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A New Quantum Statistical Evaluation Method for Time Correlation Functions

D. Loss[1] and H. Schoeller[1]

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Considering a system of N identical interacting particles, which obey Fermi–Dirac or Bose–Einstein statistics, we derive new formulas for correlation functions of the type $C(t) = \langle \sum_{i=1}^{N} A_i(t) \sum_{j=1}^{N} B_j \rangle$ (where B_j is diagonal in the free-particle states) in the thermodynamic limit. Thereby we apply and extend a superoperator formalism, recently developed for the derivation of long-time tails in semiclassical systems. As an illustrative application, the Boltzmann equation value of the time-integrated correlation function $C(t)$ is derived in a straightforward manner. Due to exchange effects, the obtained $\hat{t}$-matrix and the resulting scattering cross section, which occurs in the Boltzmann collision operator, are now functionals of the Fermi–Dirac or Bose–Einstein distribution.

KEY WORDS: Time correlation functions; Liouville operators; cluster expansion; exchange effects.

1. INTRODUCTION

In our previous work on long time tails[1] (hereafter referred to as I), we presented a new microscopic evaluation method for time correlation functions, in particular for the momentum autocorrelation function associated with self-diffusion processes. Using the superoperator formalism, in particular Liouville operators and projectors, we investigated the long-time behavior of the autocorrelation function for a fluid whose identical particles interact with a translationally invariant and short-range repulsive potential (with no bound states). Thereby the dynamics of the system is treated quantum mechanically, whereas the particles are assumed to obey classical, i.e., Boltzmann statistics. By introducing a new concept, the P_q-rule and the P_q-singularity (the latter being a generalization of van Hove's diagonal singularity[2]), we systematically discussed the various

[1] Institut für Theoretische Physik der Universität Zürich, CH-8001 Zürich, Switzerland.

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terms occurring in the cluster expansion (density expansion) of the autocorrelation function in the thermodynamic and long-time limit. By resumming a first class of divergent terms (due to "uncorrelated binary collisions") and then a second one (due to "ring events"[3]), we obtained the same long-time tails for this semiclassical system as the ones first derived by Dorfman and Cohen[4,5] (see ref. 5 for a bibliography) for a purely classical system of hard-sphere (disk) molecules.

It is the objective of the present paper to start an analogous analysis for the more general case, where the N interacting particles obey Fermi–Dirac or Bose–Einstein statistics. In particular, the central quantity of interest here is a time correlation function of the type $C(t) = \langle \sum_{i=1}^{N} A_i(t) \sum_{j=1}^{N} B_j \rangle$, as occurs, for instance, in the Green–Kubo formulas for transport coefficients obtained by linear response theory.[6] Introducing new projectors ($\bar{P}$ and $\bar{Q}$) and using cluster expansion techniques and the P_q-rule extensively discussed in I, we derive here new inversion formulas [see Eqs. (3.44) and (3.45), respectively] for the Laplace transform of the correlation function $C(\varepsilon)$ which are valid in the thermodynamic limit and hold for all $\varepsilon > 0$. These formulas, being a generalization of the formula (3.60) derived in I, are especially suited for the evaluation of the correlation function in the long-time limit. This is because a certain class of divergences, which occurs in the naive cluster expansion, has been eliminated by the help of the projectors $\bar{P}$ and $\bar{Q}$ (in the same way as was done in I and ref. 7). Therefore, these formulas can be regarded as a first step in the investigation of the long-time behavior of $C(t)$ for low-temperature N-particle systems, where degeneracy effects must be taken into account. In future work we intend to elaborate the next most singular terms on the basis of the present formalism. We note in this connection that these terms might not be given by the semiclassical ring terms, as the investigation of the Lorentz gas by Kirkpatrick and Dorfman[8] suggests.

Moreover, as in other studies[9–14],[2] directed at generalizing classical kinetic theories to normal quantum fluids, a further motivation for the present approach is to "provide a means to capitalize on the advanced state of classical kinetic theory, for quantum systems."[9]

As a first straightforward application of the formalism developed here, the binary collision approximation of $C(\varepsilon)$ (for $\varepsilon \to 0$) is then considered. As result, the Boltzmann equation value of the time-integrated correlation function is obtained, where the linearized Boltzmann collision operator is given with the full quantum statistical scattering cross section, which differs from its semiclassical counterpart in that the former takes account of the

[2] For the Brussels school formalism see ref. 14.

relative occupancy of the intermediate states[9] and which, as a consequence, depends now on the Fermi–Dirac or Bose–Einstein distribution. Besides the demonstration of the utility of the inversion formulas, the presentation of this example also allows us to clearly exhibit the parallels and differences between the quantum statistical case treated here and the semiclassical case considered in I.

We note that this generalized Boltzmann collision operator (which goes beyond the Born approximation) was first derived explicitly by Boercker and Dufty[9] within their formalism, being a quantum statistical generalization of the so-called algebraic approach.[15] Although in this algebraic approach an exact formal closure of the quantum statistical Bogoliubov–Born–Green–Kirkwood–Yvon[16] (BBGKY) hierarchy is accomplished in a simple way, the reduction of the obtained (super) operator expressions (with cluster expansions) to the generalized linear Boltzmann operator is a rather involved procedure. In contrast to this, by deducing the factorization formula (3.42), which corresponds to a closure of the BBGKY hierarchy, we arrive at a quite explicit form of the above-mentioned inversion formula, from which the generalized linear Boltzmann operator can be obtained systematically. In a subsequent paper, we shall derive the quantum statistical nonlinear Boltzmann equation (Uehling–Uhlenbeck equation[16] with degeneracy-modified t-matrix), and, in particular, its first correction, i.e., the quantum statistical version of the classical Choh–Uhlenbeck equation.[18]

The work is organized as follows. In Section 2 the quantities of interest are defined and some technical tools (e.g., superoperators, phase-space representation,[19] etc.) are provided. In Section 3, which represents the main part of this paper, we first discuss the naive cluster expansion together with the divergences occurring there. After the motivation for the choice of the new projectors $\bar{P}$ and $\bar{Q}$, by which the new features introduced by the statistics are taken into account, the above-mentioned inversion formulas are derived. The section is concluded by some remarks, in particular on the reduced distribution operators, defined in the canonical and grand canonical ensemble. In this connection an exact formula for the Fermi–Dirac (Bose–Einstein) distribution in the canonical ensemble is given [see Eq. (3.55)]. In Section 4, finally, the binary collision approximation and its consequences are discussed.

2. SOME DEFINITIONS

We consider a quantum mechanical N-particle system in a periodicity volume Ω at temperature $T=(\beta k_B)^{-1}$, where k_B is Boltzmann's constant.

The N-particle Hamiltonian operator H of this system is given by

$$H = H_0 + V = \sum_{i=1}^{N} H_0(i) + \sum_{i<j} V_{ij} \tag{2.1}$$

with

$$H_0(i) = \hat{\mathbf{p}}_i^2/2m \tag{2.2}$$

and

$$V_{ij} = V(|\mathbf{x}_i - \mathbf{x}_j|) \tag{2.3}$$

where $\hat{\mathbf{p}}_i$ is the momentum operator of the ith particle and m is its mass. V is a short-range pair-interaction potential with no bound states which depends only on the relative coordinates of the particles i and j, i.e., the system is translationally invariant. In the following we are concerned with a correlation function of the form

$$C(t) = \sum_{i,j}^{N} \langle A_i(t)\, B_j \rangle = \sum_{i,j}^{N} \operatorname{Tr} \rho A_i(t)\, B_j \tag{2.4}$$

i.e., the observables in which we are interested are represented by sums of single-particle operators A_i and B_j, respectively. In addition, we assume that B_i is diagonal in the eigenstates of H_0 and that

$$\langle A_i \rangle = 0, \qquad 1 \leqslant i \leqslant N \tag{2.5}$$

which can always be achieved by replacing A_i by $\bar{A}_i = A_i - \langle A_i \rangle$. Such correlation functions occur, e.g., in the kinetic part of transport coefficients (such as the shear viscosity or the thermal conductivity) or in forms of the fluctuation-dissipation theorem,[6,20] etc.

Furthermore, ρ is the canonical density matrix

$$\rho = Z_N^{-1} e^{-\beta H}, \qquad Z_N = \operatorname{Tr} e^{-\beta H} \tag{2.6}$$

The Heisenberg operator $A_i(t)$ is given by (we set $\hbar = 1$)

$$A_i(t) = e^{iHt} A_i e^{-iHt} = e^{iLt} A_i \tag{2.7}$$

where we have introduced the Liouville operator L defined by

$$L = L_0 + L_V = \sum_{i=1}^{N} L_0(i) + \sum_{i<j}^{N} L_{ij} \tag{2.8}$$

with

$$L_0(i)A = [H_0(i), A] \tag{2.9}$$

$$L_{ij}A = [V_{ij}, A] \tag{2.10}$$

and therefore $LA = [H, A]$, where A is an ordinary Hilbert-space operator. The Liouville operator belongs to the class of superoperators which are formally defined as linear operators acting on ordinary Hilbert-space operators (for more details about superoperators see, e.g., refs. 20 and 21).

The trace, Tr, in Eq. (2.4) is to be taken over a complete set of symmetrized (antisymmetrized) states for bosons (fermions). These states may be chosen as eigenstates of the total momentum and are of the form

$$\left(\frac{N!}{\prod_i n_i!}\right)^{1/2} \pi \, |\mathbf{k}_1 \cdots \mathbf{k}_N\rangle \tag{2.11}$$

Here,

$$|\mathbf{k}_1 \cdots \mathbf{k}_N\rangle = |\mathbf{k}_1\rangle \times \cdots \times |\mathbf{k}_N\rangle \equiv |k\rangle \tag{2.12}$$

is the direct product of single-particle momentum eigenstates; π denotes the projecting operator, which (anti)symmetrizes the product states:

$$\pi = \frac{1}{N!}\pi^{1\cdots N} = \frac{1}{N!}\sum_{\sigma \in S_N} \pi_\sigma \tag{2.13}$$

$$\pi_\sigma \, |k\rangle = \eta^{|\sigma|} \, |\mathbf{k}_{\sigma(1)} \cdots \mathbf{k}_{\sigma(N)}\rangle \tag{2.14}$$

$$|\sigma| = \begin{cases} 2 & \text{for even permutations} \\ 1 & \text{for odd permutations} \end{cases}$$

$$\eta = \begin{cases} 1 & \text{for bosons} \\ -1 & \text{for fermions} \end{cases}$$

$\sum_{\sigma \in S_N}$ denotes the sum over all permutations σ of N particles. n_i indicates the number of identical $\mathbf{k}$-vectors of the sort i. For further reference we note that $\pi^{1\cdots N}$ can be represented, e.g., in the form

$$\pi^{1\cdots N} = (1 + \pi_{12})(1 + \pi_{13} + \pi_{23}) \cdots (1 + \pi_{1N} + \cdots + \pi_{N-1N}) \tag{2.15}$$

with

$$\pi_{ij} \, |\mathbf{k}_1 \cdots \mathbf{k}_i \cdots \mathbf{k}_j \cdots \mathbf{k}_N\rangle = \eta \, |\mathbf{k}_1 \cdots \mathbf{k}_j \cdots \mathbf{k}_i \cdots \mathbf{k}_N\rangle \tag{2.14a}$$

Since the state (2.11) remains unchanged under a permutation of the vectors $\mathbf{k}_i$ (apart from the sign in the fermionic case), only those states of

the form (2.11) need to be considered in the trace in Eq. (2.4) whose sets $\{\mathbf{k}_1,..., \mathbf{k}_N\}$ are different. Equation (2.4) therefore reads

$$C(t) = \sum_{i,j}^{N} \sum_{\{\mathbf{k}_1,...,\mathbf{k}_N\}} \frac{N!}{\prod_i n_i!} \langle k| \pi B_j(\rho A_i)(t)\, \pi\, |k\rangle$$
$$= \sum_{i,j}^{N} \sum_{\mathbf{k}_1,...,\mathbf{k}_N} \langle k| \pi B_j(\rho A_i)(t)\, \pi\, |k\rangle$$

Finally, since $\pi\pi = \pi$ and therefore

$$\pi \sum_{j}^{N} B_j\left(\rho \sum_{i}^{N} A_i\right)(t)\, \pi = \sum_{j}^{N} B_j\left(f \sum_{i}^{N} A_i\right)(t)$$

with

$$f = \rho\pi = \pi\rho \tag{2.16}$$

the correlation function (2.4) takes the form

$$C(t) = \sum_{i,j}^{N} \sum_{\mathbf{k}_1,...,\mathbf{k}_N} \langle k| B_j(fA_i)(t)\, |k\rangle \equiv \sum_{i,j}^{N} \mathrm{Tr}_{1\ldots N} B_j(fA_i)(t) \tag{2.17}$$

where $\mathrm{Tr}_{1\ldots N} \equiv \mathrm{Tr}_1 \cdots \mathrm{Tr}_N$ denotes the trace for Boltzmann statistics.

Next, the matrix elements of an ordinary operator are given by

$$A_{kq} = \langle k| A\, |q\rangle \tag{2.18}$$

whereas the matrix elements of a superoperator S are defined through the relation

$$(SA)_{kq} = \sum_{k'',q''} S_{kq|k''q''} A_{k''q''} \tag{2.19a}$$

or more explicitly (choose $A = |k'\rangle\langle q'|$)

$$S_{kq|k''q''} = (S\, |k'\rangle\langle q'|)_{kq} \tag{2.19b}$$

In particular, one easily finds

$$(L_0)_{kq|k'q'} = \delta_{kk'}\delta_{qq'}(\varepsilon_k - \varepsilon_q) \tag{2.20}$$

$$(L_V)_{kq|k'q'} = \delta_{qq'} V_{kk'} - \delta_{kk'} V_{q'q} \tag{2.21}$$

where

$$\varepsilon_k = \frac{k^2}{2m} = \sum_{i=1}^{N} \frac{\mathbf{k}_i}{2m} \tag{2.22}$$

is the kinetic energy of the N particles.

For what follows it is very convenient to introduce superoperators projecting on special matrix elements in the product state representation. First we define the superoperators P and Q projecting on diagonal and nondiagonal matrix elements, respectively. We have

$$(PA)_{kk'} = A_{kk'}\delta_{kk'} \tag{2.23}$$

with

$$\delta_{kk'} = \delta_{\mathbf{k}_1\mathbf{k}_1'} \cdots \delta_{\mathbf{k}_N\mathbf{k}_N'} \tag{2.24}$$

and $Q = 1 - P$. Here, A is an ordinary operator. Obviously one has

$$P^2 = P, \qquad QP = PQ = 0 \tag{2.25}$$

and

$$P \equiv P^{1\cdots N} = P^1 \cdots P^N, \qquad (P^i A)_{kk'} = A_{kk'}\delta_{\mathbf{k}_i\mathbf{k}_i'} \tag{2.26}$$

These projectors are useful in the case with Boltzmann statistics, as has been extensively discussed in I. However, we shall see in the next section that for Fermi–Dirac or Bose–Einstein statistics, generalized projectors $\bar{P} = \bar{P}(1\cdots N)$ and $\bar{Q} = \bar{Q}(1\cdots N)$ are relevant for the removal of the so-called first divergences (see I and Section 3). They are defined by

$$(\bar{P}A)_{kk'} = A_{kk'}\delta_{\{k\},\{k'\}} \tag{2.27}$$

and $\bar{Q} = 1 - \bar{P}$, where $\delta_{\{k\},\{k'\}}$ equals 1 if the sets $\{k\} = \{\mathbf{k}_1,..., \mathbf{k}_N\}$ and $\{k'\} = \{\mathbf{k}_1',..., \mathbf{k}_N'\}$ are equal and 0 otherwise. We note that this definition holds equally for bosons and fermions. Here, too, one finds

$$\bar{P}^2 = \bar{P}, \qquad \bar{P}\bar{Q} = \bar{Q}\bar{P} = 0 \tag{2.28}$$

Moreover, we see that

$$P^{s+1\cdots N}\bar{P} = \bar{P}P^{s+1\cdots N} = P^{s+1\cdots N}\bar{P}(1\cdots s) \tag{2.29}$$

in particular,

$$P\bar{P} = \bar{P}P = P \tag{2.30}$$

For the following it is very convenient to introduce a more explicit representation of $\bar{P}(1\cdots s)$ for $s \ll N$, which is given by

$$\bar{P}^{1\cdots s} = \sum_{\sigma \in S_s} \pi_\sigma P^{1\cdots s}\pi_\sigma^{-1} \tag{2.31}$$

where π_σ^{-1} denotes the inverse permutation of π_σ (note that η^σ drops out). In matrix representation this reads

$$(\bar{P}^{1\cdots s}A)_{kk'} = \sum_{\sigma\in S_s} \langle \pi_\sigma^{-1}k|\, P^{1\cdots s}\pi_\sigma^{-1}A\,|k'\rangle = A_{kk'} \sum_{\sigma\in S_s} \delta_{k^s,\sigma(k'^s)} \quad (2.32)$$

where $k^s=(\mathbf{k}_1,...,\mathbf{k}_s)$ and $\sigma(k')=(\mathbf{k}'_{\sigma(1)},...,\mathbf{k}'_{\sigma(s)})$. Now we would like to point out that in $\sum_{\sigma\in S_s}\delta_{k^s,\sigma(k'^s)}$ some terms are counted more than once if, for instance, $\mathbf{k}_i=\mathbf{k}_j$ for $1\leqslant i<j\leqslant s$. This stands in contrast to $\delta_{\{k^s\},\{k'^s\}}$, where all terms occur only once. Therefore, $\bar{P}^{1\cdots s}$ and $\bar{P}(1\cdots s)$ are not exactly equal. However, since in the following we only consider matrix elements over which a summation $\sum_{k^s,k'^s}$ is to be performed, the terms with e.g., $\mathbf{k}_i=\mathbf{k}_j$ give a negligible contribution in the thermodynamic limit (i.e., for $N,\Omega\to\infty$ with $n=N/\Omega$ finite) as long as $s\ll N$. Hence, we may write

$$\bar{P}^{1\cdots s}=\bar{P}(1\cdots s) \qquad \text{for} \quad \Omega\to\infty \quad \text{and } s \text{ finite} \quad (2.33)$$

Finally, let us note that, if $s\sim N$, the foregoing relation is not valid any more. This is because the number of equal terms in $\bar{P}^{1\cdots s}$ then becomes proportional to N and therefore these terms are no longer negligible in the thermodynamic limit.

We conclude this section by briefly discussing the phase-space representation[19] of (super)operators (for details we refer to I). The reason for introducing this phase-space representation is first that quantum mechanical quantities take a form which is very similar to their classical counterparts [this holds, in particular, for the Liouville operator; see, e.g., Eqs. (I.2.33), (I.2.31), and (I.34)], and second that the P_q-rule extensively used in the following is most easily established in this representation (see also Section 4 of I). Now, a phase function $A^{\mathrm{ph}}(x,p)$, depending on the c-number variables $x=(\mathbf{x}_1,...,\mathbf{x}_N)$ and $p=(\mathbf{p}_1,...,\mathbf{p}_N)$, is defined as the Weyl transform of the ordinary operator A,

$$A^{\mathrm{ph}}(x,p)=\sum_k e^{ikx}A_{p+k/2,\,p-k/2} \quad (2.34)$$

For the product AB one obtains the relation [see (I.2.28)]

$$(AB)^{\mathrm{ph}}(x,p)=e^D A^{\mathrm{ph}}(x,p)\,B^{\mathrm{ph}}(x,p) \quad (2.35)$$

Here the differential operator $D\equiv D(1\cdots N)$ is given by

$$D=\frac{1}{2i}\left(\frac{\partial^B}{\partial x}\frac{\partial^A}{\partial p}-\frac{\partial^A}{\partial x}\frac{\partial^B}{\partial p}\right) \quad (2.36)$$

where $\partial^A/\partial x$ acts on A^{ph}, etc. A phase operator S^{ph}, which corresponds to a superoperator S and which acts on phase functions, is defined by

$$S^{\text{ph}}A^{\text{ph}}(x, p) = (SA)^{\text{ph}}(x, p) \tag{2.37}$$

from which it follows that

$$(S_1 S_2)^{\text{ph}} = S_1^{\text{ph}} S_2^{\text{ph}} \tag{2.38}$$

Using Eq. (2.37), one finds,[19] in particular [see (I.2.30), (I.2.31), (I.2.40)]

$$L_0^{\text{ph}} = -\frac{i}{m} p \cdot \frac{\partial}{\partial x} \tag{2.39}$$

$$L_{ij}^{\text{ph}} = 2i \left\{ \sin \left[\frac{1}{2} \frac{\partial^V}{\partial \mathbf{x}_i} \left(\frac{\partial}{\partial \mathbf{p}_i} - \frac{\partial}{\partial \mathbf{p}_j} \right) \right] \right\} V_{ij} \tag{2.40}$$

and

$$P^{\text{ph}} = \frac{1}{\Omega^N} \int dx \tag{2.41}$$

3. INVERSION FORMULAS

The objective of this section is to derive new inversion formulas which are well suited for the evaluation of the correlation function $C(t)$ first in the thermodynamic limit of the system and second for long times t. The derivation is based on cluster expansions and on the P_q-rule derived in I.

To motivate the following procedure, we first perform a "naive" cluster expansion of the dynamical part in $C(t)$ (see also I). Since it is more convenient to work with the resolvent of e^{iLt}, let us introduce the Laplace transform of $C(t)$:

$$C(\varepsilon) = \int_0^\infty dt\, e^{-\varepsilon t} C(t), \qquad \varepsilon > 0 \tag{3.1}$$

where now the small-ε behavior of $C(\varepsilon)$ determines the long-time behavior of $C(t)$. Explicitly, we have from Eq. (2.17)

$$C(\varepsilon) = N \sum_{i=1}^{N} \text{Tr}_{1 \dots N} B_1 \bar{P} \frac{1}{\varepsilon - iL} f A_i \tag{3.2}$$

where we have used Eq. (2.30) and the facts that the N particles are

identical and that B_i is diagonal. Now, since $\bar{P}L_0 = 0$, we obtain for the resolvent

$$\bar{P}\frac{1}{\varepsilon - iL} = \frac{1}{\varepsilon}\bar{P}\left(1 + \sum_{i<j} iL_{ij}\frac{1}{\varepsilon - iL}\right) \tag{3.3}$$

where we have used the identity

$$\frac{1}{X-Y} = \frac{1}{X} + \frac{1}{X}Y\frac{1}{X-Y} \tag{3.4}$$

The simplest way to obtain the desired cluster expansion is to decompose L in the following manner [see also (I.3.9)–(I.3.14)]:

$$L = L(ij) + L(N-ij) + \sum_{k}^{N\prime}(L_{ik} + L_{jk}) \tag{3.5}$$

$$= L(ijk) + L(N-ijk) + \sum_{l}^{N\prime}(L_{il} + L_{jl} + L_{kl}) \tag{3.6}$$

$$= L(ijkl) + L(N-ijkl) + \sum_{m}^{N\prime}(L_{im} + L_{jm} + L_{km} + L_{lm}) \tag{3.7}$$

etc., where $L(i\cdots j)$, $1 \leqslant i,\ldots, j \leqslant N$, obviously is the full Liouville operator of the subsystem constituted by the particles $i,\ldots, j$, and $L(N-i\cdots j)$ is the full Liouville operator of the subsystem constituted by the remaining particles. These two particle groups are connected by the interaction term $\sum_k'^N (L_{ik} + \cdots + L_{jk})$, where the prime excludes the indices $i,\ldots, j$ in the sum. Making successive use of the decompositions (3.5), (3.6), (3.7), etc., and of Eq. (3.4), one obtains, with the help of the relation

$$\mathrm{Tr}_{i\ldots j} L(i\cdots j)\, A = \mathrm{Tr}_{i\ldots j}[H(i\cdots j), A] = 0 \tag{3.8}$$

the "naive" cluster expansion of $C(\varepsilon)$

$$\begin{aligned} C(\varepsilon) = {} & \frac{1}{\varepsilon}\mathrm{Tr}_1 B_1(f_1 A_1 + \mathrm{Tr}_2 f_{12} A_2) \\ & + \frac{1}{\varepsilon}\mathrm{Tr}_{12} B_1 \bar{P} G_{12}\left(f_{12}\sum_{i=1}^{2} A_i + \mathrm{Tr}_3 f_{123} A_3\right) \\ & + \cdots + \frac{1}{\varepsilon}\mathrm{Tr}_{1\ldots s} B_1 \bar{P} G_{1\ldots s}\left(f_{1\ldots s}\sum_{i=1}^{s} A_i + \mathrm{Tr}_{s+1} f_{1\ldots s+1} A_{s+1}\right) \\ & + \cdots \end{aligned} \tag{3.9}$$

where the cluster superoperators $G_{1\cdots s}$, $2 \leqslant s \leqslant N$, are defined by

$$G_{12} = iL_{12} \frac{1}{\varepsilon - iL(12)} \tag{3.10}$$

$$\vdots$$

$$G_{1\cdots s} = iL_{12} \frac{1}{\varepsilon - iL(12)} i(L_{13} + L_{23}) \frac{1}{\varepsilon - iL(123)} \cdots i(L_{1s} + \cdots + L_{s-1s}) \frac{1}{\varepsilon - iL(1\cdots s)} \tag{3.11}$$

In deriving Eq. (3.9) we have introduced the reduced density operator defined by

$$f_{1\cdots s} = \frac{N!}{(N-s)!} \operatorname{Tr}_{s+1\cdots N} f \tag{3.12}$$

Now we show that $\bar{P}G_{1\cdots s}$ is not defined for $\varepsilon \to 0$. For that purpose we insert $\bar{P} + \bar{Q} = 1$ into $\bar{P}G_{1\cdots s}$ after each resolvent, which yields

$$\bar{P}G_{1\cdots s} = \bar{P}iL_{12} \frac{1}{\varepsilon - iL(12)} [\bar{P}(12) + \bar{Q}(12)]\, i(L_{13} + L_{23}) \times \frac{1}{\varepsilon - iL(123)} [\bar{P}(123) + \bar{Q}(123)] \cdots \frac{1}{\varepsilon - iL(1\cdots s)} [\bar{P}(1\cdots s) + \bar{Q}(1\cdots s)] \tag{3.13}$$

where we have used Eq. (2.29). As regards van Hove's diagonal singularity,[2] which occurs in this connection, we refer the interested reader to I (pp. 211–215) and ref. 7, where this concept has been thoroughly discussed. Since $L_0(1\cdots k)\, \bar{P}(1\cdots k) = 0$, we have

$$\frac{1}{\varepsilon - iL(1\cdots k)} \bar{P}(1\cdots k) = \frac{1}{\varepsilon} \left(1 + \frac{1}{\varepsilon - iL(1\cdots k)} iL_{\nu}(1\cdots k) \right) \bar{P}(1\cdots k) \tag{3.14}$$

Therefore we see that, for $\varepsilon \to 0$, the part with the largest number of $\bar{P}$'s in (3.13) diverges (at least) like $1/\varepsilon^{s-1}$, $2 \leqslant s \leqslant N$. We refer to these divergences, which obtain their $1/\varepsilon$ factors from the zero-particle free resolvent $[1/(\varepsilon - iL_0)]\, \bar{P} = (1/\varepsilon)\, \bar{P}$, as the first divergences. On the other hand, since

$$\left(\frac{1}{\varepsilon - iL_0} \bar{Q} \right)_{kq|k'q'} = \delta_{kk'} \delta_{qq'} \frac{1}{\varepsilon - i(\varepsilon_k - \varepsilon_q)} (1 - \delta_{\{k\},\{q\}}) \tag{3.15}$$

we recognize that $[1/(\varepsilon - iL_0)]\,\bar{Q}$ does not give a full $1/\varepsilon$ factor in the thermodynamic limit (the contribution of terms with $\varepsilon_k = \varepsilon_q$ for $\{k\} \neq \{q\}$ is then negligible[7]). Of course, this does not exclude the possibility that $[1/(\varepsilon - iL_0)]\,\bar{Q}$ leads to further divergences as $\varepsilon \to 0$ (see, e.g., the second divergences of the ring terms[3,4] discussed in I); they are, however, always less divergent than the ones coming from $[1/(\varepsilon - iL_0)]\,\bar{P} = (1/\varepsilon)\,\bar{P}$. In this connection we would like to point out that the projectors P and Q, which have been used for the case with Boltzmann statistics (see I), are not useful in the case of Fermi–Dirac or Bose–Einstein statistics considered in this work. The reason for this is that in (3.9) there would be nonvanishing terms, e.g., of the form (after insertion of $P + Q = 1$)

$$\frac{1}{\varepsilon - iL_0} Q\pi P\rho A_i = \frac{1}{\varepsilon} Q\pi P\rho A_i \tag{3.16}$$

which obviously give also a $1/\varepsilon$ factor like $[1/(\varepsilon - iL_0)]\,P = (1/\varepsilon)\,P$. Hence, a decomposition with P and Q would not be useful in order to single out the first divergences in (3.13), whereas a decomposition with the generalized projectors $\bar{P}$ and $\bar{Q}$ serves this purpose, as Eq. (3.15) shows. In particular, we see that the analog of (3.16) yields zero, because $\bar{Q}\pi P = 0$ (or, more generally, $\bar{Q}\pi\bar{P} = 0$), which follows from $\bar{P}\pi = \pi\bar{P}$ and Eqs. (2.28) and (2.30).

After these motivations we now start the actual derivation of the inversion formulas, in which these first divergences no longer occur. To this end, we go back to Eq. (3.2) and transform $\bar{P}[1/(\varepsilon - iL)]$ in the same way as was done in I and ref. 7. Making use of $\bar{P} + \bar{Q} = 1$, $(XY)^{-1} = Y^{-1}X^{-1}$, and $\bar{P}\bar{Q} = 0$, one finds

$$\begin{aligned}
\bar{P}\frac{1}{\varepsilon - iL} &= \bar{P}\frac{1}{\{1 - i\bar{P}L[1/(\varepsilon - i\bar{Q}L)]\}(\varepsilon - i\bar{Q}L)} \\
&= \bar{P}\frac{1}{\varepsilon - i\bar{Q}L}\frac{1}{1 - i\bar{P}L[1/(\varepsilon - i\bar{Q}L)]} \\
&= \bar{P}\frac{1}{\varepsilon - i\varepsilon\bar{P}L[1/(\varepsilon - i\bar{Q}L)]}
\end{aligned} \tag{3.17}$$

By virtue of the identity

$$\begin{aligned}
&\bar{P}\frac{1}{1 - i\bar{P}L[1/(\varepsilon - i\bar{Q}L)](\bar{P} + \bar{Q})} \\
&\quad = \bar{P}\frac{1}{1 - i\bar{P}L[1/(\varepsilon - i\bar{Q}L)]}\bar{P}\left(1 + i\bar{P}L\frac{1}{\varepsilon - i\bar{Q}L}\bar{Q}\right)
\end{aligned} \tag{3.18}$$

where we have used Eq. (3.4) and $\bar{Q}\bar{P}=0$, we finally arrive at

$$\bar{P}\frac{1}{\varepsilon-iL}=\frac{1}{\varepsilon-i\varepsilon\bar{P}L_V[1/(\varepsilon-i\bar{Q}L)]\,\bar{P}}\,\bar{P}\left(1+i\bar{P}L_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{Q}\right) \tag{3.19}$$

Now the first divergences have been resummed in the denominator on the rhs of the foregoing equation. Next we show (see also I) that, when Eq. (3.19) is inserted into (3.2), this denominator can be replaced by a one-particle superoperator (cf. Eq. (3.45) below). To begin with, we rewrite Eq. (3.19) in the form

$$\bar{P}\frac{1}{\varepsilon-iL}=i\bar{P}L_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{P}\frac{1}{\varepsilon-iL}+\frac{1}{\varepsilon}\,\bar{P}\left(1+i\bar{P}L_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{Q}\right) \tag{3.20}$$

By applying both sides to $f\sum_{i=1}^{N}A_i$ and by taking the trace $\mathrm{Tr}_{2\ldots N}$ on both sides, we are left with

$$\begin{aligned}\frac{1}{N}\Phi_1(\varepsilon)=\mathrm{Tr}_{2\ldots N}i\bar{P}L_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{P}f\frac{1}{\varepsilon-iL}\sum_{i=1}^{N}A_i\\ +\frac{1}{\varepsilon}\,\mathrm{Tr}_{2\ldots N}\,\bar{P}\left(1+\bar{P}iL_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{Q}\right)f\sum_{i=1}^{N}A_i\end{aligned} \tag{3.21}$$

with

$$\Phi_{1\ldots s}(\varepsilon):=\frac{N!}{(N-s)!}\,\mathrm{Tr}_{s+1\ldots N}\,\bar{P}f\frac{1}{\varepsilon-iL}\sum_{i=1}^{N}A_i \tag{3.22}$$

where we have used the fact that $Lf\sum_i A_i=fL\sum_i A_i$. By making use of Eqs. (2.29), (2.33), and (2.31) and the relation $\pi_\sigma f=f$, we may rewrite $\Phi_{1\ldots s}(\varepsilon)$ in the useful form

$$\Phi_{1\ldots s}(\varepsilon)=\frac{N!}{(N-s)!}\,\pi^{1\cdots s}\,\mathrm{Tr}_{s+1\ldots N}\,Pf\frac{1}{\varepsilon-iL}\sum_{i=1}^{N}A_i \tag{3.23}$$

We now consider the first term on the rhs of Eq. (3.21) in more detail. By performing the same cluster expansion as the one leading to Eq. (3.9) (the presence of the $\bar{Q}$'s has no influence), we obtain here

$$\begin{aligned}&\mathrm{Tr}_{2\ldots N}\,i\bar{P}L_V\frac{1}{\varepsilon-i\bar{Q}L}\,\bar{P}f\frac{1}{\varepsilon-iL}\sum_i A_i\\ &\quad=\frac{1}{N}\sum_{s=2}^{N}\mathrm{Tr}_{2\ldots s}\,\bar{P}(1\cdots s)\,\bar{G}_{1\ldots s}\bar{P}(1\cdots s)\,\Phi_{1\ldots s}(\varepsilon)\end{aligned} \tag{3.24}$$

with

$$\bar{G}_{1\dots s} := iL_{12}\frac{1}{\varepsilon - i\bar{Q}(12)\,L(12)}\,i\bar{Q}(12)(L_{13}+L_{23})\frac{1}{\varepsilon - i\bar{Q}(123)\,L(123)}\,i\bar{Q}(123)$$
$$\cdots i\bar{Q}(1\cdots s-1)(L_{1s}+\cdots+L_{s-1s})\frac{1}{\varepsilon - i\bar{Q}(1\cdots s)\,L(1\cdots s)} \tag{3.25}$$

Let us go back to time space for a moment and split $\Phi_{1\dots s}(t)$ into two parts,

$$\Phi_{1\dots s}(t) = \pi^{1\cdots s}\left(\sum_{i=1}^{s}\Phi^{1,i}+\Phi^{2}\right) \tag{3.26}$$

with

$$\Phi^{1,i} = \frac{N!}{(N-s)!}\,\mathrm{Tr}_{s+1\cdots N}\,Pfe^{iLt}A_i, \qquad 1\leqslant i\leqslant s \tag{3.27}$$

$$\Phi^{2} = \frac{N!}{(N-s-1)!}\,\mathrm{Tr}_{s+1\cdots N}\,Pfe^{iLt}A_{s+1} \tag{3.28}$$

Next we perform a cluster expansion for e^{iLt}. Explicitly, we have

$$e^{iLt} = \sum_{l=1}^{N}\sum_{I_1,\dots,I_l} U(I_1)\cdots U(I_l) \tag{3.29}$$

where $I_1\cup\cdots\cup I_l=\{1,\dots,N\}$, $I_i\cap I_j=\varnothing$, and $U(I)\equiv 1$ if $I=\varnothing$. Inserting this cluster expansion into $\Phi^{1,i}$ and taking into account that $U(I)\,A_i=0$ if $|I|\geqslant 2$ and $i\notin I$, we obtain

$$\Phi^{1,i} = \sum_{J_i}\sum_{d\geqslant 0}\mathrm{Tr}_{I_d}\,Pf_{1\dots sI_d}U(iJ_iI_d)\,A_i \tag{3.30}$$

where $I_d=\{s+1,\dots,s+d\}$ $(I_d=\varnothing$ for $d=0)$ and $J_i\subset\{1,\dots,s\}\backslash\{i\}$. Similarly, we perform the usual cluster expansion for the reduced density operator

$$f_{1\dots sI_d} = \sum_{l=1}^{s+d}\sum_{I_1,\dots,I_l} g_{I_1}\cdots g_{I_l} \tag{3.31}$$

where the notation is analogous to the one introduced in Eq. (3.29). This can be rewritten in a more appropriate form as

$$f_{1\dots sI_d} = f_{iI_d}\prod_{j(\neq i)}^{s} f_j + g(1\mid\cdots\mid i-1\mid iI_d\mid i+1\mid\cdots\mid s) \tag{3.32}$$

Here, the cluster operator g connects (by V_{kl} or/and π_{kl}) any particle(s) from iI_d with any particle(s) from $\{1,..., s\}\backslash\{i\}$ or two (or more) particles from $\{1,..., s\}\backslash\{i\}$ with one another. Inserting this cluster decomposition into Eq. (3.30) and going over to the phase space representation, we then obtain with Eq. (2.35)

$$(\Phi^{1,i})^{\mathrm{ph}} = \sum_{J_i} \sum_{d\geqslant 0} \sum_{\mathbf{p}_{s+1},\ldots,\mathbf{p}_{s+d}} P^{\mathrm{ph}} e^{D(1\cdots s+d)} \times \left(f_{iI_d} \prod_{j(\neq i)}^{s} f_j + g \right)^{\mathrm{ph}} U(iJ_iI_d)^{\mathrm{ph}} A_i^{\mathrm{ph}} \tag{3.33}$$

Now, due to the cluster property of g^{ph} and U^{ph} (see I), we see with Eq. (2.41) and $f_i = P^i f_i$ (due to the translational invariance) that the terms with g's or/and $J_i \neq \varnothing$ are smaller at least by a factor Ω^{-1} compared to the other terms. Thus, by going back to the operator representation and retaining only the leading contributions, we have

$$\Phi^{1,i} = \sum_{d\geqslant 0} \mathrm{Tr}_{I_d} P \prod_{j(\neq i)}^{s} f_j f_{iI_d} U(iI_d) A_i \qquad \text{for} \quad \Omega \to \infty \tag{3.34}$$

Then, using the relation

$$\begin{aligned} f_{iI_d} &= \frac{N!}{(N-d-1)!} \mathrm{Tr}_{N-iI_d} f(1\cdots N) \\ &= \frac{(N-s+1)!}{(N-s-d)!} \mathrm{Tr}_{s+d+1\cdots N} f(is+1\cdots N) \qquad \text{for} \quad \Omega \to \infty \end{aligned} \tag{3.35}$$

which holds for $1 \leqslant i \leqslant s \ll N$, we eventually find, with $U(I) A_i = 0$, if $i \notin I(|I| \geqslant 2)$,

$$\Phi^{1,i} = NP^{1\cdots s} \prod_{j(\neq i)}^{s} f_j \, \mathrm{Tr}_{N-i} P f e^{iLt} A_i \qquad \text{for} \quad \Omega \to \infty \tag{3.36}$$

We note that $P^{1\cdots s}$ can be omitted in the foregoing expression, for f_j is diagonal (i.e., $f_j = P^j f_j$).

Next we transform Φ^2 in a similar way. Substituting for e^{iLt} its cluster expansion into (3.28), we obtain [again with $U(I) A_{s+1} = 0$ if $s+1 \notin I$, $|I| \geqslant 2$]

$$\Phi^2 = \sum_{d\geqslant 1} \mathrm{Tr}_{I_d} P f_{1\cdots sI_d} \left\{ \sum_{i=1}^{s} \sum_{J_i} U(iJ_iI_d) + U(I_d) \right\} A_{s+1} \tag{3.37}$$

where I_d and J_i are the same sets as in Eq. (3.30). By replacing f by the cluster expansion (3.32), the first term in the braces of the foregoing

equation can be treated as above. For the second term we substitute for f the following cluster expansion [being an alternative form of Eq. (3.31)]

$$f_{1\cdots sI_d} = f_{1\cdots s} f_{I_d} + \sum_{i=1}^{s} g(i\,|\,I_d) \prod_{j(\neq i)}^{s} f_j + \bar{g}(1\cdots s\,|\,I_d) \tag{3.38}$$

where g connects any particle(s) from I_d with particle i, and $\bar{g}$ contains the remaining terms. Using the same arguments as above for $\Phi^{1,i}$, one finds

$$\Phi^2 = \sum_{i=1}^{s} P \prod_{j(\neq i)}^{s} f_j \sum_{d\geqslant 1} \mathrm{Tr}_{I_d}\{f_{iI_d} U(iI_d) + g(i\,|\,I_d)\, U(I_d)\}\, A_{s+1}$$
$$+ P f_{1\cdots s} \sum_{d\geqslant 1} \mathrm{Tr}_{I_d} f_{I_d} U(I_d)\, A_{s+1} \qquad \text{for} \quad \Omega \to \infty \tag{3.39}$$

With the help of Eq. (3.35) we see, however, that the last term vanishes, since

$$\mathrm{Tr}_{s+1\cdots N} f(s+1\cdots N)\, e^{iL(s+1\cdots N)t} A_{s+1} \sim \langle A_{s+1}\rangle = 0 \tag{3.40}$$

For the same reason we can replace $g(i\,|\,I_d)$ by f_{iI_d}, since obviously $g(i\,|\,I_d) = f_{iI_d} - f_i f_{I_d}$. Hence, after some manipulations, we are left with

$$\Phi^2 = N \sum_{i=1}^{s} P^{1\cdots s} \prod_{j(\neq i)}^{s} f_j\, \mathrm{Tr}_{N-i}\, P f e^{iLt} \sum_{k(\neq i)}^{N} A_k \qquad \text{for} \quad \Omega \to \infty \tag{3.41}$$

Combining this result for Φ^2 together with $\Phi^{1,i}$ given in Eq. (3.36), we find from (3.26) the *factorization formula*

$$\Phi_{1\cdots s}(\varepsilon) = \pi^{1\cdots s} P^{1\cdots s} \sum_{i=1}^{s} \sigma_{1i} \Phi_1(\varepsilon)\, f_2 \cdots f_s \qquad \text{for} \quad \Omega \to \infty \tag{3.42}$$

Here, we have introduced the permutation superoperator σ_{ij} defined by

$$\sigma_{ij} A(1\cdots i\cdots j\cdots N) = A(1\cdots j\cdots i\cdots N) \tag{3.43}$$

where A is an ordinary operator. Now, we insert this result for $\Phi_{1\cdots s}(\varepsilon)$ back into Eq. (3.24) and solve Eq. (3.21) for $N^{-1}\Phi_1(\varepsilon)$. Then, after some simple manipulations, the Laplace transform of the correlation function $C(t)$ [defined in (2.4)] takes the final form

$$C(\varepsilon) = \mathrm{Tr}_1\, B_1 \frac{1}{\varepsilon - \varepsilon \sum_{s=2}^{\infty} \mathrm{Tr}_{2\cdots s} P^1 \bar{G}_{1\cdots s} \pi^{1\cdots s} P \sum_{i=1}^{s} \sigma_{1i} f_2 \cdots f_s}$$
$$\times N\, \mathrm{Tr}_{2\cdots N} P \left(1 + iPL_V \frac{1}{\varepsilon - i\bar{Q}L} \bar{Q}\right) f \sum_{i=1}^{N} A_i \qquad \text{for} \quad \Omega \to \infty \tag{3.44}$$

where $\bar{G}_{1\ldots s}$ is given in Eq. (3.25) In Appendix A we show that the foregoing result can be brought to the following equivalent but more compact form:

$$C(\varepsilon) =$$

$$\mathrm{Tr}_1 B_1 \frac{1}{\varepsilon - \varepsilon N \,\mathrm{Tr}_{2\ldots N} i\bar{P}L_V[1/(\varepsilon - i\bar{Q}L)]\,\bar{P}f(1+N\sigma_{12})(f_1 + \mathrm{Tr}_k f_{1k}\sigma_{1k})^{-1}}$$

$$\times N \,\mathrm{Tr}_{2\ldots N} \bar{P}\left(1 + i\bar{P}L_V \frac{1}{\varepsilon - i\bar{Q}L}\bar{Q}\right) f(1+N\sigma_{12})\, A_1 \qquad \text{for} \quad \Omega \to \infty \tag{3.45}$$

Let us make some remarks on the inversion formulas (3.44) and (3.45), respectively, which represent the main result of this work. First, we note that these formulas, which are exact in the thermodynamic limit, have been derived for a translationally invariant and short-range potential and hold for systems obeying Bose–Einstein or Fermi–Dirac statistics. Although Eqs. (3.44) and (3.45) are valid for all $\varepsilon > 0$, they are especially suited as starting points for the evaluation of $C(\varepsilon)$ in the limit $\varepsilon \to 0$. This is because the most divergent terms as $\varepsilon \to 0$, namely the first divergences, no longer occur due to the action of the $\bar{Q}$'s in $\bar{G}_{1\ldots s}$ and $(\varepsilon - i\bar{Q}L)^{-1}$ (see the discussion at the outset of this section). In this connection, it is worth noting that only the $\bar{Q}$'s in the numerator of $\bar{G}_{1\ldots s}$ must be retained, whereas the $\bar{Q}$'s in the denominator of $\bar{G}_{1\ldots s}$ can be replaced by 1, since there the $\bar{P}$ part in $\bar{Q} = 1 - \bar{P}$ leads to a negligible contribution in the thermodynamic limit due to the P_q-rule established in I (see also Appendix B). Moreover, in Appendix B we show that, after some simple manipulations, $\bar{G}_{1\ldots s}\pi^{1\cdots s}A$ (where A is a symmetric operator) can be brought to a very convenient form, where all remaining $\bar{Q}$'s are replaced by the simpler projectors Q. Explicitly, one finds

$$\begin{aligned}
\bar{G}_{1\ldots s}\pi^{1\cdots s}A = i\bar{L}_{12}\frac{1}{\varepsilon - iL(12)} iQ^{12}(\bar{L}_{13} + \bar{L}_{23} + \bar{L}_{12,3})\frac{1}{\varepsilon - iL(123)} iQ^{123} \\
\times (\bar{L}_{14} + \bar{L}_{24} + \bar{L}_{34} + \bar{L}_{12,4} + \bar{L}_{13,4} + \bar{L}_{23,4})\frac{1}{\varepsilon - iL(1234)} iQ^{1234} \\
\times \cdots \frac{1}{\varepsilon - iL(1\cdots s-1)} iQ^{1\cdots s-1} \\
\times \left(\bar{L}_{1s} + \cdots + \bar{L}_{s-1\,s} + \sum_{i<j}^{s-1} \bar{L}_{ij,s}\right)\frac{1}{\varepsilon - iL(1\cdots s)}
\end{aligned} \tag{3.46}$$

where the new Liouville operators are defined by

$$\bar{L}_{ij}A = [\bar{V}_{ij}, A], \qquad \bar{V}_{ij} = V_{ij}(1+\pi_{ij}) \tag{3.47}$$

$$\bar{L}_{ij,k}A = (\pi_{ik}+\pi_{jk})\, V_{ij}A - AV_{ij}(\pi_{ik}+\pi_{jk}) \tag{3.48}$$

Starting from the inversion formula (3.44) and the preceding representation for $\bar{G}_{1\ldots s}$, it is a straightforward matter to derive the Boltzmann equation value of $C(\varepsilon)$ for $\varepsilon \to 0$, as we shall demonstrate in Section 4.

As regards the small-ε behavior of $C(\varepsilon)$, we point out that further divergences (due to, e.g., the ring terms[1]) appear in $\bar{G}_{1\ldots s}$ for $s \geqslant 3$ (4) in 2 (3) dimensions as $\varepsilon \to 0$, as we know from the classical case[3,4] or from the semiclassical case with Boltzmann statistics,[1] which is obtained by replacing π by 1 and $\bar{P}$ by P everywhere in the formulas (3.44) and (3.45). Whether these ring terms are the next leading divergences or whether there are equally or more divergent terms (as one should expect from the discussion of the Lorentz gas[8]) needs further investigation.

Finally, we remark that, for large systems, the reduced distribution operator $f_{1\ldots s}$, defined in the canonical ensemble, can be replaced by the grand canonical reduced distribution operator $n_{1\ldots s}$. The latter is defined by

$$n_{1\ldots s} = \sum_{N \geqslant s} \frac{N!}{(N-S)!} \mathrm{Tr}_{s+1\ldots N}\, \pi\rho_G \tag{3.49}$$

with

$$\rho_G = Z_G^{-1} e^{-\beta(H-\mu N)}, \qquad Z_G = \sum_{N \geqslant 0} e^{\beta N\mu} Z_N \tag{3.50}$$

where μ is the chemical potential. Making use of the second quantization formalism, it is not difficult to obtain an explicit representation especially of the unperturbed (i.e., $V=0$) reduced distribution operator $n^0_{1\ldots s}$. First we note the well-known relation

$$\langle \mathbf{k}'_1 \cdots \mathbf{k}'_s |\, n_{1\ldots s}\, | \mathbf{k}_1 \cdots \mathbf{k}_s \rangle = \langle a^+_{\mathbf{k}_1} \cdots a^+_{\mathbf{k}_s} a_{\mathbf{k}'_s} \cdots a_{\mathbf{k}'_1} \rangle_G \tag{3.51}$$

where $a^+_{\mathbf{k}}$ ($a_{\mathbf{k}}$) is a creation (annihilation) operator satisfying the usual commutation relations for bosons or anticommutation relations for fermions. The expectation value on the rhs of Eq. (3.51) is to be evaluated with ρ_G in the Fock space. Setting $V=0$ in Eq. (3.51) and using Wick's theorem for time-independent operators, one obtains

$$n^0_{1\ldots s} = \pi^{1\cdots s} n^0_1 \cdots n^0_s \tag{3.52}$$

Here, n_i^0 is the momentum distribution operator for free bosons ($\eta = 1$) or fermions ($\eta = -1$),

$$n_i^0 = (e^{\beta[H_0(i) - \mu_0]} - \eta)^{-1} \tag{3.53}$$

where μ_0 is the unperturbed chemical potential.

For the sake of completeness, however, let us finally show that Eq. (3.52) (which can be regarded as Wick's theorem in operator form) together with Eq. (3.53) may be derived completely within the canonical ensemble formalism. First, noting that $f^0_{1\cdots s} = \bar{P}(1\cdots s) f^0_{1\cdots s}$ and making use of Eqs. (2.33), (2.31), and (3.31) and the P_q-rule, one immediately finds

$$f^0_{1\cdots s} = \pi^{1\cdots s} f^0_1 \cdots f^0_s + O(1/\Omega) \tag{3.54}$$

In Appendix C we derive the exact formula

$$f^0_1[N] = \left(\frac{Z^0_N}{Z^0_{N-1}} e^{\beta H_0(1)} - \eta \right)^{-1} \{1 - \eta(f^0_1[N] - f^0_1[N-1])\} \tag{3.55}$$

which holds for all $N > 1$. Here, $f^0_1[N]$ ($\equiv f^0_1$) and the unperturbed partition function Z^0_N belong to the N-particle system, whereas $f^0_1[N-1]$ and Z^0_{N-1} belong to the $(N-1)$-particle system. Since

$$Z^0_N / Z^0_{N-1} = e^{-\beta\mu_0} + O(\partial\mu_0/\partial N)$$

where $\partial\mu_0/\partial N \sim N^{-1}$, as is well known from thermodynamics, and since, with $\partial f^0_1[N]/\partial N \sim O(\partial\mu_0/\partial N)$, $f^0_1[N] - f^0_1[N-1] \sim N^{-1}$ [which is a special case of Eq. (3.35)], Eq. (3.55) reduces to the expected result

$$f^0_1 = n^0_1 + O(1/\Omega) \tag{3.56}$$

4. BINARY COLLISION APPROXIMATION

To illustrate the utility of the formalism derived in the previous sections, the binary collision approximation of the inversion formula (3.44) for $\varepsilon \to 0$ will be considered in the following. In particular, this means that we shall obtain the Boltzmann equation value of the time-integrated correlation function $C(t)$, where the linearized Boltzmann collision operator is given with the full (exchange modified) scattering cross section. A further reason for deriving this known result[9] with the help of the present formalism is to exhibit clearly some important differences between the semiclassical case with Boltzmann statistics (as treated in I) and the quantum statistical case considered here.

To begin with, we introduce the notation

$$C = \lim_{\varepsilon \to 0^+} C(\varepsilon) = \int_0^\infty dt\, C(t) \tag{4.1}$$

and write for the inversion formula (3.44)

$$C = \lim_{\varepsilon \to 0^+} \mathrm{Tr}_1 B_1 \frac{1}{\varepsilon - \mathscr{D}_1(\varepsilon)} N \mathrm{Tr}_{2\ldots N} P \left(1 + iPL_V \frac{1}{\varepsilon - i\bar{Q}L} \bar{Q}\right) f \sum_{i=1}^{N} A_i \tag{4.2}$$

Here the superoperator $\mathscr{D}_1(\varepsilon) = P^1 \mathscr{D}_1(\varepsilon)\, P^1$ is defined by

$$\mathscr{D}_1(\varepsilon)\, X_1 = \varepsilon \sum_{s=2}^{\infty} \mathrm{Tr}_{2\ldots s} P^{1\cdots s} \bar{G}_{1\ldots s} \pi^{1\cdots s} \sum_{i=1}^{s} \sigma_{1i} X_1 f_2 \cdots f_s \tag{4.3}$$

where X_1 is an arbitrary diagonal one-particle operator (i.e., $P^1 X_1 = X_1$). For the further evaluation of $\mathscr{D}_1$ it is very convenient to rewrite (4.3) in a more symmetric form. By means of the identity

$$\sum_{i=1}^{s} \sigma_{1i} X_1 f_2 \cdots f_s = \frac{\partial}{\partial \lambda}\bigg|_{\lambda=0} \tilde{f}_1 \cdots \tilde{f}_s \tag{4.4}$$

where

$$\tilde{f}_i = f_i + \lambda X_i \tag{4.5}$$

one has

$$D_1^\lambda(\varepsilon) = \varepsilon \sum_{s=2}^{\infty} \mathrm{Tr}_{2\ldots s} P^{1\cdots s} \bar{G}_{1\ldots s} \pi^{1\cdots s} \tilde{f}_1 \cdots \tilde{f}_s \tag{4.6}$$

with

$$\mathscr{D}_1(\varepsilon)\, X_1 = \frac{\partial}{\partial \lambda}\bigg|_{\lambda=0} D_1^\lambda(\varepsilon) \tag{4.7}$$

Up to this point everything is exact. To obtain the binary collision approximation, we now retain only those terms in $\bar{G}_{1\ldots s}$ [see Eq. (3.46)] and in D_1^λ, respectively, which involve at most two particles. The decisive point now is to realize that the Liouville operator $\bar{L}_{ij,k}$, which apparently depends on three particles, can reduce to a two-particle operator in special cases. By using the identity

$$\mathrm{Tr}_j \pi_{ij} = \eta \tag{4.8}$$

one finds, for instance,

$$\mathrm{Tr}_k\, \bar{L}_{ij,k} \tilde{f}_k^0 A_{ij} = \tilde{L}_{ij} A_{ij} \qquad (k \neq i, j) \tag{4.9}$$

with

$$\tilde{L}_{ij} A_{ij} = \eta(\tilde{f}_i^0 + \tilde{f}_j^0)\, V_{ij} A_{ij} - \eta A_{ij} V_{ij} (\tilde{f}_i^0 + \tilde{f}_j^0) \tag{4.10}$$

where $\tilde{f}_i^0$ is the unperturbed value of $\tilde{f}_i$ and A_{ij} is an arbitrary two-particle operator. On the other hand, a term, e.g., of the form $\mathrm{Tr}_k\, \bar{L}_{ij,k} \tilde{f}_k V_{ik}$ obviously cannot be reduced to a two-particle operator. Taking this fact into account, one immediately convinces oneself that in the binary collision approximation only the Liouville operators $\bar{L}_{12}$, $\bar{L}_{12,l}$ $(3 \leqslant l \leqslant s)$, and L_{12} have to be retained in Eq. (3.46). In addition, $\tilde{f}_i$ can be replaced by $\tilde{f}_i^0$ in this approximation. Hence, Eq. (4.6) takes the form

$$D_1^\lambda(\varepsilon) = \varepsilon \sum_{s=2}^{\infty} P^1\, \mathrm{Tr}_{2\ldots s}\, i\bar{L}_{12} \frac{1}{\varepsilon - iL(12)}\, iQ^{12}\bar{L}_{12,3} \frac{1}{\varepsilon - iL(12)} \cdots \frac{1}{\varepsilon - iL(12)}\, iQ^{12}\bar{L}_{12,s} \frac{1}{\varepsilon - iL(12)} \tilde{f}_1^0 \cdots \tilde{f}_s^0 + \mathrm{MC} \tag{4.11}$$

where the multiple collision term MC contains all irreducible contributions which involve more than two particles. Next, noting that the Q's can be omitted in the preceding equation due to the P_q-rule and making use of Eq. (4.9), one can perform the summation over s explicitly and obtain

$$D_1^\lambda(\varepsilon) = \mathscr{B}_1^\lambda(\varepsilon)\, \tilde{f}_1^0 + MC \tag{4.12}$$

Here, the superoperator $\mathscr{B}_1^\lambda(\varepsilon) = P^1 \mathscr{B}_1^\lambda(\varepsilon)\, P^1$ is defined by

$$\mathscr{B}_1^\lambda(\varepsilon) = -\mathrm{Tr}_2\, P^{12} \hat{T}_{12}^\lambda P^{12} \tilde{f}_2^0 \tag{4.13}$$

where $\hat{T}_{12}^\lambda$ is the exchange-modified Liouville T-matrix

$$\hat{T}_{12}^\lambda = -i\bar{L}_{12} \frac{1}{\varepsilon - i\hat{L}^\lambda(12)} [\varepsilon - iL_0(12)] \tag{4.14}$$

with

$$\hat{L}^\lambda(12) = L(12) + \tilde{L}_{12} \tag{4.15}$$

In Appendix D, it is shown that $\mathscr{B}_1^\lambda = \lim_{\varepsilon \to 0^+} \mathscr{B}_1^\lambda(\varepsilon)$ represents the Boltzmann collision operator with the full scattering cross section, where

the relative occupancy of the intermediate states has been taken into account by the factor $(1+\eta\tilde{f}_1^0+\eta\tilde{f}_2^0)$. Explicitly, we find there

$$(\mathscr{B}_1^\lambda \tilde{f}_1^0)_{\mathbf{k}_1\mathbf{k}_1} = -4\pi \sum_{\mathbf{k}_2,\mathbf{k}_1',\mathbf{k}_2'} |[\hat{t}_{12}^-(\varepsilon_{\mathbf{k}_1}+\varepsilon_{\mathbf{k}_2};\lambda)\tfrac{1}{2}(1+\pi_{12})]_{\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_1'\mathbf{k}_2'}|^2$$
$$\times \delta(\varepsilon_{\mathbf{k}_1}+\varepsilon_{\mathbf{k}_2}-\varepsilon_{\mathbf{k}_1'}-\varepsilon_{\mathbf{k}_2'})\{\tilde{f}_{\mathbf{k}_1'}^0\tilde{f}_{\mathbf{k}_2'}^0(1+\eta\tilde{f}_{\mathbf{k}_1}^0)(1+\eta\tilde{f}_{\mathbf{k}_2}^0)$$
$$-(1+\eta\tilde{f}_{\mathbf{k}_1}^0)(1+\eta\tilde{f}_{\mathbf{k}_2}^0)\tilde{f}_{\mathbf{k}_1'}^0\tilde{f}_{\mathbf{k}_2'}^0\} \tag{4.16}$$

where $\tilde{f}_{\mathbf{k}_1}^0=(\tilde{f}_1^0)_{\mathbf{k}_1\mathbf{k}_1}$, etc., and where the t-matrix $\hat{t}_{12}^-(E;\lambda)=\lim_{\varepsilon\to 0^+}\hat{t}_{12}^-(E-i\varepsilon;\lambda)$ is given by

$$\hat{t}_{12}^-(E-i\varepsilon;\lambda)=V_{12}\frac{1}{\varepsilon-i[\hat{H}_\lambda(12)-E]}\{\varepsilon-i[H_0(12)-E]\} \tag{4.17}$$

with

$$\hat{H}_\lambda(12)=H_0(12)+V_{12}(1+\eta\tilde{f}_1^0+\eta\tilde{f}_2^0) \tag{4.18}$$

Next, to obtain $\mathscr{D}_1X_1:=\lim_{\varepsilon\to 0}\mathscr{D}_1(\varepsilon)X_1$ we take the derivative of $\lim_{\varepsilon\to 0}D_1^\lambda(\varepsilon)=\mathscr{B}_1^\lambda\tilde{f}_1^0+\mathrm{MC}$ with respect to λ [see Eqs. (4.7) and (4.12)]. Since in Eq. (4.16) for $\lambda=0$ the terms in the braces cancel due to energy conservation, only the derivative of the $\tilde{f}$'s in the braces has to be calculated. Using again the relation

$$f_{\mathbf{k}_1}^0 f_{\mathbf{k}_2}^0(1+\eta f_{\mathbf{k}_1'}^0)(1+\eta f_{\mathbf{k}_2'}^0)=(1+\eta f_{\mathbf{k}_1}^0)(1+\eta f_{\mathbf{k}_2}^0)f_{\mathbf{k}_1'}^0 f_{\mathbf{k}_2'}^0$$

which holds on the energy shell, one then finds after some simple algebra

$$\mathscr{D}_1X_1=\mathscr{B}_1X_1+\mathrm{MC} \tag{4.19}$$

where $\mathscr{B}_1=(\partial/\partial\lambda)|_{\lambda=0}\mathscr{B}_1^\lambda$. Explicitly,

$$(\mathscr{B}_1X_1)_{\mathbf{k}_1\mathbf{k}_1}=-4\pi\sum_{\mathbf{k}_2,\mathbf{k}_1',\mathbf{k}_2'}\left|\left[\hat{t}_{12}^-(\varepsilon_{\mathbf{k}_1}+\varepsilon_{\mathbf{k}_2})\frac{1}{2}(1+\pi_{12})\right]_{\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_1'\mathbf{k}_2'}\right|^2$$
$$\times\delta(\varepsilon_{\mathbf{k}_1}+\varepsilon_{\mathbf{k}_2}-\varepsilon_{\mathbf{k}_1'}-\varepsilon_{\mathbf{k}_2'})(1+\eta f_{\mathbf{k}_1}^0)(1+\eta f_{\mathbf{k}_2}^0)$$
$$\times f_{\mathbf{k}_1'}^0 f_{\mathbf{k}_2'}^0\{\bar{X}_{\mathbf{k}_1}+\bar{X}_{\mathbf{k}_2}-\bar{X}_{\mathbf{k}_1'}-\bar{X}_{\mathbf{k}_2'}\} \tag{4.20}$$

where

$$\bar{X}_{\mathbf{k}_1}=(\bar{X}_1)_{\mathbf{k}_1\mathbf{k}_1}=X_{\mathbf{k}_1}[(1+\eta f_{\mathbf{k}_1}^0)f_{\mathbf{k}_1}^0]^{-1}$$

etc., and $\hat{t}_{12}^-(E)=\hat{t}_{12}^-(E;\lambda=0)$. Evidently, $\mathscr{B}_1$ represents the linearized quantum statistical Boltzmann collision operator with the full (exchange-

modified) cross section, as was first obtained by Boercker and Dufty.[9],[3] We point out that the $\hat{t}$-matrix and therefore the scattering cross section in $\mathscr{B}_1$ are now functionals of the Fermi or Bose distribution.

To obtain the final result for C, we return to Eq. (4.2) and write

$$C = \lim_{\varepsilon \to 0^+} \mathrm{Tr}_1 \, B_1 \frac{1}{(1/\mathscr{M}_1)[\varepsilon - \mathscr{D}_1(\varepsilon)]} A_1 \tag{4.21}$$

where

$$\mathscr{M}_1 = N \, \mathrm{Tr}_{2 \cdots N} P \left(1 + iPL_V \frac{1}{\varepsilon - i\bar{Q}L} \bar{Q} \right) f \sum_{i=1}^{N} \sigma_{1i} \tag{4.22}$$

Now, since $\mathscr{D}_1(\varepsilon) = \mathscr{B}_1(\varepsilon) + \mathrm{MC}$, it is obvious that in $\mathscr{M}_1$ only the terms involving one particle at most have to be retained in the binary collision approximation. Thus, the second term in the parentheses in $\mathscr{M}_1$ can be omitted in this approximation, because this term involves at least two particles due to the presence of L_V. In contrast to this, the first term in $\mathscr{M}_1$ contains a one-particle contribution, which we extract as follows. First we note that, with $f_{12} = f_1 f_2 + g_{12}$ and Eq. (2.5), $\mathrm{Tr}_2 f_{12} A_2$ reduces to $\mathrm{Tr}_2 g_{12} A_2$. Then, using the fact that only the cluster $g_{12}^0 = \pi_{12} f_1^0 f_2^0$ (which occurs in g_{12}) can contribute in the considered approximation, we find, with $\mathrm{Tr}_2 \pi_{12} = \eta$,

$$N \, \mathrm{Tr}_{2 \cdots N} Pf \sum_{i=1}^{N} A_i = P^1 A_1 f_1^0 (1 + \eta f_1^0) + \mathrm{BC} \tag{4.23}$$

and consequently

$$\mathscr{M}_1 A_1 = P^1 A_1 f_1^0 (1 + \eta f_1^0) + \mathrm{BC} \tag{4.24}$$

where BC contains the terms involving more than one particle. Therefore, the binary collision approximation of the time-integrated correlation function C finally reads

$$C = \lim_{\varepsilon \to 0^+} \mathrm{Tr}_1 \, B_1 \frac{1}{\varepsilon - \mathscr{B}_1} A_1 f_1^0 (1 + \eta f_1^0) + \mathrm{MC} \tag{4.25}$$

where now P^1 has been omitted because B_1 and f_1^0 are diagonal.

We conclude this section with some remarks. As is evident from the above derivation, the presence of the permutation operator $\pi^{1 \cdots s}$ makes the explicit evaluation of $\bar{G}_{1 \ldots s}$ more complicated in comparison to the

[3] For a discussion of this $\hat{t}$-matrix see also ref. 10.

semiclassical case. There, the derivation of the linearized Boltzmann collision operator is quite straightforward, because only G_{12} must be taken into account, as one can see, e.g., from Eq. (4.11). In the quantum statistical case, however, one has to resum all two-particle contributions contained in $\bar{G}_{12}$, $\bar{G}_{123}$, etc., in order to obtain the full cross section, which, as a consequence of this resummation, is now a functional of the reduced distribution operator f_i^0. Despite this complication, let us point out, however, that the above result, Eq. (4.22), has been obtained in a direct and clear manner, being a great advantage of the formalism developed here. Due to this fact, it is possible to discuss the triple, quadruple, etc., collision terms (coming from the dynamical part) in an analogous way, as will be shown in a subsequent work.

Finally, we remark that in the course of the above derivation the Boltzmann collision operator $\mathscr{B}_1^{\lambda}$ has been obtained [see Eq. (4.16)]. This suggests that similar methods, leading to the inversion formula (3.44), can be used to derive the nonlinear quantum statistical Boltzmann equation (Uehling–Uhlenbeck equation[17] with degeneracy-modified t-matrix) in the binary collision approximation, and, moreover, the quantum statistical version of the Choh–Uhlenbeck equation in the triple collision approximation. This is indeed the case and will be demonstrated in a subsequent paper.

APPENDIX A

In this appendix we derive formula (3.45). For that purpose, let us go back to Eq. (3.24) and abbreviate its lhs by D. Then, using Eq. (3.42), we obtain

$$D = \frac{1}{N} \sum_{s=2}^{\infty} \mathrm{Tr}_{2\ldots s} P\bar{G}_{1\ldots s}\pi^{1\cdots s}P^{1\cdots s} \sum_{i=1}^{s} \sigma_{1i}\Phi_1 f_2 \cdots f_s \tag{A.1}$$

Next we replace Φ_1 by the identity

$$\Phi_1 = N\,\mathrm{Tr}_{2\ldots N} f \sum_{i=1}^{N} \sigma_{1i} f_1^{-1}\bar{\Phi}_1 = (\bar{\Phi}_1 + \mathrm{Tr}_k f_{1k} f_k^{-1}\bar{\Phi}_k), \qquad k > 1 \tag{A.2}$$

where

$$\bar{\Phi}_1 = \left(N\,\mathrm{Tr}_{2\ldots N} f \sum_{i=1}^{N} \sigma_{1i} f_1^{-1} \right)^{-1} \Phi_1 \tag{A.3}$$

This leads to

$$D = \frac{1}{N} \sum_{s=2}^{\infty} \mathrm{Tr}_{2\ldots s} P\bar{G}_{1\ldots s}\pi^{1\cdots s}P^{1\cdots s} \left(f_{1\ldots s} \sum_{i=1}^{s} f_i^{-1}\bar{\Phi}_i + \sum_{i=1}^{s} \sigma_{1i} f_{2\ldots s}\,\mathrm{Tr}_k f_{1k} f_k^{-1}\bar{\Phi}_k \right), \qquad k > s \tag{A.4}$$

where we have used the fact that $Pf_1 \cdots f_s = Pf_{1\ldots s}[1 + O(1/\Omega)]$. (only the leading terms for $\Omega \to \infty$ are retained). Now we transform the second term in the parentheses in Eq. (A.4), which we abbreviate by ② for the moment. Since $f_{ik} = f_i f_k + g_{ik}$ and $\mathrm{Tr}_k \bar{\Phi}_k = 0$ (see below), we find

$$② = P \,\mathrm{Tr}_k \sum_{i=1}^{s} \sigma_{1i} f_{2\ldots s} g_{1k} f_k^{-1} \bar{\Phi}_k \tag{A.5}$$

Further, taking account of the cluster expansion (3.31), it is not difficult to see that

$$P\left(f_{1\ldots s} f_k + \sum_{i=1}^{s} \sigma_{1i} f_{2\ldots s} g_{1k} \right) = Pf_{1\ldots sk}[1 + O(1/\Omega)] \tag{A.6}$$

Hence,

$$② = P \,\mathrm{Tr}_k \, f_{1\ldots sk} f_k^{-1} \bar{\Phi}_k \tag{A.7}$$

Inserting this result back into Eq. (A.4), one gets, with Eq. (3.12),

$$D = \frac{1}{N} \mathrm{Tr}_{2\ldots N} P \sum_{s=2}^{\infty} \frac{N!}{(N-s)!} \bar{G}_{1\ldots s} \bar{P}^{1\cdots s} f \sum_{i=1}^{N} \sigma_{1i} f_1^{-1} \bar{\Phi}_1 \tag{A.8}$$

where we have used $\pi_\sigma^{-1} f = f$. Replacing $\bar{P}^{1\cdots s}$ by $\bar{P}(1 \cdots s)$ and using the identity $P^{s+1\cdots N} \bar{P}(1 \cdots s) = P^{s+1\cdots N} \bar{P}$, we see that the sum in (A.8) can be performed to yield

$$D = \mathrm{Tr}_{2\ldots N} PiL_V \frac{1}{\varepsilon - i\bar{Q}L} \bar{P} f \sum_{i=1}^{N} \sigma_{1i} f_1^{-1} \bar{\Phi}_1 \tag{A.9}$$

Substituting the foregoing result into Eq. (3.21) and solving for $N^{-1}\Phi_1(\varepsilon)$, one finally arrives at formula (3.45).

To complete the derivation, we eventually show that $\mathrm{Tr}_k \bar{\Phi}_k = 0$. Making use of the identity (3.4), one finds from Eq. (A.3)

$$\mathrm{Tr}_k \bar{\Phi}_k = \mathrm{Tr}_k \Phi_k - \mathrm{Tr}_{kl} f_{kl} f_l^{-1} \sigma_{kl} (1 + \mathrm{Tr}_j f_{kj} f_j^{-1} \sigma_{kj})^{-1} \Phi_k \tag{A.10}$$

The first term vanishes due to Eqs. (3.22) and (2.5). The second term can be transformed to give $(N-1)\,\mathrm{Tr}_k \bar{\Phi}_k$, which immediately leads to the desired result.

APPENDIX B

In this appendix we derive Eq. (3.46). To begin with, we note the obvious relations

$$L(1 \cdots s)\, \pi^{1\cdots s} A = \pi^{1\cdots s} L(1 \cdots s)\, A$$

and

$$\sum_{i=1}^{s-1} L_{is}\pi^{1\cdots s-1}A = \pi^{1\cdots s-1}\sum_{i=1}^{s-1} L_{is}A$$

for a symmetric operator A. With

$$\bar{Q}(1\cdots s)\,\pi^{1\cdots s} = \pi^{1\cdots s}\bar{Q}(1\cdots s)$$

and Eq. (2.16) one then finds for $\bar{G}_{1\ldots s}$ given in Eq. (3.25)

$$\begin{aligned}\bar{G}_{1\ldots s}&\pi^{1\cdots s}A\\ &= i\bar{L}_{12}\frac{1}{\varepsilon - i\bar{Q}^{12}L(12)}\,i\bar{Q}^{12}(L_{13}+L_{23})(1+\pi_{13}+\pi_{23})\frac{1}{\varepsilon - i\bar{Q}^{123}L(123)}\\ &\quad\cdots\frac{1}{\varepsilon - i\bar{Q}^{1\cdots s-1}L(1\cdots s-1)}\,i\bar{Q}^{1\cdots s-1}(L_{1s}+\cdots+L_{s-1s})\\ &\quad\times(1+\pi_{1s}+\cdots+\pi_{s-1s})\frac{1}{\varepsilon - i\bar{Q}^{1\cdots s}L(1\cdots s)}\end{aligned}\tag{B.1}$$

where $\bar{L}_{12}$ is defined in Eq. (3.47). Replacing in the denominators of the foregoing expression all $\bar{Q}^{1\cdots s}$ by $1-\bar{P}^{1\cdots s}$, we see that these $\bar{Q}$'s can be replaced by 1 for $\Omega\to\infty$ due to the P_q-rule[1] (the presence of π_σ in $\bar{P}^{1\cdots s}$ has no influence). The $\bar{Q}$'s in the numerator can be transformed as follows. First we note that

$$\pi^{1\cdots s-1}\bar{Q}^{1\cdots s-1} = \pi^{1\cdots s-1}(1-P^{1\cdots s-1}\pi^{1\cdots s-1})$$

Since in (B.1) to the left of $\bar{Q}^{1\cdots s-1}$ the particles $1,\ldots,s-1$ are connected by L_{ij}, $P^{1\cdots s-1}\pi^{1\cdots s-1}$ can be replaced by $P^{1\cdots s-1}+O(\Omega^{-1})$ again due to the P_q-rule [note that $\pi_{ij}^{\mathrm{ph}} = (2\pi)^3\,\delta(\mathbf{p}_i-\mathbf{p}_j)\,\delta(\mathbf{x}_i-\mathbf{x}_j)$ and therefore, e.g., $(P^{ij}\pi_{ij})^{\mathrm{ph}}\sim\Omega^{-1}$]. Hence $\bar{Q}^{1\cdots s-1}$ can be replaced by $Q^{1\cdots s-1}$ for $\Omega\to\infty$. Proceeding in this way from the right to the left in (B.1), we see that the $\bar{Q}$'s in the numerator may be replaced by Q.

Finally, using the relation

$$(L_{13}\pi_{23}+L_{23}\pi_{13})\,A = \bar{L}_{12,3}A\tag{B.2}$$

where $\bar{L}_{12,3}$ is defined in Eq. (3.48), one easily proves by induction

$$\sum_{i=1}^{s-1} L_{is}\left(1+\sum_{i=1}^{s-1}\pi_{is}\right)A = \left(\sum_{i=1}^{s-1}\bar{L}_{is}+\sum_{i<j}^{s-1}\bar{L}_{ij,s}\right)A,\quad s\geqslant 2\tag{B.3}$$

Insertion of (B.3) into Eq. (B.1) immediately yields Eq. (3.46).

APPENDIX C

In this appendix we derive formula (3.55). Due to the definition (3.12), $f_1^0 \equiv f_1^0[N]$ reads

$$f_1^0[N] = \frac{N}{Z_N^0} \operatorname{Tr}_{[N-1]} \pi[N]\, e^{-\beta H_0[N]} \tag{C.1}$$

where $[N-i\cdots j] = \{1,..., N\}\backslash\{i,..., j\}$, $\pi[N] = (1/N!)\,\pi^{1\cdots N}$, $H_0[N] = H_0(1\cdots N)$, and

$$Z_N^0 = \operatorname{Tr}_{[N]} \pi[N]\, e^{-\beta H_0[N]} \tag{C.2}$$

Next we note that $\pi[N]$ can be represented as

$$\pi[N] = \frac{1}{N}(1 + \pi_{12} + \cdots \pi_{1N})\,\pi[N-1] \tag{C.3}$$

where

$$\pi[N-1] = \frac{1}{(N-1)!}\,\pi^{2\cdots N}$$

Insertion of Eq. (C.3) into Eq. (C.1) then yields

$$f_1^0[N] = \frac{1}{Z_N^0}\{\operatorname{Tr}_{[N-1]} \pi[N-1]\, e^{-\beta H_0[N-1]} e^{-\beta H_0(1)} + (N-1)\operatorname{Tr}_{[N-1]} \pi_{12}\pi[N-1]\, e^{-\beta H_0[N]}\} \tag{C.4}$$

The first term in the braces is equal to $Z_{N-1}^0 e^{-\beta H_0(1)}$. Then, by using the identities

$$\pi_{12}\pi[N-1] = \pi[N-2]\,\pi_{12}, \qquad \pi_{12} e^{-\beta H_0[N]} = e^{-\beta H_0[N-2]} \pi_{12} e^{-\beta H_0(1)}$$

and $\operatorname{Tr}_2 \pi_{12} = \eta$, one immediately finds for the second term

$$\eta(N-1)\operatorname{Tr}_{[N-12]} \pi[N-2]\, e^{-\beta H_0[N-2]} e^{-\beta H_0(1)} \tag{C.5}$$

which, due to (C.1), is equal to

$$\eta Z_{N-1}^0 f_1^0[N-1]\, e^{-\beta H_0(1)} \tag{C.6}$$

Hence, we have

$$f_1^0[N] = \frac{Z_{N-1}^0}{Z_N^0}\, e^{-\beta H_0(1)}(1 + \eta f_1^0[N-1]) \tag{C.7}$$

Adding and subtracting the term $\eta f_1^0[N]$ in the parentheses and then solving the resulting equation for $f_1^0[N]$, one finally arrives at formula (3.55).

APPENDIX D

In this last appendix we express the Liouville T-matrix $\hat{T}_{12}^{\lambda}$ (in the following we suppress the explicit indication of the λ dependence) by ordinary Hilbert-space t-matrices and derive Eq. (4.16). The following treatment generalizes the one given in Appendix A of I. We start by introducing some abbreviations:

$$\hat{L} = \hat{L}(12) \tag{D.1}$$

$$\hat{H} = H_0 + SV_{12}, \qquad H_0 = H_0(12) \tag{D.2}$$

$$S = 1 + \eta \tilde{f}_1^0 + \eta \tilde{f}_2^0 \tag{D.3}$$

Since $(\tilde{f}_1^0)^+ = \tilde{f}_1^0$, one has $\hat{H}^+ = H_0 + V_{12}S$. Now we note the identity

$$[\exp(i\hat{L}t)]\, A = [\exp(i\hat{H}t)]\, A \exp(-i\hat{H}^+ t) \tag{D.4}$$

which is easily established by showing that both sides obey the same differential equation (the initial values are obviously equal). It then follows that

$$\frac{1}{2\varepsilon - i\hat{L}} A = \int_0^\infty dt\, [\exp(-2\varepsilon t) \exp(i\hat{H}t)]\, A \exp(-i\hat{H}^+ t) \tag{D.5}$$

Making use of the relations

$$e^{-2\varepsilon t} = e^{-\varepsilon t} \int_0^\infty dt'\, \delta(t - t')\, e^{-\varepsilon t'}, \qquad t > 0 \tag{D.6}$$

and

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE\, e^{-iEt} \tag{D.7}$$

one finds

$$\frac{1}{2\varepsilon - i\hat{L}} A = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE \frac{1}{\varepsilon - i(\hat{H} - E)} A \frac{1}{\varepsilon + i(\hat{H}^+ - E)} \tag{D.8}$$

Then, introducing the exchange-modified Hilbert-space t-matrix,

$$\hat{t}_{12}^{-}(E^-) = V_{12} \frac{1}{\varepsilon - i(\hat{H} - E)} [\varepsilon - i(H_0 - E)] \tag{D.9}$$

where $E^{\pm} = E \pm i\varepsilon$, one obtains (after one iteration)

$$\frac{1}{\varepsilon - i(\hat{H} - E)} = \left[1 + \frac{1}{\varepsilon - i(H_0 - E)} iS\hat{t}_{12}^{-}(E^{-})\right] \frac{1}{\varepsilon - i(H_0 - E)} \tag{D.10}$$

and

$$\frac{1}{\varepsilon + i(\hat{H}^{+} - E)} = \frac{1}{\varepsilon + i(H_0 - E)} \left[1 - \hat{t}_{12}^{+}(E^{+})\, iS \frac{1}{\varepsilon + i(H_0 - E)}\right] \tag{D.11}$$

where

$$\hat{t}_{12}^{+}(E^{+}) = [\hat{t}_{12}^{-}(E^{-})]^{+} \tag{D.12}$$

Thus, it follows from Eq. (D.8) that

$$\begin{aligned} L_{12} \frac{1}{2\varepsilon - i\hat{L}} A = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE \\ \times \left\{ \hat{t}_{12}^{-}(E^{-}) \frac{1}{\varepsilon - i(H_0 - E)} A \frac{1}{\varepsilon + i(H_0 - E)} \right. \\ \times \left[1 - \hat{t}_{12}^{+}(E^{+})\, iS \frac{1}{\varepsilon + i(H_0 - E)}\right] \\ - \left[1 + \frac{1}{\varepsilon - i(H_0 - E)} iS\hat{t}_{12}^{-}(E^{-})\right] \\ \left. \times \frac{1}{\varepsilon - i(H_0 - E)} A \frac{1}{\varepsilon + i(H_0 - E)} \hat{t}_{12}^{+}(E^{+}) \right\} \end{aligned} \tag{D.13}$$

Then, for $A = P^{12}B$, one finds

$$\begin{aligned} \lim_{\varepsilon \to 0^{+}} P^{12} L_{12} \frac{2\varepsilon}{2\varepsilon - i\hat{L}} P^{12} B \\ = 2\pi \int_{-\infty}^{\infty} dE\, P^{12} \\ \times \left\{ [\hat{t}_{12}^{-}(E) - \hat{t}_{12}^{+}(E)] \frac{1}{2\pi} \delta(H_0 - E)\, P^{12} B \right. \\ \left. - \hat{t}_{12}^{-}(E)\, \delta(H_0 - E)(P^{12} B)\, \hat{t}_{12}^{+}(E)\, iS\, \delta(H_0 - E) \right\} \end{aligned} \tag{D.14}$$

where $\hat{t}_{12}^{\pm}(E) = \lim_{\varepsilon \to 0^{+}} \hat{t}_{12}^{\pm}(E \pm i\varepsilon)$. Next, we note that

$$\begin{aligned} \hat{t}_{12}^{-}(E^{-}) - \hat{t}_{12}^{+}(E^{+}) = V_{12} \left(1 + \frac{1}{\varepsilon - i(\hat{H} - E)} iSV_{12}\right) \\ - \left(1 - iS \frac{1}{\varepsilon + i(\hat{H}^{+} - E)}\right) V_{12} \end{aligned} \tag{D.15}$$

from which the generalized optical theorem follows {note that $iS[\varepsilon + i(\hat{H}^+ - E)]^{-1} = [\varepsilon + i(\hat{H} - E)]^{-1} iS$}, i.e.,

$$\hat{t}_{12}^-(E^-) - \hat{t}_{12}^+(E^+) = \hat{t}_{12}^-(E^-)\, iS \frac{2\varepsilon}{\varepsilon^2 + (H_0 - E)^2}\, \hat{t}_{12}^+(E^+) \tag{D.16}$$

Therefore, Eq. (D.14) reduces to

$$\begin{aligned} &\lim_{\varepsilon \to 0^+} P^{12} L_{12} \frac{1}{2\varepsilon - i\hat{L}} P^{12} B \\ &\quad = -2\pi i \int_{-\infty}^{\infty} dE\, P^{12} \hat{t}_{12}^-(E)\, \delta(H_0 - E) \\ &\qquad \times \{(P^{12}B)\, \hat{t}_{12}^+(E)\, S - S\hat{t}_{12}^+(E)(P^{12}B)\}\, \delta(H_0 - E) \end{aligned} \tag{D.17}$$

Now, setting $B = \bar{f}_1^0 \bar{f}_2^0$ and noting that $S = (1 + \eta \bar{f}_1^0)(1 + \eta \bar{f}_2^0) - \bar{f}_1^0 \bar{f}_2^0$, we arrive at

$$\begin{aligned} &\lim_{\varepsilon \to 0^+} iP^{12} L_{12} \frac{2\varepsilon}{2\varepsilon - i\hat{L}} P^{12} \bar{f}_1^0 \bar{f}_2^0 \\ &\quad = 2\pi \int_{-\infty}^{\infty} dE\, P^{12} \hat{t}_{12}^-(E)\, \delta(H_0 - E) \\ &\qquad \times \{\bar{f}_1^0 \bar{f}_2^0 \hat{t}_{12}^+(E)(1 + \eta \bar{f}_1^0)(1 + \eta \bar{f}_2^0) \\ &\qquad - (1 + \eta \bar{f}_1^0)(1 + \eta \bar{f}_2^0)\, \hat{t}_{12}^+(E)\, \bar{f}_1^0 \bar{f}_2^0\}\, \delta(H_0 - E) \end{aligned} \tag{D.18}$$

Finally, to obtain $P^{12}\hat{T}_{12}P^{12}$, we note that the same derivation leading to Eq. (D.18) goes through if we replace V_{12} by $V_{12}(1 + \pi_{12})/2$. Since $[\frac{1}{2}(1 + \pi_{12})]^n = \frac{1}{2}(1 + \pi_{12})$ for all $n \geqslant 1$, we see that in Eq. (D.18), $\hat{t}_{12}^+$ has to be replaced by $\hat{t}_{12}^+(1 + \pi_{12})/2$. Therefore, by taking matrix elements of (D.18) and using that $(\hat{t}_{12}^+)^+ = \hat{t}_{12}^-$, we obtain

$$\begin{aligned} &\lim_{\varepsilon \to 0^+} (P^{12}\hat{T}_{12}P^{12}\bar{f}_1^0 \bar{f}_2^0)_{\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_1\mathbf{k}_2} \\ &\quad = 4\pi \sum_{\mathbf{k}_1',\mathbf{k}_2'} \left| [\hat{t}_{12}^-(\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2}) \frac{1}{2}(1 + \pi_{12})]_{\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_1'\mathbf{k}_2'} \right|^2 \\ &\qquad \times \delta(\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_1'} - \varepsilon_{\mathbf{k}_2'}) \{\bar{f}_{\mathbf{k}_1'}^0 \bar{f}_{\mathbf{k}_2'}^0 (1 + \eta \bar{f}_{\mathbf{k}_1}^0)(1 + \eta \bar{f}_{\mathbf{k}_2}^0) \\ &\qquad - (1 + \eta \bar{f}_{\mathbf{k}_1'}^0)(1 + \eta \hat{f}_{\mathbf{k}_2'}^0)\, \hat{f}_{\mathbf{k}_1}^0 \bar{f}_{\mathbf{k}_2}^0\} \end{aligned} \tag{D.19}$$

which immediately leads to Eq. (4.16).

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