) \), and Eqn. (35) for \( \vec{w}_i^A(\vec{Q}, t) \) do not change explicitly, but they do change implicitly for the presence of external fields.

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

\[
\vec{f}_i^A(\vec{q}, t) = - N(A) \left[ \sum_{B=1}^{N_s} (N(B) - \delta_{AB}) \int d\vec{Q}_1^A D(\vec{Q}_1^A(q), t) \nabla V^{AB}(|\vec{q} - \vec{q}_N^B|) \right] \\
+ \frac{e_i^A}{m_A} \rho_i^A(\vec{q}, t) \left[ \vec{E}(\vec{q}, t) + \vec{v}_i^A(\vec{q}, t) \times \vec{B}(\vec{q}, t) \right].
\]  (133)

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

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

\[
\vec{f}^{\text{tot}}(\vec{q}, t) = - \sum_{A=1}^{N_s} \left\{ N(A) \left[ \sum_{B=1}^{N_s} (N(B) - \delta_{AB}) \int d\vec{Q}_1^A D(\vec{Q}_1^A(q), t) \nabla V^{AB}(|\vec{q} - \vec{q}_N^B|) \right] \\
+ \frac{e_i^A}{m_A} \rho_i^A(\vec{q}, t) \left[ \vec{E}(\vec{q}, t) + \vec{v}_i^A(\vec{q}, t) \times \vec{B}(\vec{q}, t) \right] \right\},
\]  (134)

which replaces Eqn. (51).

In addition, in the old calculations we found two different representations for the momentum flow density tensor elements \( \Pi_{\alpha\beta}^A(q, t) \) of the sort A. The first one is Eqn. (64), which contains components of the canonical momentum flow operator \( \hat{D}_1^A \). 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 \( \hat{\mathcal{D}}_1^A \):

\[
\Pi_{\alpha\beta}^A(q, t) = N(A) \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \frac{1}{4m_A} \times \\
\left[ \Psi^\dagger \left( \hat{D}_{1\beta}^A \hat{D}_{1\alpha}^A \Psi \right) + \left( \hat{D}_{1\beta}^A \Psi \right)^\dagger \left( \hat{D}_{1\alpha}^A \Psi \right) + \left( \hat{D}_{1\alpha}^A \Psi \right)^\dagger \left( \hat{D}_{1\beta}^A \Psi \right) + \left( \hat{D}_{1\beta}^A \hat{D}_{1\alpha}^A \Psi \right)^\dagger \Psi \right].
\]  (135)

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

It can be found for the pressure tensor elements \( p_{\alpha\beta}^A(q, t) \) and \( p_{\alpha\beta}^{\text{tot}}(q, t) \) that the corresponding Eqns. (102) and (104) remain valid explicitly. However, implicit changes occur due
to the components of the velocities $\vec{u}_A^1(\vec{Q}, t)$ and $\vec{u}_A^1(\vec{Q}, t)$ appearing in Eqn. (102) or Eqn. (104), respectively.

Taking all these changes into account for the different quantities discussed above, we eventually find that both for a certain sort of particles $A$ and the total particle ensemble the corresponding MPCEs, MPEEMs, and the MPQCEs, given in Eqns. (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 $\Pi$ and $p$ tensors

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

3.1 Kuzmenkov tensors $\Pi^{KA}$ and $p^{KA}$

In the calculations above we found the formula (69) for the elements of the momentum flow density tensor $\Pi^A(\vec{q}, t)$, and the formula (102) for the elements of the pressure tensor $p^A(\vec{q}, t)$. Since these equations are similar to results stated in [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 Eqns. (78) and (113), the classical Kuzmenkov tensors $\Pi^{KA,cl}(\vec{q}, t)$ and $p^{KA,cl}(\vec{q}, t)$ are related to dyadic products $\vec{w}^A_1 \otimes \vec{w}^A_1$ or $\vec{u}^A_1 \otimes \vec{u}^A_1$, respectively. So – as mentioned above – these tensors are related to the momentum-flow density tensor $\Pi$ or to the pressure tensor $p$, respectively, in classical hydrodynamics, and their interpretation is clear.

However, a clear interpretation for the quantum quantities $\Pi^{KA,qu}(\vec{q}, t)$, $p^{KA,qu}(\vec{q}, t)$ is missing except for the aspect that they are related to quantum effects. This problem occurs because the term $D (\nabla^A_1 \otimes \nabla^A_1) \ln D$ appearing in Eqn. (117) for these quantities is difficult to understand. In order to close this gap, an alternative to the Kuzmenkov versions $\Pi^{KA}(\vec{q}, t)$ and $p^{KA}(\vec{q}, t)$ of the momentum flow density tensor and the pressure tensor is analyzed in the following Sec. 3.2.
3.2 Wyatt tensors $\Pi^{WA}$ and $p^{WA}$

The formula (1.57) in R. E. Wyatts book [42], p. 31, implies that the momentum flow density tensor $\Pi^{\alpha}(\vec{q}, t)$ can be calculated in the following manner (here, $\mathbb{1}$ is the unit matrix):

$$\Pi^{WA}(\vec{q}, t) = \mathbb{1}P_{\alpha} + \sum_{i=1}^{N(A)} m_{\alpha} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) D \left[(\vec{w}_i^A \otimes \vec{w}_i^A) + (\vec{d}_i^A \otimes \vec{d}_i^A)\right],$$  \hspace{1cm} (136)

so that its elements are given for Cartesian coordinates by:

$$\Pi^{WA}_{\alpha\beta}(\vec{q}, t) = P_{\alpha} \delta_{\alpha\beta} + \sum_{i=1}^{N(A)} m_{\alpha} \int d\vec{Q} \delta(\vec{q} - \vec{q}_i^A) D \left[w_{i\alpha}^A w_{i\beta}^A + d_{i\alpha}^A d_{i\beta}^A\right].$$  \hspace{1cm} (137)

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

The quantity $P_{\alpha}$ appearing in Eqns. (136) and (137) is the scalar quantum pressure given by:

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

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

In addition, in Eqn. (136), the dyadic product of a vector $d_i^A$ appears; this vector is defined by

$$\vec{d}_i^A(\vec{Q}, t) = -\frac{\hbar}{2m_{\alpha}} \nabla_i^A \frac{D}{D}. \hspace{1cm} (139)$$

This vector $\vec{d}_i^A(\vec{Q}, t)$ is named osmotic velocity of the $(A, i)$-particle corresponding to the nomenclature in [42], p. 327. It is the quantum analog to the particle velocity $\vec{w}_i^A(\vec{Q}, t)$, 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 osmotical velocity $\vec{d}_i^A(\vec{Q}, t)$ relative to the coordinate $\vec{q}_i^A$ vanishes:

$$\nabla_i^A \times \vec{d}_i^A(\vec{Q}, t) = -\frac{\hbar}{2m_{\alpha}} \nabla_i^A \times \left(\frac{1}{D} \nabla_i^A D\right)$$

$$= -\frac{\hbar}{2m_{\alpha}} \left\{ \frac{1}{D} \nabla_i^A \times (\nabla_i^A D) + \left[ \nabla_i^A \left(\frac{1}{D}\right) \right] \times (\nabla_i^A D) \right\}.$$  \hspace{1cm} (32)
\[
= \frac{\hbar}{2m_A} D^2 \left[ (\nabla^A D) \times (\nabla^A D) \right].
\] (140)

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

\[
\Pi^W A (\vec{q}, t) = 1 P_A + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left[ (\vec{w}_1^A \otimes \vec{w}_1^A) + (\vec{d}_1^A \otimes \vec{d}_1^A) \right],
\] (141)

\[
\Pi^{WA}_{\alpha\beta} (\vec{q}, t) = P_A \delta_{\alpha\beta} + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left( w_{1\alpha}^A w_{1\beta}^A + d_{1\alpha}^A d_{1\beta}^A \right),
\] (142)

\[
P_A (\vec{q}, t) = -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \Delta_1^A D.
\] (143)

In order to achieve a better understanding for the different meanings of the particle velocities \(\vec{d}_i^A (\vec{Q}, t)\) and \(\vec{w}_i^A (\vec{Q}, t)\), we calculate, as a small excursion, the velocities \(w\) and \(d\) for an one-dimensional free Gaussian wave packet for a single particle at the start time \(t = 0\). In literature ([13, 21, 22], and [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:

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

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

\[
S(x, 0) = \hbar k_0 x,
\] (145)

\[
D(x, 0) = \left( \frac{1}{2\pi\sigma^2} \right)^{\frac{1}{4}} e^{-x^2/(2\sigma^2)},
\] (146)

and the velocities \(w\) and \(d\) are given by:

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

\[
d(x, 0) = -\frac{\hbar}{2m} \frac{1}{D} \frac{\partial D}{\partial x} = -\frac{\hbar}{2m\sigma^2} x.
\] (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 \(\hat{p} = \frac{\hbar}{\sigma} \frac{\partial}{\partial x}\) for the wave function \(\Psi(x, 0)\) is given by

\[
\langle \hat{p} \rangle = \langle \Psi(x, 0) | \hat{p} | \Psi(x, 0) \rangle = \hbar k_0 = mw.
\] (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, and for $x < 0$, it is negative and is related to a rear movement of the backward wave packet shoulder (see for this dispersion discussion also [13] and [12], p. 327).

Resuming our general analysis, as can be realized by Eqns. (82) and (101), one can get the pressure tensor by substituting the particle velocities $\vec{\omega}^A_1(\vec{q}, t)$ in the equation for the momentum flow density tensor by the corresponding relative velocities $\vec{u}^A_1(\vec{Q}, t)$. So, using Eqn. (141) for $\Pi^{WA}(\vec{q}, t)$ as a starting point, we get a “Wyatt version” $p^{WA}(\vec{q}, t)$ of the pressure tensor. This tensor and its elements are:

$$
p^{WA}(\vec{q}, t) = P_A + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( (\vec{u}^A_1 \otimes \vec{u}^A_1) + (\vec{d}^A_1 \otimes \vec{d}^A_1) \right), \quad (150)
$$

$$
p^{WA}_{\alpha\beta}(\vec{q}, t) = P_A \delta_{\alpha\beta} + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( \vec{u}^A_{1\alpha} \vec{u}^A_{1\beta} + \vec{d}^A_{1\alpha} \vec{d}^A_{1\beta} \right). \quad (151)
$$

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

$$
\Pi^{WA}(\vec{q}, t) = \Pi^{WA,cl}(\vec{q}, t) + \Pi^{WA,qu}(\vec{q}, t), \quad (152)
$$

$$
\Pi^{WA,cl}(\vec{q}, t) = \Pi^{KA,cl}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( \vec{u}^A_1 \otimes \vec{u}^A_1 \right), \quad (153)
$$

$$
\Pi^{WA,qu}(\vec{q}, t) = 1 P_A + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( \vec{d}^A_1 \otimes \vec{d}^A_1 \right), \quad (154)
$$

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

$$
p^{WA,cl}(\vec{q}, t) = p^{KA,cl}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( \vec{u}^A_1 \otimes \vec{u}^A_1 \right), \quad (156)
$$

$$
p^{WA,qu}(\vec{q}, t) = \Pi^{WA,qu}(\vec{q}, t) = 1 P_A + N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}^A_1) D \left( \vec{d}^A_1 \otimes \vec{d}^A_1 \right). \quad (157)
$$

By the equations above we realize that for the Wyatt tensors $\Pi^{WA}(\vec{q}, t)$ and $p^{WA}(\vec{q}, t)$, their quantum parts are related to dyadic products $\vec{d}^A_1 \otimes \vec{d}^A_1$ of the osmotic velocity $\vec{d}^A_1(\vec{Q}, t)$ and to the scalar quantum pressure $P_A(\vec{q}, t)$. So, the advantage of the Wyatt tensor versions $\Pi^{WA}(\vec{q}, t)$ and $p^{WA}(\vec{q}, t)$ relative to the corresponding Kuzmenkov tensors is that their quantum parts $\Pi^{WA,qu}(\vec{q}, t)$ and $p^{WA,qu}(\vec{q}, t)$, which are identical, are more clearly to interpret.
Now, it remains to show that the Wyatt tensors $\Pi^W(q, t)$ and $p^W(q, t)$ are physically equivalent to the corresponding Kuzmenkov tensors $\Pi^K(q, t)$ or $p^K(q, t)$, respectively. First, we explain this proof for the pressure tensors $p^W(q, t)$ and $p^K(q, t)$:

As will be shown below, the Wyatt pressure tensor $p^W(q, t)$ is in general not equal to the Kuzmenkov pressure tensor $p^K(q, t)$:

$$p^W(q, t) \neq p^K(q, t).$$ (158)

However, it will be shown below, too, that

$$\nabla p^W(q, t) = \nabla p^K(q, t)$$ (159)

holds, so that both tensors lead to an equivalent input in the MPQCE – and this is the property which makes them physically equivalent.

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

$$\nabla p(q, t) = \left( \frac{\partial p_{xx}}{\partial x} + \frac{\partial p_{yx}}{\partial y} + \frac{\partial p_{zx}}{\partial z}, \frac{\partial p_{xy}}{\partial x} + \frac{\partial p_{yy}}{\partial y} + \frac{\partial p_{zy}}{\partial z}, \frac{\partial p_{xz}}{\partial x} + \frac{\partial p_{yz}}{\partial y} + \frac{\partial p_{zz}}{\partial z} \right),$$ (160)

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

In this sense, we can understand the definition (151) for the Wyatt pressure tensor $p^W(q, t)$ 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 $p^W_{\alpha \beta}(q, t)$ explained above, there are other versions for the pressure tensor $p^A(q, t)$ where this physical interpretation is not so clear – and the Kuzmenkov pressure tensor $p^K_A(q, t)$ is one of these other versions.
At this point, we notice that it was already mentioned in [23, 28] that there exist several versions of the pressure tensor \( p(\vec{q}, t) \). In addition, Sonego discussed already in [13] the reason mentioned above for the ambiguity of the pressure tensor \( p(\vec{q}, t) \). In contrast to our discussion, Sonego restricts the allowed transformations of this tensor to transformations which 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 \( \nabla p(\vec{q}, t) \) 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 \( p^K(\vec{q}, t) \) and the Wyatt pressure tensor \( p^W(\vec{q}, t) \).

But in contrast to our work, Sonego prefers using the Kuzmenkov pressure tensor \( p^K(\vec{q}, t) \) to using the Wyatt pressure tensor \( p^W(\vec{q}, t) \). His reason for this is that he uses a function called Wigner function to describe the system in the phase space which yields as a result the Kuzmenkov pressure tensor \( p^K(\vec{q}, t) \). 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: (...)” [13], p. 1166. In this sense, we think that it is still reasonable to prefer the Wyatt pressure tensor \( p^W(\vec{q}, t) \).

We now finish our discussion about the ambiguity of the pressure tensor \( p(\vec{q}, t) \) 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 \( T(\vec{q}, t) \) 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 [54]. Another example is the gauge ambiguity of the vector potential \( \vec{A}(\vec{q}, t) \) and the scalar potential \( \Phi(\vec{q}, t) \) in electrodynamics:

There is the Lorenz gauge

\[
\nabla \vec{A}(\vec{q}, t) + \frac{1}{c^2} \frac{\partial}{\partial t} \Phi(\vec{q}, t) = 0,
\]

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 [55], p. 179-181, 377-380.

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

\[
\nabla \vec{A}(\vec{q}, t) = 0
\]

as well, where the divergence of the vector potential \( \vec{A}(\vec{q}, t) \) vanishes. The Coulomb gauge can be advantageous for applications where no charges are present. For more details see [55], p. 181-183.

In order to prove now Eqns. (158) and (159), we first transform the term \(-\frac{h^2}{4m_A} \frac{\partial^2 \ln D}{\partial \vec{q}_{\alpha} \cdot \partial \vec{q}_{\beta}}\)
appearing in Eqn. (102) for the matrix elements $p_{\alpha\beta}^{KA}(\vec{q}, t)$ using Eqn. (139):

$$-rac{\hbar^2}{4m_A} \frac{\partial^2 \ln D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A} = -\frac{\hbar^2}{4m_A} \frac{\partial}{\partial q_{1\alpha}^A} \left( \frac{1}{D} \frac{\partial D}{\partial q_{1\beta}^A} \right)$$

$$= \frac{\hbar^2}{4m_A} \frac{\partial D}{D^2} \frac{\partial D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A} - \frac{\hbar^2}{4m_A} \frac{1}{D} \frac{\partial^2 D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A}.$$

(163)

As a next step, we insert the intermediate result (163) into Eqn. (102) for $p_{\alpha\beta}^{KA}(\vec{q}, t)$. Now, $p_{\alpha\beta}^{KA}(\vec{q}, t)$ can be splitted in a sum

$$p_{\alpha\beta}^{KA}(\vec{q}, t) = p_{\alpha\beta}^{KA,1}(\vec{q}, t) + p_{\alpha\beta}^{KA,2}(\vec{q}, t),$$

(164)

where

$$p_{\alpha\beta}^{KA,1}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left( u_{1\alpha}^A u_{1\beta}^A + d_{1\alpha}^A d_{1\beta}^A \right),$$

(165)

$$p_{\alpha\beta}^{KA,2}(\vec{q}, t) = -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) \frac{\partial^2 D}{\partial q_{1\alpha}^A \partial q_{1\beta}^A}. $$

(166)

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

In an analogous manner, we can also split the corresponding Wyatt matrix element $p_{\alpha\beta}^{WA}(\vec{q}, t)$ in two summands using Eqn. (151):

$$p_{\alpha\beta}^{WA}(\vec{q}, t) = p_{\alpha\beta}^{WA,1}(\vec{q}, t) + p_{\alpha\beta}^{WA,2}(\vec{q}, t).$$

(167)

Here, the summands $p_{\alpha\beta}^{WA,1}(\vec{q}, t)$ and $p_{\alpha\beta}^{WA,2}(\vec{q}, t)$ are given by:

$$p_{\alpha\beta}^{WA,1}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left( u_{1\alpha}^A u_{1\beta}^A + d_{1\alpha}^A d_{1\beta}^A \right) = p_{\alpha\beta}^{KA,1}(\vec{q}, t),$$

(168)

$$p_{\alpha\beta}^{WA,2}(\vec{q}, t) = P_A(\vec{q}, t) \delta_{\alpha\beta}. $$

(169)

So, the summands $p_{\alpha\beta}^{WA,1}(\vec{q}, t)$ and $p_{\alpha\beta}^{KA,1}(\vec{q}, t)$ are equal. But in general, $p_{\alpha\beta}^{KA,2}(\vec{q}, t)$ and $p_{\alpha\beta}^{WA,2}(\vec{q}, t)$ are not equal – in particular, $p_{\alpha\beta}^{WA,2}(\vec{q}, t)$ is always diagonal, and $p_{\alpha\beta}^{KA,2}(\vec{q}, t)$ is in general non-diagonal.
Thus, first, we have proven the inequation (158) that in general \( p^W_A(q, t) \) and \( p^K_A(q, t) \) are not equal.

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

\[
\nabla p^K_A(q, t) = \nabla p^W_A(q, t).
\]

The proof for this equation can be done with the following straightforward calculation: We analyze the \( \beta \)-component of the tensor divergence \( \nabla p^K_A(q, t) \) in Cartesian coordinates:

\[
\left[ \nabla p^K_A(q, t) \right]_\beta = \sum_{\alpha \in K_{Ca}} \frac{\partial p^K_A(q, t)}{\partial q_\alpha} = \sum_{\alpha \in K_{Ca}} \frac{\partial}{\partial q_\alpha} \left[ -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(q - \vec{q}_A) \frac{\partial^2 D}{\partial q_{\alpha_{\beta}} \partial q_{\alpha_{\beta}}} \right]_\beta
\]

\[
= \sum_{\alpha \in K_{Ca}} \frac{\partial}{\partial q_\alpha} \left[ -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(q - \vec{q}_A) \frac{\partial}{\partial q_{\alpha_{\beta}}} \frac{\partial^2 D}{\partial q_{\alpha_{\beta}} \partial q_{\alpha_{\beta}}} \right]_\beta
\]

\[
= \sum_{\alpha \in K_{Ca}} \frac{\partial}{\partial q_\alpha} \left[ -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(q - \vec{q}_A) \Delta^A D \right]_\beta
\]

\[
= \sum_{\alpha \in K_{Ca}} \frac{\partial}{\partial q_\alpha} \left[ P_A(q, t) \delta_{\alpha_{\beta}} \right]_\beta
\]

\[
= \sum_{\alpha \in K_{Ca}} \frac{\partial}{\partial q_\alpha} \left[ \nabla p^K_A(q, t) \right]_\beta
\]

\[
\implies \nabla p^K_A(q, t) = \nabla p^W_A(q, t).
\]

The crucial steps of the proof shown above occur between Eqns. (171) and (172), where a rearrangement of the spatial derivations is done. This rearrangement is possible due to the sum \( \sum_{\alpha \in K_{Ca}} \) appearing both in Eqn. (171) and Eqn. (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 – Eqn. (160) is an illustration of this fact. The rearrangement above changes each of the three summands in this sum but doing
this, the value of the total sum remains unchanged.

Finally, with the proof of Eqn. (170), we have the evidence that Eqn. (159) is true – thus, both the Kuzmenkov pressure tensor \( p^{KA}(\vec{q}, t) \) and the Wyatt pressure tensor \( p^{WA}(\vec{q}, t) \) lead to an equivalent input in the MPQCE (90), and therefore, they are physically equivalent.

Now, it remains to prove that the momentum-flow density tensors \( \Pi^{WA}(\vec{q}, t) \) and \( \Pi^{KA}(\vec{q}, t) \) are physically equivalent. Analogously to our analysis for the pressure tensors, we will show below that in general \( \Pi^{WA}(\vec{q}, t) \) and \( \Pi^{KA}(\vec{q}, t) \) are not equal:

\[
\Pi^{WA}(\vec{q}, t) \neq \Pi^{KA}(\vec{q}, t). \tag{174}
\]

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

\[
\nabla \Pi^{WA}(\vec{q}, t) = \nabla \Pi^{KA}(\vec{q}, t). \tag{175}
\]

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

The first step to prove Eqns. (174) and (175) is inserting Eqn. (163) into Eqn. (69) for the Kuzmenkov tensor elements \( \Pi^{KA}_{\alpha\beta}(\vec{q}, t) \), and to split each of them into a term \( \Pi^{KA,1}_{\alpha\beta}(\vec{q}, t) \) containing products of two factors being first-order Cartesian derivations of \( S(\vec{Q}, t) \) or \( D(\vec{Q}, t) \), and a term \( \Pi^{KA,2}_{\alpha\beta}(\vec{q}, t) \) containing products of second-order Cartesian derivations of \( D(\vec{Q}, t) \). Thus, we get:

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

\[
\Pi^{KA,1}_{\alpha\beta}(\vec{q}, t) = N(A) m_A \int d\vec{Q} \delta(\vec{q} - \vec{q}_1^A) D \left( w_{1\alpha}^A w_{1\beta}^A + d_{1\alpha}^A d_{1\beta}^A \right), \tag{177}
\]

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

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

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

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

\[
\Pi^{WA,2}_{\alpha\beta}(\vec{q}, t) = \Pi^{WA,2}_{\alpha\beta}(\vec{q}, t). \tag{181}
\]

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 inequation (174) is proven that in general \( \Pi^{WA}(\vec{q}, t) \) and \( \Pi^{KA}(\vec{q}, t) \) are not equal.

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

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

As an intermediate conclusion, we found that the Wyatt and the Kuzmenkov pressure tensors $p^{WA}(\vec{q}, t)$, $p^{KA}(\vec{q}, t)$ are physically equivalent, and the same holds for the Wyatt and Kuzmenkov momentum flow density tensors $\Pi^{WA}(\vec{q}, t)$, $\Pi^{KA}(\vec{q}, t)$. Moreover, the quantum parts of the Wyatt tensors are more easily to interpret 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 $p^{WA}(\vec{q}, t)$ is more easily to calculate than the divergence of the Kuzmenkov pressure tensor $p^{KA}(\vec{q}, t)$, so, the clearer interpretation is not the only advantage of the Wyatt pressure tensor $p^{WA}(\vec{q}, t)$.

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

$$\vec{q} = q_x \vec{e}_x + q_y \vec{e}_y + q_z \vec{e}_z,$$

(184)

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

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

Now, we introduce the radius $\rho$, the phase $\varphi$, and the coordinates $x$, $y$, and $z$, depending on $q_x$, $q_y$, and $q_z$ by

$$q_x \equiv x = \rho \cos \varphi,$$

(185)

$$q_y \equiv y = \rho \sin \varphi,$$

(186)

$$q_z \equiv z.$$  

(187)

We will show how the cylindrical vector components $q_\rho$, $q_\varphi$, and $q_z$ depend on $\rho$, $\varphi$, and $z$ – in particular we will find that $q_\varphi$ vanishes.

The transformation between the basis vectors $\vec{e}_\rho$, $\vec{e}_\varphi$, $\vec{e}_z$ in cylindrical coordinates and the basis vectors in Cartesian coordinates is described by what is called rotation matrix $\Lambda(\varphi)$. This rotation matrix $\Lambda(\varphi)$ depends on the geometrical orientation of the position vector $\vec{q}$ via the phase $\varphi$, and its matrix elements $\Lambda_{\alpha'\alpha}(\varphi)$ have the following form ([56], p. 231):

$$\begin{pmatrix} \vec{e}_\rho \\ \vec{e}_\varphi \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \Lambda_{\rho\rho} & \Lambda_{\rho\varphi} & \Lambda_{\rho z} \\ \Lambda_{\varphi\rho} & \Lambda_{\varphi\varphi} & \Lambda_{\varphi z} \\ \Lambda_{z\rho} & \Lambda_{z\varphi} & \Lambda_{z z} \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix} = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix}. \quad (188)$$
As a convention for notation, we write in the following matrix elements of a tensor field $T(\vec{q})$ 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 $\alpha, \beta$ are elements of the set $K_{Ca} = \{x, y, z\}$, and the cylindrical indices $\alpha', \beta'$ are elements of the set $K_{cy} = \{\rho, \phi, z\}$.

As a consequence of Eqn. (188), vector components $b_{\alpha}(\vec{q})$ and tensor elements $T_{\alpha\beta}(\vec{q})$ are transformed via (57, p. 4ff.):

$$b_{\alpha'}(\vec{q}) = \sum_{\alpha \in K_{Ca}} \Lambda_{\alpha' \alpha}(\phi) b_{\alpha}(\vec{q}), \quad (189)$$

$$T_{\alpha'\beta'}(\vec{q}) = \sum_{\alpha \in K_{Ca}} \sum_{\beta \in K_{Ca}} \Lambda_{\alpha' \alpha}(\phi) \Lambda_{\beta' \beta}(\phi) T_{\alpha\beta}(\vec{q}). \quad (190)$$

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

$$\vec{q} = \rho \vec{e}_\rho + z \vec{e}_z, \quad (191)$$

so $q_{\rho} \equiv \rho$, and $q_\phi$ vanishes. However, for vectors $\vec{b}(\vec{q})$ which are not equal to the position vector $\vec{q}$ itself the component $b_\phi(\vec{q})$ 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 $\Psi$ 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 $\phi_{iA}$ of all the $(A, i)$-particles for a certain sort of particles A.

An example for a system with such a wave function is a $\textrm{H}_2^+$ molecule in its electronic and rotational ground state because for fixed nuclei we can choose the coordinate system in a manner that the wave function is independent of the polar angle $\phi_e$ 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 $i = 1, 2, \ldots, N(A)$:

$$\frac{\partial^n S}{\partial \phi_{iA}^n} = 0, \quad (192)$$

$$\frac{\partial^n D}{\partial \phi_{iA}^n} = 0. \quad (193)$$

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

\[ p_{\alpha\beta}^{XA}(\vec{q},t) = p_{\beta\alpha}^{XA}(\vec{q},t). \]  

(194)

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

\[ p_{\beta'\alpha'}^{XA}(\vec{q},t) = \sum_{\alpha \in K_{Ca}} \sum_{\beta \in K_{Ca}} \Lambda_{\beta'\alpha}(\varphi) \Lambda_{\alpha'\beta}(\varphi) p_{\alpha\beta}^{XA}(\vec{q},t) \]

\[ = \sum_{\beta \in K_{Ca}} \sum_{\alpha \in K_{Ca}} \Lambda_{\alpha'\alpha}(\varphi) \Lambda_{\beta'\beta}(\varphi) p_{\alpha\beta}^{XA}(\vec{q},t) \]

\[ = p_{\alpha'\beta'}^{XA}(\vec{q},t). \]  

(195)

For the following analysis, it is advantageous to split the pressure tensor elements \( p_{\alpha\beta}^{XA}(\vec{q},t) \) into two parts \( p_{\alpha\beta}^{XA,1}(\vec{q},t) \) and \( p_{\alpha\beta}^{XA,2}(\vec{q},t) \), analogously to the discussions above. Then, we transform each part separately into corresponding cylindrical coordinate matrix elements \( p_{\alpha'\beta'}^{XA,1}(\vec{q},t) \) or \( p_{\alpha'\beta'}^{XA,2}(\vec{q},t) \), respectively. Because of Eqns. (165), (166), (168), and (169), the Cartesian coordinate matrix elements \( p_{\alpha\beta}^{XA,1}(\vec{q},t) \) and \( p_{\alpha\beta}^{XA,2}(\vec{q},t) \) are symmetric:

\[ p_{\alpha\beta}^{XA,1}(\vec{q},t) = p_{\beta\alpha}^{XA,1}(\vec{q},t), \]  

(196)

\[ p_{\alpha\beta}^{XA,2}(\vec{q},t) = p_{\beta\alpha}^{XA,2}(\vec{q},t). \]  

(197)

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

\[ p_{\beta'\alpha'}^{XA,1}(\vec{q},t) = p_{\alpha'\beta'}^{XA,1}(\vec{q},t), \]  

(198)

\[ p_{\beta'\alpha'}^{XA,2}(\vec{q},t) = p_{\alpha'\beta'}^{XA,2}(\vec{q},t). \]  

(199)

Now, we regard these four points to make the transformations \( p_{\alpha\beta}^{XA,1}(\vec{q},t) \to p_{\alpha'\beta'}^{XA,1}(\vec{q},t) \) and \( p_{\alpha\beta}^{XA,2}(\vec{q},t) \to p_{\alpha'\beta'}^{XA,2}(\vec{q},t) \):

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

\[ p_{\alpha'\beta'}^{XA,1}(\vec{q},t) = \sum_{\alpha \in K_{Ca}} \sum_{\beta \in K_{Ca}} \Lambda_{\alpha'\alpha}(\varphi) \Lambda_{\beta'\beta}(\varphi) p_{\alpha\beta}^{XA,1}(\vec{q},t), \]  

(200)

\[ p_{\alpha'\beta'}^{XA,2}(\vec{q},t) = \sum_{\alpha \in K_{Ca}} \sum_{\beta \in K_{Ca}} \Lambda_{\alpha'\alpha}(\varphi) \Lambda_{\beta'\beta}(\varphi) p_{\alpha\beta}^{XA,2}(\vec{q},t). \]  

(201)
Second, the Cartesian matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$ depend on the Cartesian vector components $u_{1\alpha}^\lambda(\vec{q}, t), d_{1\alpha}^\lambda(\vec{q}, t)$ (see Eqn. (168)). So, when one calculates the matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$ using Eqn. (200), one has to transform the Cartesian vector components $u_{1\alpha}^\lambda(\vec{q}, t), d_{1\alpha}^\lambda(\vec{q}, t)$ using Eqn. (189) into the vector components $u_{1\alpha'}^\lambda(\vec{q}, t), d_{1\alpha'}^\lambda(\vec{q}, t)$ for each of the Cartesian matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$, which appear on the right side of Eqn. (200). These velocity components $u_{1\alpha'}^\lambda(\vec{q}, t)$ and $d_{1\alpha'}^\lambda(\vec{q}, t)$ can be calculated from the quantities $S(\vec{q}, t)$ and $D(\vec{q}, t)$ by using Eqsns. (13), (23), (26), (30), (31), and (139). We regard for this calculation that the divergence $\nabla_i S(\vec{q}, t)$ appears in Eqn. (26), and that the divergence $\nabla_i D(\vec{q}, t)$ appears in Eqn. (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 $\rho^i$ is given in cylindrical coordinates by:

$$\nabla_i \Phi(\vec{q}, t) = \frac{\partial \Phi}{\partial \rho^i} = \frac{\partial \Phi}{\partial \rho^i} \varepsilon^i + \frac{\partial \Phi}{\partial \varphi^i} \varphi^i + \frac{\partial \Phi}{\partial z^i} z^i. \quad (202)$$

Third, the Cartesian coordinate derivations $\frac{\partial}{\partial x^{1A}} = \frac{\partial}{\partial x^{1A}} \equiv \frac{\partial}{\partial x^{1A}}$ and $\frac{\partial}{\partial y_1} = \frac{\partial}{\partial y_1} \equiv \frac{\partial}{\partial y_1}$ are present in Eqn. (169) for all of the Cartesian matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$ (besides the $zz$-element). Thus, when one calculates the matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$, one has to transform the Cartesian coordinate derivations $\frac{\partial}{\partial x^{1A}} \equiv \frac{\partial}{\partial x^{1A}}$ and $\frac{\partial}{\partial y_1} \equiv \frac{\partial}{\partial y_1}$ for the Cartesian matrix elements $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$, which appear on the right side of Eqn. (201) for $X = K$. Hereby, one has to regard:

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial x_1} \equiv \frac{\partial}{\partial x_1} = \cos \varphi_1 \frac{\partial}{\partial \varphi_1} - \sin \varphi_1 \frac{\partial}{\partial \rho_1}, \quad (203)$$

$$\frac{\partial}{\partial y_1} = \frac{\partial}{\partial y_1} \equiv \frac{\partial}{\partial y_1} = \sin \varphi_1 \frac{\partial}{\partial \varphi_1} + \cos \varphi_1 \frac{\partial}{\partial \rho_1}. \quad (204)$$

Fourth, one can simplify the transformation calculations by taking into account the symmetry properties (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 derivation relative to the $\varphi_1$-coordinate in Eqsns. (203) and (204) – this is important for the calculation of the matrix element $p_{\alpha\beta}^{X\alpha\beta\lambda}(\vec{q}, t)$.

Then, we find for the first-order tensor components $p_{\alpha'\beta'}^{X\alpha\beta\lambda}(\vec{q}, t)$:

$$p_{\alpha'\beta'}^{X\alpha\beta\lambda}(\vec{q}, t) = p_{\alpha'\beta'}^{W\alpha\beta\lambda}(\vec{q}, t) = \frac{\partial}{\partial x_1} (\delta(\vec{q} - \vec{q}_A) \quad (205)$$
That \( p^{KA,1}_\alpha(\vec{q}, t) \) and \( p^{WA,1}_\alpha(\vec{q}, t) \) are equal is trivial since the corresponding Cartesian matrix elements are equal (see Eqn. (168)). Here, we note that the velocity components \( u^A_1 \varphi \) and \( d^A_1 \varphi \) vanish because of Eqn. (202) and the symmetry properties described by Eqns. (192) and (193):

\[
w^A_1 \varphi = \frac{1}{m_A} \frac{1}{\rho_{1A}} \frac{\partial S}{\partial \varphi_{1A}} = 0 \implies u^A_1 \varphi = 0, \tag{206}
\]

\[
d^A_1 \varphi = -\frac{\hbar}{2m_A} \frac{1}{\rho_{1A}} \frac{\partial D}{\partial \varphi_{1A}} = 0. \tag{207}
\]

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

Moreover, the calculation of the Kuzmenkov second-order tensor elements \( p^{KA,2}_\alpha(\vec{q}, t) \) yields these results:

For the \( \rho \rho \)-matrix element:

\[
p^{KA,2}_{\rho \rho}(\vec{q}, t) = -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^1) \frac{\partial^2 D}{\partial \rho_{1A}^2}. \tag{208}
\]

For the \( \rho \varphi \)-matrix element:

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

For the \( \rho z \)-matrix element:

\[
p^{KA,2}_{\rho z}(\vec{q}, t) = -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^1) \frac{\partial^2 D}{\partial \rho_{1A} \partial z_{1A}}. \tag{210}
\]

For the \( \varphi \varphi \)-matrix element:

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

For the \( \varphi z \)-matrix element:

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

For the \( zz \)-matrix element:

\[
p^{KA,2}_{zz}(\vec{q}, t) = -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \delta(\vec{q} - \vec{q}_A^1) \frac{\partial^2 D}{\partial z_{1A}^2}. \tag{213}
\]

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Hereby, 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 Eqn. (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 Eqn. (169), $P_A(\vec{q},t)\equiv 1$ 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 Eqn. (190):

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

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

$$p^{WA,2}_{\alpha'\beta'}(\vec{q},t) = P_A(\vec{q},t) \delta_{\alpha'\beta'}.$$ (215)

We mention that the quantity $P_A(\vec{q},t)$ does not change itself under a coordinate transformation because it is a scalar field. However, the coordinate transformation from Cartesian to cylindrical coordinates changes as follows how $P_A(\vec{q},t)$ is calculated:

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

$$\Delta^A = \frac{\partial^2}{\partial \rho_1^A \partial \rho_1^A} + \frac{1}{\rho_1^A} \frac{\partial}{\partial \rho_1^A} \frac{\partial^2}{\partial \varphi_1^A \partial \varphi_1^A} + \frac{\partial^2}{\partial z_1^A \partial z_1^A}.$$ (216)

After having calculated the first- and second-order cylindrical elements $p^{XA,1}(\vec{q},t)$ and $p^{XA,2}(\vec{q},t)$, we calculate the corresponding tensor divergences. For this objective, the general equation for calculating the divergence of a tensor field $\nabla T(\vec{q})$ in cylindrical coordinates has to be evaluated ([58], p. 60):

$$\nabla T(\vec{q}) = \left[ \frac{\partial T_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} \left( \frac{\partial T_{\varphi\rho}}{\partial \varphi} + T_{\rho\varphi} - T_{\varphi\rho} \right) + \frac{\partial T_{z\rho}}{\partial z} \right] \vec{e}_\rho$$

$$+ \left[ \frac{\partial T_{\rho\varphi}}{\partial \rho} + \frac{1}{\rho} \left( \frac{\partial T_{\varphi\varphi}}{\partial \varphi} + T_{\rho\varphi} + T_{\varphi\rho} \right) + \frac{\partial T_{z\varphi}}{\partial z} \right] \vec{e}_\varphi$$

$$+ \left[ \frac{\partial T_{\rho z}}{\partial \rho} + \frac{1}{\rho} \left( \frac{\partial T_{\varphi z}}{\partial \varphi} + T_{\rho z} \right) + \frac{\partial T_{z z}}{\partial z} \right] \vec{e}_z.$$ (217)

Here, we mention that Andreev and Kuzmenkov analyze in [38] QHD in cylindrical coordinates, too. However, in their approach, they calculate a tensor divergence of the momentum flow density tensor $\nabla \Pi$ in cylindrical coordinates by applying the $\nabla$-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 $\alpha \in K_{cy}$, and then they treat the result of this calculation as if it were
the $\alpha$-component of the tensor divergence $\nabla_{\alpha}$. Andreev and Kuzmenkov compensate their error by this approach by introducing in their QHD equations an additional inertia force. But we think that if one applies Eqn. (217) for calculating tensor divergences instead, it is not necessary to introduce this inertia force.

Using Eqn. (217) and the symmetry $p_{\beta' \alpha'}^{KA,1}(\vec{q}, t) = p_{\alpha' \beta'}^{KA,1}(\vec{q}, t)$ for calculating the divergence of the first-order tensors $p^{XA,1}(\vec{q}, t)$, we find:

$$\nabla_{\alpha} p^{KA,1}(\vec{q}, t) = \nabla_{\alpha} p^{WA,1}(\vec{q}, t)$$

$$= \left( \frac{\partial p^{WA,1}_{\rho \rho}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho z} + \frac{1}{\rho^2} p^{WA,1}_{zz} \right) \vec{e}_\rho$$

$$+ \left( \frac{\partial p^{WA,1}_{\rho \phi}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho z} + \frac{1}{\rho^2} p^{WA,1}_{zz} \right) \vec{e}_z.$$  (218)

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

$$\nabla_{\alpha} p^{KA,2}(\vec{q}, t) = \left[ \frac{\partial p^{KA,2}_{\rho \rho}}{\partial \rho} + \frac{1}{\rho} p^{KA,2}_{\rho \phi} - p^{KA,2}_{\phi \phi} + \frac{1}{\rho^2} p^{KA,2}_{\rho z} + \frac{1}{\rho^2} p^{KA,2}_{zz} \right] \vec{e}_\rho$$

$$+ \left( \frac{\partial p^{KA,2}_{\rho \phi}}{\partial \rho} + \frac{1}{\rho} p^{KA,2}_{\rho z} + \frac{\partial p^{KA,2}_{\phi \phi}}{\partial \rho} \right) \vec{e}_z.$$  (219)

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

$$\nabla_{\alpha} p^{WA,2}(\vec{q}, t) = \frac{\partial P_A}{\partial \rho} \vec{e}_\rho + \frac{1}{\rho} \frac{\partial P_A}{\partial \phi} \vec{e}_\phi + \frac{\partial P_A}{\partial z} \vec{e}_z.$$  (220)

As a next step, we regard that the differential operators $\Delta_A^1$ and $\frac{\partial}{\partial \varphi_{1A}}$ commute – this can be proven trivially by Eqn. (216) for the Laplace operator $\Delta_A^1$ in cylindrical coordinates. From this context, we conclude that the derivative $\frac{\partial p_A(q_1)}{\partial \varphi}$ vanishes due to the symmetry property (193):

$$\frac{\partial P_A(q_1, t)}{\partial \varphi} = -\frac{\partial}{\partial \varphi} N(A) \frac{\hbar^2}{4m_A} \int d\tilde{Q} \delta(\vec{q} - \vec{q}_1^A) \Delta_1^A D$$

$$= -N(A) \frac{\hbar^2}{4m_A} \int d\tilde{Q} \delta(\vec{q} - \vec{q}_1^A) \frac{\partial}{\partial \varphi_{1A}} \Delta_1^A D$$
\[ -N(A) \frac{\hbar^2}{4m_A} \int d\vec{Q} \, \delta(\vec{q} - \vec{q}_A) \, \Delta_1^A \frac{\partial D}{\partial \varphi_1^A} = 0. \]  

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

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

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

\[ \nabla p^{KA}(\vec{q}, t) = \nabla p^{KA,1}(\vec{q}, t) + \nabla p^{KA,2}(\vec{q}, t) 
= \left[ \frac{\partial p^{WA,1}_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho\rho} + \frac{\partial p^{WA,1}_{\rho z}}{\partial z} \right] \vec{e}_\rho 
+ \left[ \frac{\partial p^{KA,2}_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} (p^{KA,2}_{\rho\rho} - p^{KA,2}_{\varphi\varphi}) + \frac{\partial p^{KA,2}_{\rho z}}{\partial z} \right] \vec{e}_z, \]  

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

\[ \nabla p^{WA}(\vec{q}, t) = \nabla p^{WA,1}(\vec{q}, t) + \nabla p^{WA,2}(\vec{q}, t) 
= \left( \frac{\partial p^{WA,1}_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} p^{WA,1}_{\rho\rho} + \frac{\partial p^{WA,1}_{\rho z}}{\partial z} + \frac{\partial p^{WA,1}_{\rho z}}{\partial \rho} \right) \vec{e}_\rho 
+ \left( \frac{\partial p^{WA,2}_{\rho\rho}}{\partial \rho} + \frac{1}{\rho} p^{WA,2}_{\rho\rho} + \frac{\partial p^{WA,2}_{\rho z}}{\partial z} + \frac{\partial p^{WA,2}_{\rho z}}{\partial \rho} \right) \vec{e}_z. \]  

As a result, both \( \nabla p^{KA}(\vec{q}, t) \) and \( \nabla p^{WA}(\vec{q}, t) \) have no \( \vec{e}_\varphi \)-component due to the symmetry properties described by Eqns. (192) and (193). Apart from this identical property of \( \nabla p^{WA}(\vec{q}, t) \) and \( \nabla p^{KA}(\vec{q}, t) \), for numerical applications – where \( \nabla p^{WA}(\vec{q}, t) \) or \( \nabla p^{KA}(\vec{q}, t) \), respectively, are input quantities in the MPQCE (90) – the use of the Wyatt pressure tensor \( p^{WA}(\vec{q}, t) \) is advantageous:
The reason for this is that the evaluation equation (222) for the calculation of the second-order part $p_{W}^{A_2}(\vec{q}, t)$ of the Wyatt pressure tensor is more compact and less complicated than the corresponding Eqn. (219) for the calculation of the second-order part $p_{K}^{A_2}(\vec{q}, t)$ 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 $\Pi_{X}^{A_1}(\vec{q}, t)$ and $\Pi_{X}^{A_2}(\vec{q}, t)$ of the momentum flow density tensor $\Pi(\vec{q}, t)$ can be derived in an analogous manner like for the parts $p_{X}^{A_1}(\vec{q}, t)$ and $p_{X}^{A_2}(\vec{q}, t)$ of the pressure tensor $p(\vec{q}, t)$:

\begin{align*}
\Pi_{\alpha'\beta'}^{K}(\vec{q}, t) & = \Pi_{\alpha'\beta'}^{W}(\vec{q}, t) \\
& = N(A) \int dQ \delta(\vec{q} - \vec{q}^A) \ D m_A \ (w^A_{1\alpha'} w^A_{1\beta'} + d^A_{1\alpha'} d^A_{1\beta'}). \quad (225)
\end{align*}

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

\begin{align*}
\Pi_{\alpha\beta}^{X}(\vec{q}, t) & = p_{\alpha\beta}^{X}(\vec{q}, t). \quad (226)
\end{align*}

So, the cylindrical coordinate matrix elements $\Pi_{\alpha'\beta'}^{X}(\vec{q}, t)$ are given by

\begin{align*}
\Pi_{\alpha'\beta'}^{X}(\vec{q}, t) & = p_{\alpha'\beta'}^{X}(\vec{q}, t). \quad (227)
\end{align*}

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

4 Summary

In this paper, we derived MPQHD 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 up the MPCEs for all the different sorts of particles. Moreover, we derived for each sort of particles two different equations of motion. The first one of these equations of motion is the MPEEM; it describes the temporal change of the mass flux density of the particles of the analysed sort – and one can derive the MPEEM by applying the Ehrenfest theorem for the calculation of this temporal change. The second one 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 particles 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 particles. The MPQCEs for the different sorts of particles 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 particles and for the total particle ensemble, a quantity appears which is 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 particles, the properties of two different versions of this tensor are discussed: The first one 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 [42], p. 31. The second one is named the “Kuzmenkov pressure tensor” because it appears in [31]. The terms contributing to the Wyatt pressure tensor can be interpreted physically better than the Kusmenkov pressure tensor. Moreover, we made a coordinate transformation of both tensor versions from Cartesian coordinates to cylindrical coordinates and calculated the tensor divergence for both versions in cylindrical coordinates. This calculation can be performed more easily for the Wyatt pressure tensor than for the Kusmenkov pressure tensor because a certain summand contributing to the Wyatt pressure tensor is just a scalar multiplied by the diagonal unit tensor, while the according summand contributing to the Kusmenkov 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 particles, 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 like 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 just analogous to that of the two corresponding pressure tensors – so, the Wyatt momentum flow density tensor is more easily to interpret and to apply than the Kuzmenkov momentum flow density tensor. These results show that the right choice of the pressure tensor can simplify quantum hydrodynamic calculations, and researchers doing quantum hydrodynamics should regard this point.
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[53] In [5], p. 44f., a Navier-Stokes equation is derived where the force density \( \vec{f} \) is neglected – but one can find in literature other versions of the Navier-Stokes equation with a non-vanishing \( \vec{f} \) [51], p. 208. Moreover, one can realize easily by comparing the calculations in [5], p. 3 and [5], p. 44f. how one can derive a Navier-Stokes equation which includes a force density \( \vec{f} \).

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