

On the Derivation of Quantum Kinetic Equations.

I. Collision Expansions

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Received May 31, 1977

A straightforward scheme for deriving quantum kinetic equations is presented. It is based on Bogoliubov's initial condition of vanishing correlations in the infinite past and consists in the elimination of an initial one-particle Wigner function between two nonlinear functionals. By performing the elimination to second order in the density the quantum analog of the Choh-Uhlenbeck three-particle collision term is obtained. The scheme may be extended to include relativistic particles as well as particles with internal degrees of freedom.

KEY WORDS: Nonequilibrium statistical mechanics; quantum kinetic equation; initial condition of Bogoliubov; in-operators; three-particle collision term.

1. INTRODUCTION

Since 1945 the derivation of kinetic equations has become one of the principal objects of statistical mechanics. This development was set into motion mainly by Bogoliubov,⁽¹⁾ who was the first to turn the basic idea that kinetic equations are special solutions of the BBGKY hierarchy into a systematic theory. In later years the theory has been worked out further by Uhlenbeck, Choh, Green, and Cohen, among others (see, e.g., Ref. 2). Simultaneously, numerous other approaches to the problem have been developed. We mention the approach of the Brussels school,⁽³⁾ which, in the classical case, seems to lead to the same results as the Bogoliubov theory.^(4,5)

All methods for finding special solutions of the hierarchy have in common

This investigation is part of the research program of the Stichting voor fundamenteel onderzoek der materie (FOM), which is financially supported by the Organisatie voor zuiver-wetenschappelijk onderzoek (ZWO).

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that at one point or another an assumption of a statistical nature has to be introduced. Such an assumption, which may be understood as a restriction on the class of dynamical systems that are being considered, appears quite explicitly both in the Bogoliubov theory (Ref. 1, Chapter 9a) and in the work of the Brussels school (Ref. 3, Chapter 16.4; Ref. 6). It may be stated as the condition that the correlations present in the initial state should have no marked influence on the behavior of the system in the limit of times long compared to the duration of a collision. It is obvious that such a condition is necessary in order that the time evolution of the system may be predicted through a knowledge of the present state alone. The problem of kinetic theory is now to prove that it is also sufficient.

In the present paper we investigate to what extent the condition that initial correlations may be ignored suffices to derive a quantum kinetic equation. The discussion is much facilitated by the concept of the so-called in-picture.⁽⁷⁾ This picture has been introduced in field theory as a means for characterizing an interacting system by its asymptotic properties. As we shall see, the in-formalism is well suited for the purpose of imposing the initial condition on the system.

Subsequently, we present a straightforward scheme for obtaining a quantum kinetic equation. It consists in writing both the Wigner function and the interaction term of the dynamical equation that it satisfies in terms of initial distribution functions. If the aforementioned condition is imposed, these expressions become nonlinear functionals of a one-particle initial distribution function. By elimination of this distribution function a kinetic equation may be obtained.

The applicability of our approach thus rests, like the classical theory of Green⁽⁸⁾ and Cohen,⁽⁹⁾ on the mathematical question of whether a satisfactory elimination scheme can be found. Obvious possibilities are a scheme based on density expansions, or on expansions in terms of the interaction strength, or on a combination of both. We shall use the first possibility to derive the quantum analog⁽¹⁰⁾ of the Choh–Uhlenbeck collision term.⁽¹¹⁾ In a subsequent paper⁽¹²⁾ we consider the derivation of the nonlocal Uehling–Uhlenbeck equation employing an expansion in terms of the interaction strength.

We mention that application of the theory is not restricted to the non-relativistic regime. Since the second quantization formalism is used throughout, it can also be generalized to the relativistic case. For dilute systems it then leads to the relativistic Boltzmann equation.⁽¹³⁾ The extension of the theory to particles with spin has also been considered.⁽¹⁴⁾ To lowest order in the density the ensuing kinetic equation is the Waldmann–Snider equation for spin particles.⁽¹⁵⁾ An implication is that the initial condition adopted by Snider⁽¹⁶⁾ is a particular instance of the initial condition as it will be formulated further on.

2. DYNAMICAL EQUATION

We consider a system described by a Hamiltonian of the form

$$H = H_0(t) + H_I(t) \quad (1)$$

where the free Hamiltonian is given by

$$H_0(t) = \int d^3p (\mathbf{p}^2/2m)a^\dagger(\mathbf{p}, t)a(\mathbf{p}, t) \quad (2)$$

and the interaction Hamiltonian by

$$\begin{aligned} H_I(t) = & \frac{1}{2}\lambda \int d^3p_1 d^3p_2 d^3p_1' d^3p_2' \\ & \times \delta^{(3)}(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2')v(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2') \\ & \times a^\dagger(\mathbf{p}_1, t)a^\dagger(\mathbf{p}_2, t)a(\mathbf{p}_2', t)a(\mathbf{p}_1', t) \end{aligned} \quad (3)$$

The function v characterizing the interaction between the particles has to satisfy the requirement

$$v(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_1', \mathbf{p}_2') = v^*(\mathbf{p}_1', \mathbf{p}_2'; \mathbf{p}_1, \mathbf{p}_2) \quad (4)$$

in order that the operator H_I is Hermitian. The construction operators satisfy the Heisenberg equation of motion

$$i\hbar \partial_t a(\mathbf{p}, t) = [a(\mathbf{p}, t), H] \quad (5)$$

and the equal-time (anti-) commutation relation

$$a(\mathbf{p}, t)a^\dagger(\mathbf{p}', t) - \eta a^\dagger(\mathbf{p}', t)a(\mathbf{p}, t) = \delta^{(3)}(\mathbf{p} - \mathbf{p}') \quad (6)$$

where η is equal to one for bosons and equal to minus one for fermions.

To describe the statistical properties of the system, one may introduce the one-particle Wigner function, which in the second quantization formalism is defined as⁽¹⁷⁾

$$f(\mathbf{x}, \mathbf{p}, t) = (2\pi\hbar)^{-3} \int d^3u [\exp(i\mathbf{u} \cdot \mathbf{x}/\hbar)] \langle a^\dagger(\mathbf{p} - \frac{1}{2}\mathbf{u}, t)a(\mathbf{p} + \frac{1}{2}\mathbf{u}, t) \rangle \quad (7)$$

The angular brackets designate the statistical average. For this Wigner function which is the quantum analog of the classical one-particle distribution function, we seek to establish a kinetic equation.

For the following we shall find it convenient to represent the Wigner function in a different but equivalent form. To this end we introduce the total momentum operator

$$\mathbf{P} = \int d^3p \mathbf{p} a^\dagger(\mathbf{p}, t)a(\mathbf{p}, t) \quad (8)$$

Its commutation rule with $a(\mathbf{p}, t)$ is

$$[a(\mathbf{p}, t), \mathbf{P}] = \mathbf{p}a(\mathbf{p}, t) \quad (9)$$

We use this fact together with the formal solution of the Heisenberg equation (5) to write the Wigner function (7) as

$$f(\mathbf{x}, \mathbf{p}, t) = \langle \exp[i(Ht - \mathbf{P} \cdot \mathbf{x})/\hbar] \psi(\mathbf{p}) \exp[-i(Ht - \mathbf{P} \cdot \mathbf{x})/\hbar] \rangle \quad (10)$$

where $\psi(\mathbf{p})$ is the operator

$$\psi(\mathbf{p}) = (2\pi\hbar)^{-3} \int d^3u a^\dagger(\mathbf{p} - \frac{1}{2}\mathbf{u})a(\mathbf{p} + \frac{1}{2}\mathbf{u}) \quad (11)$$

Here and henceforth we shall use the convention that a deleted time argument means $t = 0$.

We now derive the exact equation satisfied by the Wigner function (10) by taking its time derivative. With the explicit form (2) of the free Hamiltonian and the (anti-) commutation rule (6) one easily obtains

$$\begin{aligned} & \left(\partial_t + \frac{\mathbf{p}}{m} \cdot \nabla \right) f(\mathbf{x}, \mathbf{p}, t) \\ &= \langle \exp[i(Ht - \mathbf{P} \cdot \mathbf{x})/\hbar] \Phi(\mathbf{p}) \exp[-i(Ht - \mathbf{P} \cdot \mathbf{x})/\hbar] \rangle \end{aligned} \quad (12)$$

with the operator $\Phi(\mathbf{p})$ given by

$$\Phi(\mathbf{p}) = (i\hbar)^{-1} [\psi(\mathbf{p}), H_I] \quad (13)$$

The dynamical equation (12) together with the expression (10) for the Wigner function will serve as the starting point for our considerations.

We mention that the right-hand side of (12) may be worked out by employing the explicit form of H_I as given in (3). One then finds the first member of the quantum mechanical hierarchy, which links the time evolution of the one-particle Wigner function to that of the two-particle Wigner function.⁽¹⁷⁾ However, this fact will play no role in the theory to be developed here.

3. IN-PICTURE

In scattering theory⁽⁷⁾ one defines an evolution operator $U(t, t_0)$ which satisfies the integral equation

$$U(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}_I(t') [\exp(-\epsilon|t'|)] U(t', t_0) \quad (14)$$

By $\hat{H}_I(t)$ we denote the interaction Hamiltonian in the interaction picture:

$$\hat{H}_I(t) = e^{iH_0 t/\hbar} H_I e^{-iH_0 t/\hbar} \quad (15)$$

For the following, the Møller wave operator

$$U(0, -\infty) = \lim_{t_0 \rightarrow -\infty} U(0, t_0) \quad (16)$$

will be of particular importance. In the absence of bound states this operator is unitary

$$U^\dagger(0, -\infty) = U^{-1}(0, -\infty) \quad (17)$$

Furthermore, it satisfies the intertwining relation

$$HU(0, -\infty) = U(0, -\infty)H_0 \quad (18)$$

With the help of the Møller wave operator one may construct the so-called in-operators⁽⁷⁾

$$a_{\text{in}}(\mathbf{p}) = U(0, -\infty)a(\mathbf{p})U^\dagger(0, -\infty) \quad (19)$$

and

$$a_{\text{in}}^\dagger(\mathbf{p}) = U(0, -\infty)a^\dagger(\mathbf{p})U^\dagger(0, -\infty) \quad (20)$$

Since we exclude bound states, the Møller operator is unitary, whence the in-operators satisfy the canonical (anti-) commutation relation

$$a_{\text{in}}(\mathbf{p})a_{\text{in}}^\dagger(\mathbf{p}') - \eta a_{\text{in}}^\dagger(\mathbf{p}')a_{\text{in}}(\mathbf{p}) = \delta^{(3)}(\mathbf{p} - \mathbf{p}') \quad (21)$$

The in-picture is convenient because it gives a description of the system in terms of the initial situation in which the particles are far apart and therefore moving freely. This last feature is demonstrated by the time development law of the in-operators, which, as a consequence of the intertwining relation (18), is the same as for free particles

$$e^{iHt/\hbar}a_{\text{in}}(\mathbf{p})e^{-iHt/\hbar} = a_{\text{in}}(\mathbf{p})e^{-ip^0t/\hbar} \quad (22)$$

Here the notation p^0 is used for the energy $\mathbf{p}^2/2m$. Because of the translational invariance of the system, the Møller operator commutes with the total momentum operator (8) and we have

$$\exp(-i\mathbf{P} \cdot \mathbf{x}/\hbar) a_{\text{in}}(\mathbf{p}) \exp(i\mathbf{P} \cdot \mathbf{x}/\hbar) = a_{\text{in}}(\mathbf{p}) \exp(i\mathbf{p} \cdot \mathbf{x}/\hbar) \quad (23)$$

for the behavior of a_{in} under space translations.

The unitarity of the Møller operator implies that any operator may be written in terms of in-construction operators. In the following we shall consider in particular the operators $\psi(\mathbf{p})$ and $\Phi(\mathbf{p})$ defined in (11) and (13), respectively. We write their expansion in terms of in-operators as

$$\Phi(\mathbf{p}) = \sum_{n=2}^{\infty} \frac{1}{n!} \int d^3p^n d^3p'^n \Phi_{\text{in}}^{(n)}(\mathbf{p}^n; \mathbf{p}'^n | \mathbf{p}) a_{\text{in}}^\dagger(\mathbf{p}^n) a_{\text{in}}(\mathbf{p}'^n) \quad (24)$$

and

$$\psi(\mathbf{p}) - \psi_{\text{in}}(\mathbf{p}) = \sum_{n=2}^{\infty} \frac{1}{n!} \int d^3p^n d^3p'^n \psi_{\text{in}}^{(n)}(\mathbf{p}^n; \mathbf{p}'^n | \mathbf{p}) a_{\text{in}}^{\dagger}(\mathbf{p}^n) a_{\text{in}}(\mathbf{p}'^n) \quad (25)$$

where we have used the short-hand notations $\mathbf{p}^n = (\mathbf{p}_1, \dots, \mathbf{p}_n)$, $d^3p^n = d^3p_1 \dots d^3p_n$, and

$$a_{\text{in}}^{\dagger}(\mathbf{p}^n) = a_{\text{in}}^{\dagger}(\mathbf{p}_1) \dots a_{\text{in}}^{\dagger}(\mathbf{p}_n) \quad (26)$$

$$a_{\text{in}}(\mathbf{p}^n) = a_{\text{in}}(\mathbf{p}_1) \dots a_{\text{in}}(\mathbf{p}_n) \quad (27)$$

Note the order of the operators in the last line. The expansion coefficients $\Phi_{\text{in}}^{(n)}$ and $\psi_{\text{in}}^{(n)}$ are by definition (anti-) symmetric functions of their primed variables \mathbf{p}'^n as well as their unprimed variables \mathbf{p}^n . They may be determined with the help of perturbation theory, as we shall see in a subsequent paper.⁽¹²⁾ For the moment we confine ourselves to stating that they are related to the scattering amplitudes describing two-particle, three-particle, etc., collision processes.

4. INITIAL CONDITION

To obtain a kinetic equation from the dynamical equation (12) one needs some kind of assumption that makes it possible to express the correlations created by the interactions in terms of the one-particle Wigner function. Now experience suggests that in many systems of interest correlations decay within a few collision times. Following Bogoliubov,⁽¹⁾ we suppose that in such systems the initial correlations have no effect on the behavior of the system for times long as compared to a characteristic collision time. In other words, we assume that in this limit the initial correlations may be ignored. In our formalism the absence of initial correlations is expressed as

$$\langle a_{\text{in}}^{\dagger}(\mathbf{p}^n) a_{\text{in}}(\mathbf{p}'^n) \rangle = \sum_{\mathcal{P}} \eta^{\mathcal{P}} \langle a_{\text{in}}^{\dagger}(\mathbf{p}_1) a_{\text{in}}(\mathbf{p}_1') \rangle \dots \langle a_{\text{in}}^{\dagger}(\mathbf{p}_n) a_{\text{in}}(\mathbf{p}_n') \rangle \quad (28)$$

where the sum runs over all permutations of the labels of the primed or unprimed momenta. The exponent \mathcal{P} is even or odd depending on whether the permutation is even or odd. Formally, the factorization rule (28) may be obtained by treating the initial state as an ideal gas in equilibrium and employing the thermodynamic Wick theorem.⁽¹⁸⁾

We now proceed by applying condition (28) to the dynamical equation (12). We first substitute the expansion (24) into its right-hand side. We note that, because of (23) and the time development law (22), the exponential

operators give rise to a phase factor which can be brought outside the average. With the factorization rule (28) we then obtain

$$\begin{aligned}
 & [\partial_t + (\mathbf{p}/m) \cdot \nabla] f(\mathbf{x}, \mathbf{p}, t) \\
 &= \sum_{n=2}^{\infty} \int d^3 p^n d^3 p'^n \Phi_{\text{in}}^{(n)}(\mathbf{p}^n; \mathbf{p}'^n | \mathbf{p}) \\
 & \quad \times \exp \left\{ i \sum_{j=1}^n [(p_j^0 - p_j'^0)t - (\mathbf{p}_j - \mathbf{p}_j') \cdot \mathbf{x}] / \hbar \right\} \\
 & \quad \times \prod_{k=1}^n \langle a_{\text{in}}^\dagger(\mathbf{p}_k) a_{\text{in}}(\mathbf{p}_k') \rangle \quad (29)
 \end{aligned}$$

All $n!$ permutations have given the same contribution on account of the (anti-) symmetry properties of the functions $\Phi_{\text{in}}^{(n)}$.

Next we introduce the initial Wigner function

$$\begin{aligned}
 f_{\text{in}}(\mathbf{x}, \mathbf{p}, t) &= (2\pi\hbar)^{-3} \int d^3 u \{ \exp[i(\mathbf{u} \cdot \mathbf{x} - u^0 t) / \hbar] \} \\
 & \quad \times \langle a_{\text{in}}^\dagger(\mathbf{p} - \frac{1}{2}\mathbf{u}) a_{\text{in}}(\mathbf{p} + \frac{1}{2}\mathbf{u}) \rangle \quad (30)
 \end{aligned}$$

where u^0 stands for $\mathbf{u} \cdot \mathbf{p} / m$. We note that it satisfies the equation

$$[\partial_t + (\mathbf{p}/m) \cdot \nabla] f_{\text{in}}(\mathbf{x}, \mathbf{p}, t) = 0 \quad (31)$$

Formula (30) may be inverted to read

$$\begin{aligned}
 & \langle a_{\text{in}}^\dagger(\mathbf{p} - \frac{1}{2}\mathbf{u}) a_{\text{in}}(\mathbf{p} + \frac{1}{2}\mathbf{u}) \rangle \\
 &= \int d^3 x \{ \exp[-i(\mathbf{u} \cdot \mathbf{x} - u^0 t) / \hbar] \} f_{\text{in}}(\mathbf{x}, \mathbf{p}, t) \quad (32)
 \end{aligned}$$

If we now use this last formula in (29), after changing variables according to $\mathbf{p}_j \rightarrow \mathbf{p}_j - \frac{1}{2}\mathbf{u}_j$ and $\mathbf{p}_j' \rightarrow \mathbf{p}_j + \frac{1}{2}\mathbf{u}_j$, we get

$$\begin{aligned}
 & [\partial_t + (\mathbf{p}/m) \cdot \nabla] f(\mathbf{x}, \mathbf{p}, t) \\
 &= \sum_{n=2}^{\infty} \int d^3 x^n d^3 p^n \tilde{\Phi}_{\text{in}}^{(n)}(\mathbf{x}^n, \mathbf{p}^n | \mathbf{x}, \mathbf{p}) \prod_{j=1}^n f_{\text{in}}(\mathbf{x}_j, \mathbf{p}_j, t) \quad (33)
 \end{aligned}$$

where the functions $\tilde{\Phi}_{\text{in}}^{(n)}$ are defined as the Fourier transforms

$$\begin{aligned}
 & \tilde{\Phi}_{\text{in}}^{(n)}(\mathbf{x}^n, \mathbf{p}^n | \mathbf{x}, \mathbf{p}) \\
 &= \int d^3 u^n \left\{ \exp \left[i \sum_{j=1}^n \mathbf{u}_j \cdot (\mathbf{x} - \mathbf{x}_j) / \hbar \right] \right\} \Phi_{\text{in}}^{(n)}(\mathbf{p}^n - \frac{1}{2}\mathbf{u}^n; \mathbf{p}^n + \frac{1}{2}\mathbf{u}^n | \mathbf{p}) \quad (34)
 \end{aligned}$$

of the functions $\Phi_{\text{in}}^{(n)}$.

At this point it is a straightforward matter to establish a similar expansion for the Wigner function (10). Following the same reasoning, we find with the in-operator expansion (25) and the initial condition (28)

$$f(\mathbf{x}, \mathbf{p}, t) - f_{\text{in}}(\mathbf{x}, \mathbf{p}, t) = \sum_{n=2}^{\infty} \int d^3x^n d^3p^n \tilde{\psi}_{\text{in}}^{(n)}(\mathbf{x}^n, \mathbf{p}^n | \mathbf{x}, \mathbf{p}) \prod_{j=1}^n f_{\text{in}}(\mathbf{x}_j, \mathbf{p}_j, t) \quad (35)$$

The functions $\tilde{\psi}_{\text{in}}^{(n)}$ are Fourier transforms of the functions $\psi_{\text{in}}^{(n)}$ as in (34).

It should be appreciated that the coefficients $\tilde{\psi}_{\text{in}}^{(n)}$ and $\tilde{\Phi}_{\text{in}}^{(n)}$, which contain the dynamical information about the system, are not independent. In fact, one may be obtained from the other by integration, or, inversely, by differentiation. Indeed, applying the operator $\partial_t + (\mathbf{p}/m) \cdot \nabla$ to both sides of Eq. (35), we deduce with the help of (31) that the relation

$$\left(\frac{\mathbf{p}}{m} \cdot \nabla + \sum_{j=1}^n \frac{\mathbf{p}_j}{m} \cdot \nabla_j \right) \tilde{\psi}_{\text{in}}^{(n)}(\mathbf{x}^n, \mathbf{p}^n | \mathbf{x}, \mathbf{p}) = \tilde{\Phi}_{\text{in}}^{(n)}(\mathbf{x}^n, \mathbf{p}^n | \mathbf{x}, \mathbf{p}) \quad (36)$$

should hold.

5. DERIVATION OF A KINETIC EQUATION

The two expansions (33) and (35), which may be considered as time-independent functionals of the Wigner function f_{in} , are the central formulas of our theory. They have been obtained by means of one assumption only, namely, that initial correlations, save for those dictated by the boson or fermion symmetry, may be ignored. (Molecular chaos in the infinite past.) The physical significance of the various terms is the same as in the classical theory, where one obtains similar formulas⁽⁹⁾; the expansion is one in terms of the collisions of isolated groups of particles. The $n = 2$ terms correspond to binary collisions, the $n = 3$ terms to triple collisions, and so forth.

In concept the method for obtaining a kinetic equation is now simple. It consists in the elimination of the Wigner function f_{in} between the two expansions (33) and (35). If this can be achieved in any meaningful way, one obtains a closed Markovian equation for the one-particle Wigner function $f(\mathbf{x}, \mathbf{p}, t)$, i.e., a kinetic equation. The problem is thus to find a suitable elimination scheme.

In the classical theory one solves the analog of Eq. (35) by using the particle number as an ordering parameter. Following the same procedure here, we find by iteration up to terms quadratic in f ,

$$f_{\text{in}}(x, t) = f(x, t) - \int dx^2 \tilde{\psi}_{\text{in}}^{(2)}(x^2 | x) \prod_{j=1}^2 f(x_j, t) \quad (37)$$

with x denoting the vector pair (\mathbf{x}, \mathbf{p}) . The substitution of this result into (33) yields the kinetic equation

$$\begin{aligned}
 & [\partial_t + (\mathbf{p}/m) \cdot \nabla] f(x, t) \\
 &= \int dx^2 \tilde{\Phi}_{\text{in}}^{(2)}(x^2|x) \prod_{j=1}^2 f(x_j, t) \\
 &+ \int dx^3 [\tilde{\Phi}_{\text{in}}^{(3)}(x^3|x) - 2 \int dy \tilde{\psi}_{\text{in}}^{(2)}(x^2|y) \tilde{\Phi}_{\text{in}}^{(2)}(y, x_3|x)] \prod_{j=1}^3 f(x_j, t)
 \end{aligned} \tag{38}$$

which is valid up to terms that contain the product of three Wigner functions. If the system is sufficiently uniform in space, the first term on the right-hand side reduces to the usual Boltzmann collision term, with a quantum mechanical transition rate.⁽¹³⁾ The second term is the quantum mechanical analog of the classical three-particle collision term first derived by Choh and Uhlenbeck.⁽¹¹⁾ We shall not attempt to prove here that in the classical limit the quantum mechanical three-particle term indeed coincides with the Choh-Uhlenbeck expression. This requires a careful analysis of the relation between the quantum mechanical and classical three-particle scattering problems. It is, however, worth mentioning that the structure of the two collision terms is quite similar and that the Møller operator defined in (16) is the quantum mechanical counterpart of the streaming operators appearing in the classical theory.

In principle also the higher order correction terms to (38) could be obtained successively. However, we know from the classical theory that this iteration procedure, which uses the particle number as an ordering parameter, leads to infinite results for these higher order terms.⁽²⁾ Since we have no reason to suppose that this situation is any different in the quantum mechanical case, we shall not pursue this line of investigation.

A second approach to the elimination problem is to employ the interaction strength as an ordering parameter and to expand the functions $\Phi_{\text{in}}^{(n)}$ and $\psi_{\text{in}}^{(n)}$ into a perturbation series. In the subsequent paper⁽¹²⁾ we shall perform the calculations up to first order. It will then appear that in this order the kinetic equation (38) is in fact the nonlocal version of the well-known Uehling-Uhlenbeck equation.

ACKNOWLEDGMENTS

We are indebted to Prof. E. G. D. Cohen for stimulating discussions about the kinetic theory of dense gases and to Prof. S. R. de Groot for carefully reading the manuscript. Also, the hospitality extended to one of us (ChGvW) by the Rockefeller University is gratefully acknowledged.

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