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ORIGINAL ARTICLE

Contributions to Plasma Physics

Time-reversal invariance of quantum kinetic equations II: Density operator formalism

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Time-reversal symmetry is a fundamental property of many quantum mechanical systems. The relation between statistical physics and time reversal is subtle, and not all statistical theories conserve this particular symmetry—most notably, hydrodynamic equations and kinetic equations such as the Boltzmann equation. Here, we consider quantum kinetic generalizations of the Boltzmann equation using the method of reduced density operators, leading to the quantum generalization of the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. We demonstrate that all commonly used approximations, including Vlasov; Hartree-Fock; and the non-Markovian generalizations of the Landau, T-matrix, and Lenard-Balescu equations, are originally time-reversal invariant, and we formulate a general criterion for time reversibility of approximations to the quantum BBGKY hierarchy. Finally, we illustrate, through the example of the Born approximation, how irreversibility is introduced into quantum kinetic theory via the Markov limit, making the connection with the standard Boltzmann equation. This paper is a complement to paper I (Scharnke et al., *J. Math. Phys.*, **2017**, *58*, 061903), where the time-reversal invariance of quantum kinetic equations was analysed in the frame of the independent non-equilibrium Green functions formalism.

KEYWORDS
BBGKY-hierarchy, density operators, quantum dynamics, quantum kinetic theory, time reversibility

1 | INTRODUCTION

Q2 The time evolution of quantum many-body systems is of great interest currently in many areas of modern physics and chemistry, for example, in the context of laser–matter interaction, non-stationary transport, or dynamics following an interaction or confinement quench. The theoretical concepts used to study these dynamics are fairly broad and include (but are not limited to) wave function-based approaches, density functional theory, and quantum kinetic theory. The latter treats the time dynamics of the Wigner distribution or, more generally, the density matrix and captures the relaxation towards an equilibrium state (see, e.g., Refs. 1–4). The most famous example of a kinetic equation is the Boltzmann equation, along with quantum generalization, but this equation is known to not be applicable to the short-time dynamics. For this reason, generalized quantum kinetic equations were derived that are non-Markovian in nature (e.g., Refs. 1, 3, 5–9) and that have a number of remarkable properties, including the conservation of total energy, in contrast to kinetic energy conservation in the Boltzmann equation. It was recently demonstrated that these generalized quantum kinetic equations are well suited to study the relaxation dynamics of weakly and moderately correlated quantum systems, in very good agreement with experiments with ultra-cold atoms (e.g., Refs. 10, 11) and first-principle density matrix renormalization group methods.[12]

This success of generalized quantum kinetic equations warrants a more detailed theoretical analysis of their properties. Despite extensive work over recent decades, the aspect of time reversibility was not studied in detail. The relation between time-reversal symmetry and statistical physics is generally subtle, and not all statistical theories are invariant under time reversal, the most famous counterexample being the above-mentioned Boltzmann equation of classical statistical mechanics and its quantum generalization. In contrast, the non-Markovian generalizations of the Boltzmann equation, which can be used to improve the Boltzmann equation and consist of the latter as a limiting case, are expected to be time-reversal invariant because of the underlying quantum mechanical system. But then, questions arise about where exactly time-reversal invariance is lost, how this is related to common many-body approximations, and so on.

Among the well-established approaches to derive these generalized quantum kinetic equations, we mention density operator concepts—see, for example, Ref. 3 for an overview—and non-equilibrium Green functions (NEGF). We recently analysed the question of time-reversal invariance within the NEGF formalism in paper I.[13] It is the goal of the present article to complement the NEGF results of that paper with an analysis of the independent and technically very different density operator formalism. In this paper, we briefly recall the derivation of the quantum Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy in section 2. As the BBGKY hierarchy can be directly derived from the Heisenberg equation (von Neumann equation) for the N-particle density operator, which is time-reversal invariant, it should be expected that this hierarchy has the same symmetry properties. Nevertheless, general proof is usually missing in the literature, for example, Refs. 1–4, and a successful procedure is presented in section 4. We then demonstrate, in section 5, that important standard closure approximations to the BBGKY hierarchy also preserve time-reversal symmetry. In section 6, we demonstrate, as an example, the transition from a time-reversal invariant generalized kinetic equation to an irreversible equation of the Boltzmann type by performing the Markov limit and the weakening of initial conditions. We conclude with a summary in section 7.

2 | BBGKY HIERARCHY FOR THE REDUCED-DENSITY OPERATORS

Here, we briefly recall the basic equations of the density operator theory following Ref. 3. The generic Hamiltonian of an interacting N-particle system is given by a sum of a single particle and an interaction term

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_i + \sum_{1\le i<j\le N} \hat{V}_{ij}, \tag{1}$$

$$\hat{H}_i(t) = \frac{\hat{p}_i^2}{2m_i} + \hat{U}_i(t). \tag{2}$$

The solutions of the time-dependent N-particle Schrödinger equation with this Hamiltonian are denoted by $|\psi^{(1)}\rangle \ldots |\psi^{(M)}\rangle$ and form a complete orthonormal basis:

$$\langle \psi^{(k)} | \psi^{(l)} \rangle = \delta_{k,l}, \tag{3}$$

$$\sum_{k=1}^{M} | \psi^{(k)}\rangle\langle\psi^{(k)} | = 1. \tag{4}$$

The central quantity for the construction of quantum kinetic equations is the N-particle density operator:

$$\hat{\rho} = \sum_{k=1}^{M} W_k \, | \psi^{(k)}\rangle\langle\psi^{(k)} |, \tag{5}$$

where W_k are positive real probabilities, and $0 \le W_k \le 1$, with $\sum_{k=1}^{M} W_k = 1$, and we restrict ourselves to the case of time-independent probabilities. The density operator obeys the von Neumann equation

$$i\hbar \frac{\partial}{\partial t}\hat{\rho} - [\hat{H}, \hat{\rho}] = 0. \tag{6}$$

In order to derive the quantum BBGKY hierarchy, we introduce the reduced s-particle density operator ($s = 1 \ldots N-1$)

$$\hat{F}_{1\ldots s} = C_s^N \mathrm{Tr}_{s+1\ldots N}\ \hat{\rho}, \qquad \mathrm{Tr}_{1\ldots s}\hat{F}_{1\ldots s} = C_s^N, \tag{7}$$

where $C_s^N = \frac{N!}{(N-s)!}$. The equations of motion for the reduced density operators follow directly from the von Neumann Equation 6 and the definition 7:

$$i\hbar \frac{\partial}{\partial t}\hat{F}_{1\ldots s} - [\hat{H}_{1\ldots s}, \hat{F}_{1\ldots s}] = \mathrm{Tr}_{s+1} \sum_{i=1}^{s} [\hat{V}_{i,s+1}, \hat{F}_{1\ldots s+1}], \tag{8}$$

where $\hat{H}_{1\ldots s}$ is the s-particle Hamilton operator, which follows from the N-particle Hamiltonian, Equation 1, by substituting $N \to s$. The system 8 with $s = 1 \ldots N-1$ constitutes the quantum generalization of the BBGKY hierarchy.

In order to specify decoupling approximations to the hierarchy, we introduce the correlation operators:

$$\hat{F}_{12} = \hat{F}_1\hat{F}_2 + \hat{g}_{12}, \tag{9}$$

$$\hat{F}_{123} = \hat{F}_1\hat{F}_2\hat{F}_3 + \hat{g}_{23}\hat{F}_1 + \hat{g}_{13}\hat{F}_2 + \hat{g}_{12}\hat{F}_3 + \hat{g}_{123}, \tag{10}$$

where $\hat{g}_{12}$ describes pair correlations, $\hat{g}_{123}$ three-particle correlations, and so on, which are due to interaction effects beyond the mean field. In contrast, mean field (Vlasov, Hartree-Fock) terms are contained in the products of single-particle density operators and appear via the mean field potential $\hat{U}_i^{\mathrm{H}} = \mathrm{Tr}_j\hat{V}_{ij}\hat{F}_j$, leading to the renormalization of the single-particle and two-particle Hamiltonians $\hat{H}_i \to \hat{\hat{H}}_i = \hat{H}_i + \hat{U}_i^{\mathrm{H}}$, $\hat{H}_{ij} \to \hat{\hat{H}}_{ij} = \hat{\hat{H}}_i + \hat{\hat{H}}_j + \hat{V}_{ij}$, and so on. The BBGKY hierarchy, rewritten in terms of the correlation operators, then becomes:

$$i\hbar\frac{\partial}{\partial t}\hat{F}_1 - [\hat{\hat{H}}_1, \hat{F}_1] = \mathrm{Tr}_2[\hat{V}_{12}, \hat{g}_{12}], \tag{11}$$

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$$i\hbar\frac{\partial}{\partial t}\hat{g}_{12} - [\hat{\hat{H}}_{12}, \hat{g}_{12}] = [\hat{V}_{12}, \hat{F}_1\hat{F}_2] + $$
$$+\mathrm{Tr}_3\{[\hat{V}_{13}, \hat{F}_1\hat{g}_{23}] + [\hat{V}_{23}, \hat{F}_2\hat{g}_{13}] + [\hat{V}_{13} + \hat{V}_{23}, \hat{g}_{123}]\}, \tag{12}$$

and this is also applicable for the higher-order operators. Standard many-body approximations are easily identified from Equations 11 and 12, cf. for example, Ref. 3:

1. The *mean field (Hartree or Hartree-Fock) approximation* that leads to the non-linear Vlasov equation (or to the time-dependent Hartree-Fock) follows from letting $\hat{g}_{12} \to 0$ in Equation 11.
2. The *second-order Born approximation,* leading to the Landau equation, follows from neglecting $\hat{V}_{12}$ in $\hat{\hat{H}}_{12}$ on the left and $\hat{g}_{23} = \hat{g}_{13} = \hat{g}_{123} \to 0$ on the right side in Equation 12.
3. The *T-matrix or ladder approximation* follows from setting $\hat{g}_{23} = \hat{g}_{13} = \hat{g}_{123} \to 0$ on the right side in Equation 12.
4. The *polarization approximation* that is related to the GW approximation of Green functions theory and leads to the Lenard-Balescu equation follows from neglecting $\hat{V}_{12}$ in $\hat{\hat{H}}_{12}$ on the left and $\hat{g}_{123} \to 0$ on the right side in Equation 12.
5. The *screened ladder approximation* that is related to the parquet approximation (or "FLEX") in Green functions theory follows from $\hat{g}_{123} \to 0$ on the right side in Equation 12.

In a similar manner, higher-order decoupling schemes for the BBGKY hierarchy are introduced on the level of the equation of motion for g_{123}. Typically, approximations are derived by omitting terms of the form $[\hat{A}, \hat{B}]$, where $\hat{A}$ is a contribution to the full Hamiltonian 1 (typically an interaction potential), and $\hat{B}$ are contributions to the cluster expansion 10. This will be discussed in more detail in section 5.

Finally, we note that the cluster expansion 10 is written without an explicit account of the spin statistics. A direct (anti-)symmetrization of the hierarchy, for the case of bosons (fermions), is straightforwardly achieved by replacing the density operators according to[14] (Figure 1)

$$\hat{F}_{1\ldots s} \to \hat{F}_{1\ldots s}\Lambda^{\pm}_{1\ldots s}, \tag{13}$$

where the (anti-)symmetrization operators are given by

$$\Lambda^{\pm}_{12} = 1 \pm P_{12},$$
$$\Lambda^{\pm}_{123} = 1 \pm P_{12} \pm P_{13} \pm P_{23} + P_{12}P_{13} + P_{12}P_{23},$$

and so on, where P_{ij} is the permutation operator of particles i and j, and the upper (lower) sign refers to bosons (fermions). (Anti-)symmetrization is then achieved by applying the s-particle operator $\Lambda^{\pm}_{1\ldots s}$ to the s-th equation of the BBGKY hierarchy, term by term. We illustrate this procedure for the (anti-)symmetrization of the Hartree mean field term on the l.h.s. of

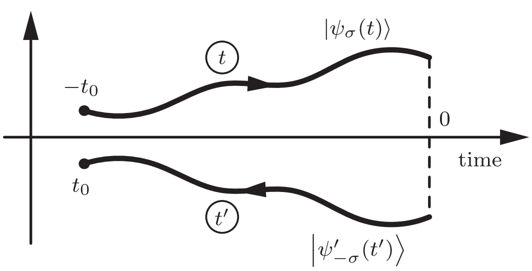

FIGURE 1 Illustration of the forward and backward solutions of the time-dependent Schrödinger equation. Upper trajectory: forward solution $|\psi_\sigma(t)\rangle$. Lower trajectory: backward solution $|\psi'_{-\sigma}(t')\rangle$. Note that we choose the limits of the forward trajectory as $t = -t_0$ and $t = 0$, whereas the backward one runs from $t' = 0$ to $t' = t_0$. The time reversal occurs at $t = 0$

Equation 11, which is obtained by replacing $\hat{F}_1\hat{F}_2 \to \hat{F}_1\hat{F}_2\Lambda^{\pm}_{12}$:

$$[\hat{U}^{\rm H}_1, \hat{F}_1] \to [\hat{U}^{\rm HF}_1, \hat{F}_1] = {\rm Tr}_2[\hat{V}_{12}, \hat{F}_1\hat{F}_2\Lambda^{\pm}_{12}],$$
$$\text{with} \quad \hat{U}^{\rm HF}_i = {\rm Tr}_j \hat{V}_{ij}\hat{F}_j\Lambda^{\pm}_{ij}, \tag{14}$$

The full (anti-)symmetrized equations are given in Ref. [3]. However, we will not need these equations below. This is because the (anti-)symmetrization operators commute with the time-reversal operator $\hat{T}$, cf. section 3. Therefore, (anti-)symmetrization does not affect the time-reversal properties of the resulting equations and approximations, allowing us to restrict ourselves to the simpler Equations 11, 12 in this study.

3 | TIME-REVERSAL INVARIANCE IN QUANTUM MANY-BODY THEORY

3.1 | Time-reversal invariance of the equations of motion of quantum mechanics

Let us recall the concept of time reversibility as was discussed in Ref. 13; for text book discussions, see Refs. 15, 16. Consider the time-dependent N-particle Schrödinger equation on an arbitrary finite interval of time, $-t_0 \le t \le 0$, with a given initial condition $|\psi_0\rangle$:

$$i\hbar\partial_t \mid \psi(t)\rangle = \hat{H} \mid \psi(t)\rangle \ , \tag{15}$$

$$\mid \psi(-t_0)\rangle = \mid \psi_0\rangle. \tag{16}$$

This equation is called time-reversal invariant if:

i. for any solution $|\psi(t)\rangle$, there exists another solution $|\psi'(t')\rangle$ with $t' \in [0, t_0]$ and $t' = -t$ and
ii. there exists a unique relation between the two:

$$\mid \psi'(t')\rangle = \hat{T} \mid \psi(t)\rangle, \tag{17}$$

for which the time-reversal operator $\hat{T}$ will be specified below. Both solutions describe the same physical state; therefore, the associated probability densities must coincide:

$$||\psi_\sigma(t)\rangle|^2 = ||\psi'_{-\sigma}(-t)\rangle|^2, \tag{18}$$

where we indicated explicitly that, on the backward trajectory $|\psi'(t')\rangle$, the spin projections σ of all particles are inverted. Analogously, momenta and angular momenta (their eigenvalues) are inverted, as in classical mechanics. To motivate the choice of $\hat{T}$, we rewrite the Schrödinger dynamics 15 in terms of the standard time-evolution operator $\hat{U}$:

$$\mid \psi(t)\rangle = \hat{U}(t, -t_0) \mid \psi_0\rangle, \tag{19}$$

$$\hat{U}(t, t') = Te^{-\frac{i}{\hbar}\int_{t'}^{t} {\rm d}\bar{t}\hat{\bar{H}}(\bar{t})}. \tag{20}$$

Backward evolution in time is, obviously, achieved by the complex conjugation of U. This brings us to the following choice of the time-reversal operator $\hat{T}$, which is originally due to Wigner[17]:

$\hat{T}$ is an anti-unitary operator, that is, $\hat{T} = \hat{K}\hat{W}$, where $\hat{W}$ is a unitary operator that assures the spin flip in Equation 18, and $\hat{K}$ performs complex conjugation. Here, we will not treat the spin explicitly and will, therefore, use $\hat{W} \to 1$. As a result, Equation 17 becomes:

$$\mid \psi'(t')\rangle = \hat{T} \mid \psi(t)\rangle = \mid \psi(-t)\rangle^*, \tag{21}$$

An operator $\hat{A}'$ acting on the time-reversed solution is obtained from the original operator $\hat{A}$ via

$$\hat{A}' = \hat{T}\hat{A}\hat{T}^{-1} \tag{22}$$

$\hat{T}$ is anti-linear, that is,

$$\hat{T}\{|\psi_1\rangle + {\rm i}|\psi_2\rangle\} = \hat{T} \mid \psi_1\rangle - {\rm i}\hat{T} \mid \psi_2\rangle, \tag{23}$$

$$\hat{T}\{\hat{A} + {\rm i}\hat{B}\}\hat{T}^{-1} = \hat{T}\hat{A}\hat{T}^{-1} - {\rm i}\hat{T}\hat{B}\hat{T}^{-1}, \tag{24}$$

for any two states and any two operators.

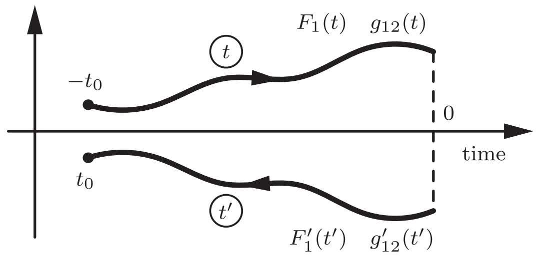

FIGURE 2 Illustration of the forward and backward solutions of the quantum BBGKY hierarchy. Upper trajectory: forward solution $\{F_1(t), g_{12}(t), \dots\}$ on the interval $-t_0 \le t \le 0$. Lower trajectory: backward solution $\{F_1'(t'), g_{12}'(t'), \dots\}$ on the same interval with $0 \le t' \le t_0$, Time reversal occurs at $t=0$, cf. Figure 1

As a test, we apply the operator $\hat{T}$ to both sides of Equation 15:

$$\begin{aligned} \hat{T} i\hbar\partial_t \mid \psi\rangle &= \hat{T}\hat{H} \mid \psi\rangle \\ \Longleftrightarrow \quad \underbrace{-i\hbar\partial_t}_{i\hbar\partial_{(-t)}} \hat{T} \mid \psi\rangle &= \hat{T}\hat{H}\hat{T}^{-1}\hat{T} \mid \psi\rangle \ , \end{aligned} \tag{25}$$

which means that, indeed, $\mid \psi'\rangle = \hat{T} \mid \psi\rangle$ solves the time-reversed Schrödinger equation

$$i\hbar\partial_{(-t)} \mid \psi'\rangle = \hat{H} \mid \psi'\rangle \tag{26}$$

if and only if

$$\hat{H} = \hat{T}\hat{H}\hat{T}^{-1}. \tag{27}$$

This is equivalent to $[\hat{T}, \hat{H}] = 0$, and we obtain a result found in many text books. However, we will see in section 4 that condition 27 is, in fact, not sufficient.

[Q7] Next, we find the time-reversed values of the coordinate and momentum operators using the coordinate representation:

$$\hat{r}' = \hat{T}\hat{r}\hat{T}^{-1} = \hat{r}\hat{T}\hat{T}^{-1} = \hat{r}, \tag{28}$$

as $\hat{r}$ is real, and

$$\hat{p}' = \hat{T}\hat{p}\hat{T}^{-1} = -\hat{p}, \tag{29}$$

as $\hat{p} = \frac{\hbar}{\mathrm{i}}\nabla$ is purely imaginary. This is again consistent with the time-reversal properties of classical mechanics. Furthermore, Equation 29 also shows that relation 27 excludes certain classes of Hamiltonians, such as those containing odd powers of the momentum (Figure 2). [Q8]

4 | TIME-REVERSAL INVARIANCE OF THE BBGKY HIERARCHY

The N-particle density operator $\hat{\rho}$, defined by Equation 5, extends the concept of the time-dependent Schrödinger equation to a thermodynamic ensemble while containing the dynamics of a pure state $|\psi^{(l)}\rangle$ as a special case, when $W_k = \delta_{k,l}$.

Let us now analyse the time-reversal symmetry of the von Neumann Equation 6 by applying the $\hat{T}$ operator, introduced above, from the left and its inverse from the right:

$$\begin{aligned} \hat{T} i\hbar\partial_t\hat{\rho}\hat{T}^{-1} &= \hat{T}(\hat{\rho}\hat{H} - \hat{H}\hat{\rho})\hat{T}^{-1} \\ -i\hbar\partial_t\hat{T}\hat{\rho}\hat{T}^{-1} &= \hat{T}\hat{\rho}\hat{T}^{-1}\hat{T}\hat{H}\hat{T}^{-1} - \hat{T}\hat{H}\hat{T}^{-1}\hat{T}\hat{\rho}\hat{T}^{-1} \ , \end{aligned}$$

which is equivalent to the time-reversed equation

$$i\hbar\partial_{-t}\hat{\rho}' = [\hat{\rho}', \hat{H}], \tag{30}$$

again, if and only if condition 27 is fulfilled, as in the case of the Schrödinger equation. Here, we introduced the solution of the time-reversed von Neumann equation:

$$\begin{aligned} \hat{\rho}'(-t) &= \hat{T}\hat{\rho}(t)\hat{T}^{-1} \\ &= \sum_k W_k \hat{T} \mid \psi^{(k)}(t)\rangle\langle\psi^{(k)}(t) \mid \hat{T}^{-1} \\ &= \sum_k W_k \mid \psi^{(k)'}(-t)\rangle\langle\psi^{(k)'}(-t) \mid, \end{aligned} \tag{31}$$

which is consistent with the definition of the density operator 5 in terms of the solutions of the time-reversed Schrödinger equation. Let us now return to the BBGKY hierarchy 8. Its time reversibility follows immediately from the reversibility of the von Neumann Equation 6 that was demonstrated above. Nevertheless, it is instructive to verify the time reversibility explicitly as this will be useful for the analysis of approximations to the hierarchy in section 5. Applying the operators $\hat{T}$ and $\hat{T}^{-1}$ from the left and right, respectively, we obtain:

$$i\hbar\frac{\partial}{\partial(-t)}\hat{F}'_{1\dots s} - [\hat{H}'_{1\dots s}(-t), \hat{F}'_{1\dots s}(-t)]$$
$$= \mathrm{Tr}_{s+1}\sum_{i=1}^{s}[\hat{V}'_{i,s+1}, \hat{F}'_{1\dots s+1}(-t)], \tag{32}$$

where we used the fact that the definition 7 is a real linear operation

$$\hat{T}\hat{F}_{1\dots s}(t)\hat{T}^{-1} = C_s^N \mathrm{Tr}_{s+1\dots N}\hat{T}\hat{\rho}(t)\hat{T}^{-1} =$$
$$= C_s^N \mathrm{Tr}_{s+1\dots N}\hat{\rho}'(-t) = \hat{F}'_{1\dots s}(-t), \tag{33}$$

such that $\hat{F}'_{1\dots s}(-t)$ is, indeed, the solution of the time-reversed hierarchy equation if the following conditions hold:

$$\hat{H}'_{1\dots s}(-t) \equiv \hat{T}\hat{H}_{1\dots s}(t)\hat{T}^{-1} = \hat{H}_{1\dots s}(t), \tag{34}$$

$$\hat{V}'_{ij} \equiv \hat{T}\hat{V}_{ij}\hat{T}^{-1} = \hat{V}_{ij}, \tag{35}$$

for all $i \neq j \in [1, N]$ and all $s = 1\dots N-1$, simultaneously. While for typical distance-dependent real potentials, Equation 35 is always fulfilled, Equation 34 places clear restrictions on the contributions to the system Hamiltonian.

Based on these results, we conclude that time-reversal invariance of the exact BBGKY hierarchy requires not only the time reversal symmetry of the full N-particle Hamiltonian 1, as in the case of the Schrödinger equation, cf. condition 27, but also that each of the contributions to the Hamiltonian have to obey this symmetry separately. This is, of course, a much stronger condition than 27.

5 | TIME-REVERSAL INVARIANCE OF APPROXIMATIONS TO THE HIERARCHY

As the solution of the BBGKY hierarchy is usually possible only with suitable approximations, the important question is which Q9 approximations retain the time-reversal properties of the exact system. We subsequently demonstrate that a very broad class of approximations retains time-reversal invariance. Therefore, we will restrict ourselves to real-valued Hamiltonians, $\hat{H}^* = \hat{H}$.

We start by rewriting the first two equations of the BBGKY hierarchy in terms of the correlation operators, Equations 11, 12, in a different form:

$$i\hbar\frac{\partial}{\partial t}\hat{F}_1 = \hat{J}_1 = \hat{J}_1^{\mathrm{app}} + \hat{O}_1, \tag{36}$$

$$i\hbar\frac{\partial}{\partial t}\hat{g}_{12} = \hat{J}_{12} = \hat{J}_{12}^{\mathrm{app}} + \hat{O}_{12}, \tag{37}$$

where $\hat{J}_1$ and $\hat{J}_{12}$ comprise all the remaining terms in Equations 11, 12. A decoupling approximation to the hierarchy can then be defined by specifying approximate expressions, $\hat{J}_1^{\mathrm{app}}$ and $\hat{J}_{12}^{\mathrm{app}}$, where the remainders, $\hat{O}_1$ and $\hat{O}_{12}$, are being omitted. The same procedure can be applied to decoupling approximations on the level of the third or higher-order hierarchy equations. To answer the question of whether a given decoupling approximation, $\hat{J}^{\mathrm{app}} = \{\hat{J}_1^{\mathrm{app}}, \hat{J}_{12}^{\mathrm{app}}, \dots\}$, is time reversible, we either have to analyse the resulting equations directly or, alternatively, investigate the time-reversal properties of the omitted operators, $\hat{O} = \{\hat{O}_1, \hat{O}_{12}, \dots\}$, as the exact equations are known to be time-reversal invariant. Here, it will be advantageous to use the latter approach.

In the following, we answer this question for the approximations that were introduced in section 2, starting by specifying the corresponding operators $\hat{O}$.

1. The *mean field approximation* is given by the choice $\hat{O} \equiv \hat{O}_1^{\mathrm{HF}} = \mathrm{Tr}_2[\hat{V}_{12}, \hat{g}_{12}]$.
2. The *second-order Born approximation* is given by $\hat{O} \equiv \hat{O}_{12}^{\mathrm{2B}} = [\hat{V}_{12}, \hat{g}_{12}] + Tr_3\{[\hat{V}_{13}, \hat{F}_1\hat{g}_{23}] + [\hat{V}_{23}, \hat{F}_2\hat{g}_{13}] + [\hat{V}_{13} + \hat{V}_{23}, \hat{g}_{123}]\}$.
3. The *T-matrix or ladder approximation* is given by $\hat{O} \equiv \hat{O}_{12}^{\mathrm{T}} = Tr_3\{[\hat{V}_{13}, \hat{F}_1\hat{g}_{23}] + [\hat{V}_{23}, \hat{F}_2\hat{g}_{13}] + [\hat{V}_{13} + \hat{V}_{23}, \hat{g}_{123}]\}$.
4. The *polarization approximation* is given by $\hat{O} \equiv \hat{O}_{12}^{\mathrm{POL}} = [\hat{V}_{12}, \hat{g}_{12}] + \mathrm{Tr}_3[\hat{V}_{13} + \hat{V}_{23}, \hat{g}_{123}]$.
5. The *screened ladder approximation* is given by $\hat{O} \equiv \hat{O}_{12}^{\mathrm{SCT}} = \mathrm{Tr}_3[\hat{V}_{13} + \hat{V}_{23}, \hat{g}_{123}]$.

Aside from their different physical characters, all these approximations have a common mathematical structure. They are Q10 given by a functional relation of the form

$$\hat{O}(t) = R[\hat{V}_{ij}, \hat{F}_k(t), \hat{g}_{lm}(t), \hat{g}_{nop}(t), \dots], \qquad R \in R, \tag{38}$$

/ ℝ ← replace by

where the indices are i, j, k, l, m, n, o, $p \in 1 \ldots N$, and R is a real function. The properties of expression 38 under time reversal are easily obtained. First, due to its real character, the functional form of R obviously does not change, that is, $\hat{T}R\hat{T}^{-1} = R$. Second, the properties of the arguments of R are known: as we have discussed above, standard pair potentials are always time-reversal invariant, $\hat{T}\hat{V}_{ij}\hat{T}^{-1} = \hat{V}_{ij}$. Next, the time-reversal invariance of the single-particle density operator was demonstrated in Equation 33. Finally, based on property 33, together with the cluster expansion (9, 10, …), which is a real functional relation, we easily conclude (iteratively) that all correlation operators are time-reversal invariant:

$$\hat{T}\hat{g}_{1\ldots s}(t)\hat{T}^{-1} = \hat{g}_{1\ldots s}(-t), \qquad s = 1 \ldots N-1. \tag{39}$$

Summarizing these results, we conclude that the operator 38 is time-reversal invariant:

$$\hat{T}\hat{O}(t)\hat{T}^{-1} = \hat{O}(-t). \tag{40}$$

This means that each of the approximations that were listed above (and the corresponding non-Markovian quantum kinetic equations)—time-dependent Hartree-Fock (non-linear quantum Vlasov equation), second-order Born approximation (quantum Landau equation), T-matrix (quantum Boltzmann equation), polarization approximation (quantum Lenárd-Balescu equation), and the screened ladder approximation—are time-reversal invariant. We emphasize that condition 38 is much more general than those approximations, including a broad range of decoupling schemes of the hierarchy that were proposed in the literature.

6 | BREAKING THE TIME-REVERSAL SYMMETRY: EXAMPLE OF THE BORN APPROXIMATION

The emergence of time irreversibility, starting from reversible quantum dynamics, has been discussed in great detail since the appearance of the Boltzmann kinetic Equation 18. Using our formalism, we can trace this emergence particularly clearly for the case of the quantum Landau equation that corresponds to the following first two hierarchy equations:

$$i\hbar\frac{\partial}{\partial t}\hat{F}_1 - [\hat{\bar{H}}_1, \hat{F}_1] = \mathrm{Tr}_2[\hat{V}_{12}, \hat{g}_{12}], \tag{41}$$

$$i\hbar\frac{\partial}{\partial t}\hat{g}_{12} - [\hat{\bar{H}}_{12}, \hat{g}_{12}] = [\hat{V}_{12}, \hat{F}_1\hat{F}_2]^{\pm} = \hat{J}^{2B}_{12}(t), \tag{42}$$

$$\hat{F}_1(-t_0) = \hat{F}^0_1, \qquad \hat{g}_{12}(-t_0) = \hat{g}^0_{12}, \qquad t \in [-t_0, 0], \tag{43}$$

where we added the initial conditions for both operators. These coupled, time-local equations can be numerically solved directly. The alternative route that leads to a quantum kinetic equation consists of, first, formally solving the equation for $\hat{g}_{12}$ analytically and then inserting the result into the r.h.s. of Equation 41. This is the approach we will use here. The solution of the initial value problem 41–43 is easily found[3] and consists of an initial value term (solution of the homogeneous equation) and a collision term

$$\hat{g}_{12}(t) = \hat{g}^{\mathrm{IC}}_{12}(t) + \hat{g}^{\mathrm{coll}}_{12}(t), \tag{44}$$

$$\hat{g}^{\mathrm{IC}}_{12}(t) = \hat{U}^0_{12}(t, -t_0)\hat{g}^0_{12}\hat{U}^{0\dagger}_{12}(t, -t_0), \tag{45}$$

$$\hat{g}^{\mathrm{coll}}_{12}(t) = \frac{1}{i\hbar}\int_{-t_0}^{t} \mathrm{d}\bar{t}\,\hat{U}^0_{12}(t, \bar{t})\hat{J}^0_{12}(\bar{t})\hat{U}^{0\dagger}_{12}(t, \bar{t}), \tag{46}$$

where the two-particle propagator factorizes into single-particle Hartree-Fock propagators, $\hat{U}^0_{12}(t, t') = \hat{U}_1(t, t')\hat{U}_2(t, t')$, with

$$\left\{ i\hbar\frac{\partial}{\partial t} - \hat{\bar{H}}_1(t) \right\} \hat{U}_1(t, t') = 0, \qquad \hat{U}_1(t, t) = 1, \tag{47}$$

the solution for which is analogous to that of the Schrödinger equation, cf. Equation 20. The quantum kinetic equation that is associated with the solution 44 contains two collision integrals: the first, involving $\hat{g}^{\mathrm{IC}}_{12}(t)$, is due to correlations existing in the system at the initial time moment, whereas the second is due to correlations being formed as a result of two-particle collisions while being absent at the initial moment. The characteristic feature of the latter collision integral is its non-Markovian character (i.e., the presence of the time integral), which is in striking contrast to the traditional Boltzmann equation that involves only distribution functions taken at the current time t.

To analyse the transition from the former to the latter and, thereby, from time reversibility to irreversibility, we switch from the operator form of the solution 44 to an instantaneous Hartree-Fock basis $\{|n\rangle\}$, given by $\hat{\bar{H}}_1 \mid n\rangle = E_n \mid n\rangle$. Then, the first hierarchy Equation 41 becomes

$$i\hbar\frac{\partial}{\partial t}F_{n_1,n_{1'}} - (E_{n_1} - E_{n'_1})F_{n_1,n_{1'}} =$$

$$= \sum_{n_2}\sum_{\bar{n}_1\bar{n}_2}\{V_{n,\bar{n}}g_{\bar{n},n'} - g_{n,\bar{n}}V_{\bar{n},n'}\}\Big|_{n_{2'}=n_2}, \tag{48}$$

where we introduced the short notations $n\equiv(n_1, n_2)$, $n' \equiv(n_1{}', n_2{}')$, and $\bar{n} \equiv (\bar{n}_1, \bar{n}_2)$. This is a generalized quantum kinetic equation that describes the probability of transitions between different single-particle states (dynamics of $F_{n_1,n_{1'}}$ with $n_1 \neq n_{1'}$), as well as the dynamics of the occupations of state n_1 (given by $F_{n_1} \equiv F_{n_1,n_1}$). Here, we focus on the latter as it is directly related to the evolution towards an equilibrium state. Furthermore, the emergence of irreversibility in the dynamics of F_n is sufficient for the transition of the whole system of coupled equations from reversible to irreversible.

The corresponding dynamics of the diagonal matrix elements are given by

$$i\hbar\frac{\partial}{\partial t}F_{n_1}(t) = 2\mathrm{i}\sum_{n_2}\sum_{\bar{n}_1\bar{n}_2}V_{n,\bar{n}}Im\ \ g_{\bar{n},n}(t), \tag{49}$$

where we used $g_{n,n'} = g^*_{n',n}$ and $V_{n,n'} = V_{n',n}$. To compute $Im\, g_{\bar{n},n}(t)$, we first write down the solution of Equation 47, which is given by a diagonal matrix:

$$\langle n_1|\hat{U}(tt')|n'_1\rangle = U_{n_1}(t-t')\delta_{n_1,n_{1'}},$$
$$U_{n_1}(\tau) = e^{-\frac{\mathrm{i}}{\hbar}E_{n_1}\tau}, \tag{50}$$

and the matrix of the pair correlation operator 44 becomes

$$Im\ \ g_{n,n'}(t) = Im\ \ g^{\mathrm{IC}}_{n,n'}(t) + Im\ \ g^{\mathrm{coll}}_{n,n'}(t), \tag{51}$$

$$Im\ \ g^{\mathrm{IC}}_{n,n'}(t) = Im\{e^{-\mathrm{i}\omega_{n,n'}[t-(-t_0)]}g^0_{n,n'}\} \tag{52}$$

$$Im\ \ g^{\mathrm{coll}}_{n,n'}(t) = -\frac{1}{\hbar}\int_{-t_0}^{t}\mathrm{d}\bar{t}\cos[\omega_{n,n'}(t-\bar{t})]J^{2\mathrm{B}}_{n,n'}(\bar{t}) \tag{53}$$

where we defined $\hbar\omega_{n,n'} \equiv E_{n1} + E_{n2} - E_{n1'} - E_{n2'}$ and used $J^{2B*}_{n,n\prime} = J^{2B}_{n,n\prime}$.

Let us now investigate the time-reversal symmetry of the kinetic Equation 48, that is, we apply the time-reversal operators $\hat{T}$ and $\hat{T}^{-1}$ from the left and right, respectively, as before:

$$i\hbar\frac{\partial}{\partial(-t)}F'_{n_1,n_{1'}}(t) - (E_{n_1} - E_{n'_1})F'_{n_1,n_{1'}}(t) =$$

$$= \sum_{n_2}\sum_{\bar{n}_1\bar{n}_2}\{V_{n,\bar{n}}g'_{\bar{n},n'}(t) - g'_{n,\bar{n}}(t)V_{\bar{n},n'}\}\Big|_{n_{2'}=n_2},$$

where F' is the solution of the time-reversed equation. Time-reversal symmetry again requires fulfilment of $F'_{n_1,n_{1'}}(t) \equiv \hat{T}F_{n_1,n_{1'}}(t)\hat{T}^{-1} = F_{n_1,n_{1'}}(-t)$ and is observed only when the time-reversed solution of the second equation obeys

$$Im\ \ g'_{n,n'}(t) \equiv \hat{T}Im\ \ g_{n_1,n_{1'}}(t)\hat{T}^{-1} = Im\ \ g_{n,n'}(-t). \tag{54}$$

Q13 This is easily verified by writing down the solution $g'(t)$ noticing that application of the operators $\hat{T}$ and $\hat{T}^{-1}$, from the left and right, to the second hierarchy equation again changes the sign of the time derivative, which is equivalent to replacing $\omega_{n,n'} \to -\omega_{n,n'}$, and $J^{2\mathrm{B}}_{n,n\prime} \to J^{2\mathrm{B}}_{n,n\prime}$, and the solution 52, 53 changes into

$$Im g^{\mathrm{IC}'}_{n,n'}(t) = Im\{e^{+\mathrm{i}\omega_{n,n'}[t-(-t_0)]}g^0_{n,n'}\} \tag{55}$$

$$Im\ \ g^{\mathrm{coll}'}_{n,n'}(t) = -\frac{1}{\hbar}\int_{-t_0}^{t}\mathrm{d}\bar{t}\cos[-\omega_{n,n'}(t-\bar{t})][-J^{2\mathrm{B}}_{n,n'}(\bar{t})]$$
$$= -\frac{1}{\hbar}\int_{-t}^{t_0}\mathrm{d}\bar{t}\cos[\omega_{n,n'}(-t-\bar{t})]J^{2\mathrm{B}}_{n,n'}(-\bar{t}). \tag{56}$$

It is obvious that the solutions g and g' fulfil 54, which can be seen by changing $(t, -t_0) \to (-t, t_0)$, in $g^{\mathrm{IC}'}$, and $(t, -t_0, \bar{t}) \to (-t, t_0, -\bar{t})$, in $g^{\mathrm{coll}'}$.

The mathematical transition to the conventional (quantum) Boltzmann collision integral that contains a delta function, $\delta(E_{n_1} + E_{n_2} - E_{n'_1} - E_{n'_2})$, of the single-particle energies before and after the collision involves three steps:

Decoupling of the time scales of the single-particle and two-particle dynamics. The argument here is that, during a collision, when the two-particle correlations are formed (during the correlation time $\tau_{\rm cor}$), the occupation of the single-particle states changes only weakly. Its relaxation towards an equilibrium distribution involves many collisions and, therefore, requires a relaxation time that is much larger

$$t_{\rm rel} \gg \tau_{\rm cor}. \tag{57}$$

Q14 This justifies the expansion $F_n(\bar{t})$, and with it $J^{2B}_{n,n'}(\bar{t})$, under the time integral in 53 around its value at the upper limit (the current time),

$$J^{2B}_{n,n'}(\bar{t}) = J^{2B}_{n,n'}(t) + \sum_{k=1} \frac{(\bar{t}-t)^k}{k!} \frac{{\rm d}^k}{{\rm d}t^k} J^{2B}_{n,n'}(t). \tag{58}$$

Truncating this retardation expansion 3 at the first term (0-th-order retardation approximation) leads to the following result for the pair correlations:

$$\begin{aligned} Img^{\rm coll(0)}_{n,n'}(t) &= -\frac{J^{2B}_{n,n'}(t)}{\hbar} \frac{\sin[\omega_{n,n'}(t-(-t_0))]}{\omega_{n,n'}} \\ &= Img^{\rm coll(0)}_{n,n'}(t,[F(t)]). \end{aligned} \tag{59}$$

This expression is, of course, a drastic distortion of the original result, and its accuracy depends on the fulfilment of condition 57. In fact, it is well known that, for weakly coupled systems, the two times are related by $\frac{\tau_{\rm cor}}{t_{\rm rel}} \sim \Gamma \ll 1$, where Γ is

Q15 the relevant coupling parameter. In the second line of 59, we noted explicitly that the pair correlation functions have a twofold time dependence: an explicit one (via the sine function, which is fast, for increasing time, particularly for high frequencies) and a slow one via the evolution of $F(t)$.

Note that this is still a proper (although distorted) solution of the initial value problem. It is also consistent with an (arbitrary) initial condition $g^0_{n,n'}(-t_0)$ because the collision term exactly vanishes for $t \to -t_0$. Interestingly, despite the approximate character of $g^{\rm coll(0)}_{n,n'}(t)$, it is easily seen (by performing the retardation expansion in 56) that it still satisfies the time-reversal invariance condition 54.

Markov limit. The limit of an infinitely remote initial state, $-t_0 \to -\infty$, is usually motivated by the assumption that two particles enter a scattering process in an uncorrelated manner. The result for the Markovian pair correlations is then:

$$\begin{aligned} Img^{\rm coll(M)}_{n,n'}(t) &\equiv \\ -\frac{J^{2B}_{n,n'}(t)}{\hbar} &\lim_{-t_0\to-\infty} \frac{\sin[\omega_{n,n'}(t-(-t_0))]}{\omega_{n,n'}} \\ &= -\frac{J^{2B}_{n,n'}(t)}{\hbar}\, \delta(\omega_{n,n'}). \end{aligned} \tag{60}$$

Q16 Note that it is assumed that the single-particle operators (i.e., the slow time dependence of $g^{\rm coll\,[0]}$) are not affected by the limit, which means that the limit $\Gamma \to 0$ has been considered first.

Weakening of initial correlations. Motivated by the argument that the state of the system cannot remember (and, hence, be influenced by) its infinitely remote history, particularly its correlations, the Markov limit is accompanied by the suppression of initial correlations:

$$\lim_{-t_0\to-\infty} g^0_{n,n'}(-t_0) \to 0. \tag{61}$$

This is consistent with the Markov limit because, after the procedure leading to 61, $g_{n,n'}\,[F(t)]$ does not obey an initial value problem that starts from an arbitrary initial state anymore but only adiabatically follows the dynamics of $F(t)$, according to the prescription 60. This concept is due to Bogolyubov[4] ("functional hypothesis"; "weakening of initial correlations") and has been generalized to situations where there exists a subclass of long-living correlations (such as those related to bound states or long range order; *partial weakening of initial correlations*) by Kremp et al.[18]

With the result 61, the collision integral due to initial correlations (the term $g^{\rm IC}$) vanishes, and only the collision integral involving Im $g^{\rm coll(M)}_{n,n'}$, Equation 60, remains, which is of the conventional Boltzmann-type form.

To summarize, time-reversal symmetry is lost at step 2. While the result of step 1, Im $g^{\rm coll(0)}_{n,n'}(t)$, is time-reversal invariant *for any finite value* $-t_0$, no matter how far back in the past, this property vanishes with the limit $-t_0 \to -\infty$. With this limit, the unitary operator structure that is still present in the sine function is lost together with the explicit time dependence of the pair correlations (this is particularly clear when the single-particle operators F are exactly stationary.)

7 | SUMMARY AND DISCUSSION

In this paper, we analysed the question of the time reversibility of generalized quantum kinetic equations that are derived within the reduced density operator formalism. The governing equations of the density operator theory are given by the quantum BBGKY hierarchy. Here, we demonstrated that the exact BBGKY hierarchy and the associated quantum kinetic equations are time reversible. This behaviour is in striking contrast to the conventional Boltzmann-type kinetic equations that are known to be irreversible and describe the relaxation of a many-body system to an equilibrium state, which is accompanied by an increase of its entropy (H-theorem). This is traditionally achieved by means of ad hoc assumptions, such as about "molecular chaos",[19] via Boltzmann's "Stoßzahlansatz"[20] or by similar procedures.

Although the derivation of generalized non-Markovian quantum kinetic equations goes back almost seven decades, in many communities, the existence of a systematic kinetic theory beyond the Boltzmann equation is poorly known, which warrants a detailed reconsideration of some mathematical aspects on the way from a reversible to an irreversible kinetic theory. Here, we have presented a simple procedure that allows one to directly verify the time-reversal property of the exact BBGKY hierachy and of important closure relations, as well as the transition to the conventional Boltzmann equation. Our approach is based on the use of Wigner's anti-unitary time-reversal operator $\widehat{T}$[17] that translates the solution of the Schrödinger equation into the time-reversed equation and is a mathematically well-controlled procedure that replaces the traditional heuristic arguments mentioned above.

Let us summarize our main results:

Q17

1. Our proof of time-reversal invariance of the exact quantum BBGKY hierarchy revealed a much stronger condition, Equations 34 and 35, than the commonly used condition for time reversibility of the N-particle Schrödinger equation, that is, Equation 27. We have shown that not only does the total Hamiltonian have to obey $\widehat{T}\widehat{H}\widehat{T}^{-1} = \widehat{H}$, but each of its single-particle, two-particle, and higher contributions, separately. This might seem surprising as Equation 27 is known to be necessary and sufficient for the Schrödinger and von Neumann equations. However, the N-particle dynamics have to always be consistent with the quantum dynamics of sub-complexes (of $N-1\ldots1$ particles), which follow directly from the partial integration of the N-particle equations. It is clearly impossible that the N-particles dynamics are reversible, whereas the N-s-particle dynamics are not.
2. We presented a very general condition for time-reversal invariance of approximate solutions to the BBGKY hierarchy, Equation 38, and demonstrated that it applies to many of the commonly used many-body approximations. Moreover, this condition goes far beyond those approximations, including a broad range of additional decoupling schemes of the hierarchy. This is not limited to approximations that are motivated by physical considerations and violate conservation laws. For example, the choice of the omitted term $\widehat{O} = \widehat{O}_{12} \neq \widehat{O}_{21}$ would violate the conservation of total energy, cf. Ref. 3, while still being time-reversal invariant.
3. Our results allow us to analyse the interesting question posed in Ref. 13 of how total energy conservation and time reversibility are related. While in most cases of practical relevance, both phenomena are fulfilled (or violated) simultaneously, their areas of validity are not equivalent. As shown above, there exist time-reversible models that violate energy conservation. On the other hand, there exist model Hamiltonians (e.g., those that contain odd powers of the momentum) that conserve energy but violate condition 27 and, therefore, time-reversal symmetry.
4. Our analysis of the transition to the conventional Boltzmann equation involved three successive approximations. The first one—the decoupling of the relaxation time scales of single-particle $t_{\rm rel}$ and two-particle dynamics ($\tau_{\rm cor}$) by means of a retardation expansion—allowed us to perform the memory integral and obtain a time-local result for the pair correlations, Equation 59. This result ("completed collision approximation" or "energy broadening approximation") not only conserves total energy,[3] but, here, we also demonstrated that it preserves time-reversal symmetry. The same analysis also applies to higher-order approximations in the retardation expansion 58.
5. We have demonstrated that time reversibility is lost only at the second step—the Markov limit, that is, with the shift of the initial time to the infinitely remote past, $-t_0 \to -\infty$. This destroys the unitary character of the dynamics of the pair correlations and introduces a preferred "arrow" of time because there is no possibility of the system ever returning to this state.
6. Our analysis also shows that the commonly used argument, that irreversibility is introduced into the theory via the assumption of "molecular chaos"[19] or the "Stoßzahlansatz",[20] has to be stated with some care. The requirement that the two-particle probabilities factorize and particles enter the collision uncorrelatedly—that is, in our notation, $F_{12} = F_1F_2$ or $g_{12} \equiv 0$—is not sufficient. First, transition to irreversibility is also possible in a strongly correlated system where this factorization is not possible, for example, Ref. 3. Second, the example of the Born approximation that we discussed in section 5 applied to a weakly coupled system. Choosing, as the initial condition, an uncorrelated system, that is, $g(-t_0) = g^0 = 0$, we would formally satisfy those assumptions. Nevertheless, the resulting dynamics would still be given by Equation 44 without the

initial correlation term, but it would be perfectly time reversible. The crucial point for the emergence of irreversibility is again that the factorization is introduced not at a finite initial time but in the infinitely remote past.

With the generalized quantum kinetic equations that were discussed above at our disposal, one may ask whether it is necessary at all to force the transition to conventional irreversible Boltzmann-type kinetic equations given the rather crude approximations involved. The argument for the latter has always been that macroscopic many-particle dynamics, such as transport (diffusion, heat conduction, viscosity, fluid dynamics etc.), is dissipative, and the dynamics are expected to approach thermodynamic equilibrium—the state of maximum entropy. The answer is clearly "No". Experience in solving the generalized quantum kinetic equations (e.g., Ref. 3), which are derived either from the BBGKY hierarchy or from non-equilibrium Green functions, for a sufficiently long time clearly reveals that these solutions exhibit an irreversible trend towards an asymptotic state that is consistent with thermodynamic equilibrium. However, this state is different from a Maxwellian, Fermi, or Bose momentum distribution as a result of correlations. Certainly, the present reversible dynamics will return to the initial state; however the associated Poincaré recurrence time increases exponentially with particle number. This behaviour is in complete agreement with simulation results for classical systems: solutions of the reversible equations of classical mechanics of a many-particle system by means of microcanonical molecular dynamics show perfect relaxation trends to (correlated) thermodynamic equilibrium.

Therefore, the choice between the irreversible Boltzmann-type kinetic equations and reversible generalized kinetic equations is mainly governed by the substantially increased computational effort involved in the solution of the latter. Here, in fact, proof of time reversibility of the relevant approximations that was given in this paper is of high practical value as it provides a sensitive test for the numerical accuracy and convergence, for example, Ref. 21. Time reversibility is also of importance for "echo"-type experiments (e.g., Loschmidt echo,[22] spin echo, Rabi flop etc.) where time reversal is being forced by an external pulse. The analysis of the forward and backward dynamics gives important insights into the internal properties (e.g., dissipation channels) of a many-body system, and the present generalized quantum kinetic equations are well suited for such investigation. For a recent theoretical analysis, see Ref. 23.

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