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The Inverse Conjecture for the Revised Enskog Equation

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It is shown that the pair correlation function (which is by definition the high-density factor in the revised Enskog theory) is not always a well-defined functional of the local density. Moreover, for a finite system with periodic boundary conditions and in the space homogeneous case, this function, computed at the contact value, is bounded at the maximum allowed density (i.e., a density $n_{\max}$ such that, in one dimension, $1/a - 1/L \leqslant n_{\max} < 1/a$; equality sign, which corresponds to the usual close-packing density for which L/a is an integer, being included as a particular case). At least for the one-dimensional gas model this finite value is shown to approach infinity in the thermodynamic and in the hydrodynamic limits. A new form for the revised Enskog equation, which does not depend on the inverse conjecture, is finally given.

KEY WORDS: Kinetic theory; Enskog equation; dense gases; inverse problem; close-packing density.

1. INTRODUCTION

It is well known[1,2] that the Boltzmann equation (BE) provides a successful description of gases as long as the proper volume of the molecules is very small, but that it ceases to be valid in the case of dense systems.

The first attempt to generalize Boltzmann-like arguments to higher densities is due to Enskog,[3] who proposed in 1921 a kinetic equation (SEE) for the one-particle distribution function in a dense gas of hard spheres. Two effects were taken into account: first, the *covolume* effect increasing the collision frequency, and second the *collisional transfer* leading to an instantaneous flow of significant interest in transport phenomena.

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Van Beijeren and Ernst[4] showed that Enskog's procedure has to be modified in order to obtain results which are not in conflict with irreversible thermodynamics (in fact, the Onsager symmetry relations do not hold for the SEE): an H-theorem for this revised Enskog equation (REE) was derived by Résibois[5,6] and an analogous theorem for a dense gas of rough spheres was obtained by Cercignani and Lampis[7]; the REE was also shown[8,9] to admit a local H-theorem. Recently several existence theorems for the Enskog equation (EE) under several assumptions on the high-density factor have been given.[10–16] None of them applies to the REE as first derived by Van Beijeren and Ernst and indeed it appears that a rigorous analysis of the high-density factor is required before a theorem for the latter equation can be obtained.

The aim of this paper is to study some mathematical assumptions underlying the high-density factor for the REE: in particular, the so-called *inverse conjecture*,[17,18] which may fail for a system of hard spheres. As a consequence of this, in Section 3 it is noticed that the high-density factor is not always a well-defined functional of the local density.

Another quite separate problem here examined is the following. Mathematical results on the EE which are available in the literature distinguish, in a sense, between the finiteness[5,10,11,16] and the infiniteness[12,15,16] of the external system in which the gas is confined. However, in both cases the high-density factor is implicitly assumed to be a monotone increasing function (resp., functional in RET) of the local density, becoming infinity at the close-packing density. The validity of this second conjecture for the REE is also examined in Section 3. In particular, for a finite system with periodic boundary conditions and in the space homogeneous case, it is shown that the high-density factor is bounded at the maximum allowed density (i.e., a density $n_{\max}$ such that, in one dimension, $1/a - 1/L \leqslant n_{\max} < 1/a$; equality sign, which corresponds to the usual close-packing density for which L/a is an integer, being included as a particular case). At least for the one-dimensional gas model this finite value is shown to approach infinity in the thermodynamic and hydrodynamic limits. This is done in Section 4.

A new form for the REE (which does not depend on the *inverse conjecture*) and a few open questions raised by our analysis are finally discussed in Section 5.

2. THE REVISED ENSKOG EQUATION

The SEE describes the time evolution of the one-particle distribution function $f_1(\mathbf{r}_1, \mathbf{v}_1; t)$:

$$f_1(\mathbf{r}_1, \mathbf{v}_1; t): \quad \Lambda \times R^3 \times R_+ \to R_+ \tag{2.1}$$

which gives at time t the number density of particles at point $\mathbf{r}_1$ with velocity $\mathbf{v}_1$. Here Λ is a measurable subset of R^3 representing the external volume in which the gas is confined: as previously said, Λ may be R^3 itself as well as a proper (bounded or unbounded) subset of R^3.

The above-mentioned equation is written

$$\frac{\partial f_1}{\partial t}+\mathbf{v}_1\cdot\frac{\partial f_1}{\partial \mathbf{r}_1}+\mathbf{F}\cdot\frac{\partial f_1}{\partial \mathbf{v}_1}=J^{\mathrm{E}}(f_1, f_1) \tag{2.2}$$

where $\mathbf{F}$ is the external force per unit mass, assumed to be such that $(\partial/\partial\mathbf{v})\cdot\mathbf{F}=0$, and J^{E} is the collision operator, which differs from Boltzmann's in two respects: first, because it takes into account that the centers of the molecules are, at a collision, at a distance of a sphere diameter and second, because the frequencies of these collisions are modified by the covolume effect.

Within Enskog's procedure we have for J^{E}

$$\begin{aligned} J^{\mathrm{E}}(f_1, f_1)=a^2\int_{R^3\times S^2} & d\mathbf{v}_2\, d^2\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12})\,\Theta(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12}) \\ & \times\left\{Y\left[n\left(\mathbf{r}_1-\frac{1}{2}a\boldsymbol{\varepsilon}; t\right)\right] f_1(\mathbf{r}_1, \mathbf{v}_1'; t)\, f_1(\mathbf{r}_1-a\boldsymbol{\varepsilon}, \mathbf{v}_2'; t)\right. \\ & \left. -Y\left[n\left(\mathbf{r}_1+\frac{1}{2}a\boldsymbol{\varepsilon}; t\right)\right] f_1(\mathbf{r}_1, \mathbf{v}_1; t)\, f_1(\mathbf{r}_1+a\boldsymbol{\varepsilon}, \mathbf{v}_2; t)\right\} \end{aligned} \tag{2.3}$$

Here a denotes the hard-sphere diameter; Θ is the Heaviside step function; $\boldsymbol{\varepsilon}$ is a unit vector, directed as the apsidal line, ranging over the unit sphere S^2 in R^3, or rather, because of the Heaviside function, over a half of such a sphere; $\mathbf{v}_{12}=\mathbf{v}_1-\mathbf{v}_2$, $\mathbf{v}_1'$ and $\mathbf{v}_2'$ are the velocities after the collision:

$$\mathbf{v}_1'=\mathbf{v}_1-\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12}), \qquad \mathbf{v}_2'=\mathbf{v}_2+\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12}) \tag{2.4}$$

and Y, the so-called high-density factor, is a function of the local density [see Eq. (2.22)], calculated at the contact points $\mathbf{r}_1\pm\frac{1}{2}a\boldsymbol{\varepsilon}$: in particular, Y is *assumed* to be equal to unity for a rare gas, and to increase with increasing density, becoming infinity as the density approaches its close-packing value.[19]

The original mathematical model due to Enskog was afterward modified by replacing the function Y with the correct pair distribution function g_2 defined as a functional of the local density as in a nonuniform equilibrium state[4]; the result is a new collision operator given by

$$J^{E}(f_1, f_1) = a^2 \int_{R^3 \times S^2} d\mathbf{v}_2\, d^2\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12})\,\Theta(\boldsymbol{\varepsilon}\cdot\mathbf{v}_{12})$$
$$\times [g_2(\mathbf{r}_1, \mathbf{r}_1 - a\boldsymbol{\varepsilon} \mid n(t))\, f_1(\mathbf{r}_1, \mathbf{v}_1'; t)\, f_1(\mathbf{r}_1 - a\boldsymbol{\varepsilon}, \mathbf{v}_2'; t)$$
$$- g_2(\mathbf{r}_1, \mathbf{r}_1 + a\boldsymbol{\varepsilon} \mid n(t))\, f_1(\mathbf{r}_1, \mathbf{v}_1; t)\, f_1(\mathbf{r}_1 + a\boldsymbol{\varepsilon}, \mathbf{v}_2; t)] \quad (2.5)$$

In this section we describe, following Résibois' paper,[5] the derivation of the revised Enskog collision operator as given by Eq. (2.5), with the help of two assumptions: a physical one on the N-particle time-dependent distribution function [see Eq. (2.6)] and a mathematical one on the inversion of a functional equation [see Eqs. (2.21) and (2.23)].

Concerning the first assumption, the hypothesis is made that, at all times, the reduced distribution functions of the system can be calculated from the following (grand canonical) distribution function:

$$\rho_N(t) = \frac{1}{N!} \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=1}^{N} W_i(t)/\Xi(t) \quad (2.6)$$

where the normalization factor $\Xi(t)$ is given by

$$\Xi(t) = \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\Lambda^N \times R^{3N}} d\Gamma^N \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=1}^{N} W_i(t) \quad (2.7)$$

Here Λ^N is the Cartesian product of N copies of Λ and the following notations have been introduced:

$$\Theta_{ij} = \Theta(r_{ij} - a), \qquad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \quad (2.8)$$

$$W_i(t) = W(\mathbf{r}_i, \mathbf{v}_i; t) \quad (2.9)$$

$$d\Gamma^{N-n} = d\mathbf{r}_{n+1} \cdots d\mathbf{r}_N\, d\mathbf{v}_{n+1} \cdots d\mathbf{v}_N \quad (2.10)$$

Conventionally, empty products in Eq. (2.7) are replaced by 1 and no integration is performed if $d\Gamma^N$ reduces to $d\Gamma^0$.

The function W generates the reduced particle distribution functions according to the rule

$$f_n(\mathbf{r}_1,..., \mathbf{r}_n, \mathbf{v}_1,..., \mathbf{v}_n; t) = \sum_{N=n}^{\infty} \frac{N!}{(N-n)!} \int_{\Lambda^{N-n} \times R^{3(N-n)}} d\Gamma^{N-n}\, \rho_N(t) \quad (2.11)$$

It is worth noting that we have not yet defined the function $W(\mathbf{r}, \mathbf{v}; t)$: this is done by considering Eq. (2.11) for $n = 1$,

$$f_1(\mathbf{r}_1, \mathbf{v}_1; t) \equiv f_1(\mathbf{r}_1 \mid W(t)) \quad (2.12)$$

and by *assuming* that this equation can be inverted to express W as a functional[2] of f_1: the validity of this conjecture is examined in Section 3.

However, to ensure that the approximate ρ_N is a probability density, we have at least to require W as nonnegative. As a consequence, we have

$$1 + \|W(t)\|_1 \leqslant \Xi(t) \leqslant \exp \|W(t)\|_1 \tag{2.13}$$

$$\|f_n(t)\|_1 \leqslant (\|W(t)\|_1)^n \tag{2.14}$$

Here for any arbitrary measurable function $h(\mathbf{r}_{n+1},..., \mathbf{r}_N, \mathbf{v}_{n+1},..., \mathbf{v}_N; t)$ we put

$$\|h(t)\|_1 = \int_{\Lambda^{N-n} \times R^{3(N-n)}} d\Gamma^{N-n} \, |h(\mathbf{r}_{n+1},..., \mathbf{r}_N, \mathbf{v}_{n+1},..., \mathbf{v}_N; t)| \tag{2.15}$$

and we say that $h(t) \in L^1_+(\Lambda^{N-n} \times R^{3(N-n)}, d\Gamma^{N-n})$ provided that h is, for any t, a measurable and nonnegative function such that $\|h(t)\|_1 < \infty$ (those h's which are equal almost everywhere are of course identified).

Equations (2.13) and (2.14) and the condition $W \geqslant 0$ now give

$$W(t) \in L^1_+(\Lambda \times R^3, d\Gamma) \Leftrightarrow 1 \leqslant \Xi(t) < \infty \tag{2.16}$$

$$W(t) \in L^1_+(\Lambda \times R^3, d\Gamma) \Rightarrow f_n(t) \in L^1_+(\Lambda^n \times R^{3n}, d\Gamma^n) \tag{2.17}$$

For this reason we require, in addition, that $W(t) \in L^1_+(\Lambda \times R^3, d\Gamma)$ and we consider Eq. (2.12) as a map of $L^1_+(\Lambda \times R^3, d\Gamma)$ in $L^1_+(\Lambda \times R^3, d\Gamma)$.

It is also convenient to define the quantity

$$b_n(\mathbf{r}_1,..., \mathbf{r}_n \,|\, z(t)) = \left\{ \sum_{N=n}^{\infty} \frac{1}{(N-n)!} \int_{\Lambda^{N-n} \times R^{3(N-n)}} d\Gamma^{N-n} \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=n+1}^{N} W_i(t) \right\} \Big/ \Xi(t) \tag{2.18}$$

where the notation explicitly takes into account that b_n depends functionally on W only through its spatial part $z(\mathbf{r}; t)$ defined by

$$z(\mathbf{r}; t) = \int_{R^3} W(\mathbf{r}, \mathbf{v}; t) \, d\mathbf{v} \tag{2.19}$$

A simple calculation shows that

$$b_n(\mathbf{r}_1,..., \mathbf{r}_n \,|\, z(t)) \leqslant 1 \tag{2.20}$$

We can then rewrite Eq. (2.12) as

$$f_1(\mathbf{r}_1, \mathbf{v}_1 \,|\, W(t)) = W(\mathbf{r}_1, \mathbf{v}_1; t) \, b_1(\mathbf{r}_1 \,|\, z(t)) \tag{2.21}$$

[2] The quantity $f(x; t)$ depending functionally on $W(x; t)$ for all x is written $f(x \,|\, W(t))$.

and by integrating over $\mathbf{v}_1$ we find an analogous functional relation between z and the local density n defined by

$$n(\mathbf{r};t)=\int_{R^3} f_1(\mathbf{r},\mathbf{v};t)\,d\mathbf{v} \tag{2.22}$$

The relation under consideration gives n in terms of z:

$$n(\mathbf{r}_1\,|\,z(t))=z(\mathbf{r}_1;t)\,b_1(\mathbf{r}_1\,|\,z(t)) \tag{2.23}$$

and can also be regarded as a map of $L^1_+(\Lambda, d\mathbf{r}_1)$ in $L^1_+(\Lambda, d\mathbf{r}_1)$, which is *assumed*[5] to be invertible for *any arbitrary* density $n(t)\in L^1_+(\Lambda, d\mathbf{r}_1)$ to express, functionally, z in terms of n, i.e.,

$$z(\mathbf{r};t)\equiv z(\mathbf{r}\,|\,n(t)) \tag{2.24}$$

Taking now Eq. (2.11) for $n=2$ we have

$$f_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{v}_1,\mathbf{v}_2;t)=W(\mathbf{r}_1,\mathbf{v}_1;t)\,W(\mathbf{r}_2,\mathbf{v}_2;t)\,b_2(\mathbf{r}_1,\mathbf{r}_2\,|\,z(t)) \tag{2.25}$$

and combining this expression with Eq. (2.21), we get the closure relation

$$f_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{v}_1,\mathbf{v}_2;t)=g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t))\,f_1(\mathbf{r}_1,\mathbf{v}_1;t)\,f_1(\mathbf{r}_2,\mathbf{v}_2;t) \tag{2.26}$$

where g_2 is defined by

$$\begin{aligned} g_2(\mathbf{r}_1,\mathbf{r}_2\,|\,n(t)) &= \frac{f_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{v}_1,\mathbf{v}_2;t)}{f_1(\mathbf{r}_1,\mathbf{v}_1;t)\,f_1(\mathbf{r}_2,\mathbf{v}_2;t)} \\ &= \frac{b_2(\mathbf{r}_1,\mathbf{r}_2\,|\,z(t))}{b_1(\mathbf{r}_1\,|\,z(t))\,b_1(\mathbf{r}_2\,|\,z(t))} \end{aligned} \tag{2.27}$$

and g_2 is written as a functional of the local density if the *inverse conjecture*, that is, Eq. (2.24), is valid.

The collision operator given by Eq. (2.5) for the REE is now immediately obtained by inserting Eq. (2.26) into the first BBGKY hierarchy equation.

3. THE INVERSE CONJECTURE

Inspired essentially by Stell's methods[20] involving formal series expansions, the *inverse conjecture* for the REE has been always considered to be true.[4,5,7,15]

However, disregarding the dependence on time, $n(\mathbf{r};t)$ given by Eq. (2.23) is precisely the same as the equilibrium single-particle density of a system of hard spheres, under the influence of an external potential, and we know that, in this case, there are infinitely many densities such that the *inverse conjecture* fails.

In fact, keeping in mind the correspondence rule

$$\mathbf{r} \rightleftharpoons x \tag{3.1}$$

$$n(\mathbf{r}; t) \rightleftharpoons \varrho(x) \tag{3.2}$$

$$z(\mathbf{r}; t) \rightleftharpoons \exp[-U(x)] \tag{3.3}$$

we obtain[17]:

Theorem 3.1. For any density $n(\mathbf{r}; t) \in L^1_+(\Lambda, d\mathbf{r})$ (here time t is fixed) and for every set $B(\mathbf{s}; a/2)$ [where $B(\mathbf{s}; a/2)$ is the intersection of the external volume Λ in which the gas is confined with a ball of radius $a/2$ centered at $\mathbf{s} \in R^3$], a necessary condition for the existence of a function $z(\mathbf{r}; t) \in L^1_+(\Lambda, d\mathbf{r})$, such that Eq. (2.23) holds, is

$$\int_{B(\mathbf{s}; a/2)} n(\mathbf{r}; t)\, d\mathbf{r} \leqslant 1 \tag{3.4}$$

Remark. Equation (3.4) has a simple probabilistic interpretation: if a given particle is in $B(\mathbf{s}; a/2)$, then, with probability one, all other particles are excluded.

For H-stable systems in the grand canonical ensemble it has been also established[17,18] that:

(i) If $U(x)$ is a solution of the inverse problem, for a given $\varrho \in L^1_+(\Lambda, dx)$, and is such that $\Xi(U) < \infty$, then U is unique.

(ii) If ϱ is any admissible density (i.e., there exists a solution for the inverse problem for ϱ), then ϱ' is also admissible provided that $\|\varrho - \varrho'\|_1$ is sufficiently small.

In our case, because of Eqs. (2.16) and (2.17), we thus have:

Theorem 3.2. The map given by Eq. (2.23) is, for any t, injective from $L^1_+(\Lambda, d\mathbf{r})$ in $L^1_+(\Lambda, d\mathbf{r})$.

Theorem 3.3. The set of all admissible densities $n(\mathbf{r}; t)$ is, for any t, an open set in $L^1_+(\Lambda, d\mathbf{r})$ (in the strong topology induced by the norm).

In this section we first give a simple proof that the map $n \equiv n(\cdot \mid z)$ is locally surjective [see property (ii) with $n = 0$ and $z = 0$], but not globally, and then we study the same functional relation in the space homogeneous case.

Theorem 3.4. If $n(\mathbf{r};t)$ is in $L^1_+(\Lambda, d\mathbf{r})$ and if $\|n(t)\|_1 \leqslant 1/8e$, then there exists a unique $z(\mathbf{r};t)$ in $L^1_+(\Lambda, d\mathbf{r})$ such that Eq. (2.23) holds. (Here, as usual, $e = \sum_{k=0}^{\infty} 1/k!$.)

Proof. Let $n(\mathbf{r}_1;t) \in L^1_+(\Lambda, d\mathbf{r}_1)$, $\|n(t)\|_1 = R \leqslant 1/8e$ and $\varphi \equiv \varphi_n$: $L^1_+(\Lambda, d\mathbf{r}_1) \to L^1_+(\Lambda, d\mathbf{r}_1)$ defined by

$$\varphi(z(\mathbf{r}_1;t)) = \frac{n(\mathbf{r}_1;t)}{b_1(\mathbf{r}_1 \mid z(t))} \tag{3.5}$$

and put

$$S = \{z(\mathbf{r}_1;t) \colon \|z(t)\|_1 \leqslant M(R)\} \tag{3.6}$$

$$X = S \cap L^1_+(\Lambda, d\mathbf{r}_1) \tag{3.7}$$

where $M(R)$ is implicitly defined by $R = M/4e^{2M}$ in the assigned interval $0 \leqslant R \leqslant 1/8e$ (and M is such that $0 \leqslant M \leqslant 1/2$).

We prove the theorem by showing that φ is a contraction from the complete metric space[3] X in X.

If we define

$$h_1(\mathbf{r}_1 \mid z(t)) = \sum_{N=1}^{\infty} \frac{1}{(N-1)!} \int_{\Lambda^{N-1} \times R^{3(N-1)}} d\Gamma^{N-1} \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=2}^{N} W_i(t) \tag{3.8}$$

Eq. (2.18) gives

$$b_1(\mathbf{r}_1 \mid z(t)) = \frac{h_1(\mathbf{r}_1 \mid z(t))}{\Xi(t)} \tag{3.9}$$

Integrating now Eq. (3.5) over $\mathbf{r}_1$, we find, with the help of Eq. (2.13),

$$\|\varphi(z(t))\|_1 \leqslant \|n(t)\|_1 \, \Xi(t) \leqslant Re^M < Re^{2M} = M/4 < M \tag{3.10}$$

which shows that φ is a well-defined map of X in X.

Now we show that φ is a contraction:

$$\begin{aligned} |\varphi(z(t)) - \varphi(\tilde{z}(t))| &= n(\mathbf{r}_1;t) \left| \frac{\Xi(z(t))}{h_1(\mathbf{r}_1 \mid z(t))} - \frac{\Xi(\tilde{z}(t))}{h_1(\mathbf{r}_1 \mid \tilde{z}(t))} \right| \\ &= n(\mathbf{r}_1;t) \left| \frac{\Xi(z(t)) - \Xi(\tilde{z}(t))}{h_1(\mathbf{r}_1 \mid z(t))} \right. \\ &\quad \left. + \frac{\Xi(\tilde{z}(t))[h_1(\mathbf{r}_1 \mid \tilde{z}(t)) - h_1(\mathbf{r}_1 \mid z(t))]}{h_1(\mathbf{r}_1 \mid z(t)) \, h_1(\mathbf{r}_1 \mid \tilde{z}(t))} \right| \end{aligned} \tag{3.11}$$

[3] In fact X is a close subset of $L^1(\Lambda, d\mathbf{r}_1)$ in the strong topology.

making use of the inequalities

$$h_1(\mathbf{r}_1 \mid z(t)) \geqslant 1, \qquad h_1(\mathbf{r}_1 \mid \tilde{z}(t)) \geqslant 1 \tag{3.12}$$

$$\Xi(\tilde{z}(t)) \leqslant \exp \|\tilde{z}(t)\|_1 \leqslant e^M \tag{3.13}$$

and, as we will prove later,

$$|\Xi(z(t)) - \Xi(\tilde{z}(t))| \leqslant \|z(t) - \tilde{z}(t)\|_1 \frac{e^M}{M} \tag{3.14}$$

$$|h_1(\mathbf{r}_1 \mid \tilde{z}(t)) - h_1(\mathbf{r}_1 \mid z(t))| \leqslant \|z(t) - \tilde{z}(t)\|_1 \frac{e^M}{M} \tag{3.15}$$

we obtain

$$|\varphi(z(t)) - \varphi(\tilde{z}(t))| \leqslant n(\mathbf{r}_1; t) \; \|z(t) - \tilde{z}(t))\|_1 \frac{e^M + e^{2M}}{M} \tag{3.16}$$

so that integrating over $\mathbf{r}_1$ we arrive at the desired property:

$$\begin{aligned} \|\varphi(z(t)) - \varphi(\tilde{z}(t))\|_1 &\leqslant \frac{R(e^M + e^{2M})}{M} \|z(t) - \tilde{z}(t)\|_1 \\ &\leqslant \frac{1}{2} \|z(t) - \tilde{z}(t)\|_1 \end{aligned} \tag{3.17}$$

To complete the proof, we have only to prove Eqs. (3.14) and (3.15). By definition, we have

$$\begin{aligned} &|\Xi(z(t)) - \Xi(\tilde{z}(t))| \\ &\quad \leqslant \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\Lambda^N \times R^{3N}} d\Gamma^N \prod_{i>j}^{N} = \Theta_{ij} \left| \prod_{i=1}^{N} W_i(t) - \prod_{i=1}^{N} \tilde{W}_i(t) \right| \end{aligned} \tag{3.18}$$

then, recalling the elementary equality

$$\prod_{i=1}^{N} W_i - \prod_{i=1}^{N} \tilde{W}_i = \sum_{j=1}^{N} W_1 \cdots W_{j-1}(W_j - \tilde{W}_j) \, \tilde{W}_{j+1} \cdots \tilde{W}_N$$

(here $W_0 = \tilde{W}_{N+1} = 1$), we finally obtain[4]

$$\begin{aligned} |\Xi(z(t)) - \Xi(\tilde{z}(t))| &\leqslant \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{j=1}^{N} \|z(t) - \tilde{z}(t)\|_1 \, \|z(t)\|_1^{j-1} \, \|\tilde{z}(t)\|_1^{N-j} \\ &\leqslant \|z(t) - \tilde{z}(t)\|_1 \sum_{N=0}^{\infty} \frac{M^{N-1}}{N!} \\ &= \|z(t) - \tilde{z}(t)\|_1 \frac{e^M}{M} \quad \blacksquare \end{aligned} \tag{3.19}$$

[4] Equation (3.15) follows in the same manner.

Remark. It is possible to show[17] that the bound $1/8e$ may be replaced by 1 [for example, by increasing the Lipschitz constant in Eq. (3.17)] and that, although too limited to be of physical interest, the bound $\|n(t)\|_1 \leqslant 1$ is in a sense optimal: in fact, for any constant $C > 1$, there are infinitely many functions $n(\mathbf{r}; t)$ in $L^1_+(\Lambda, d\mathbf{r})$ with $\|n(t)\|_1 = C$ such that the functional inversion given by Eq. (2.23) is impossible [for example, all the functions in $L^1_+(\Lambda, d\mathbf{r})$ with $\|n(t)\|_1 = C$ and support in $B(\mathbf{s}; a/2)$, for which Eq. (3.4) does not hold]. We also remark that, up to now, we have only required Λ to be a measurable subset of R^3.

Let us now examine the space homogeneous case, i.e., the case in which $n(\mathbf{r}; t) \equiv n(t)$. First of all we notice that the condition $n(t) \in L^1_+(\Lambda, d\mathbf{r})$ now implies that the external system Λ is a measurable subset of R^3 with finite measure V; we think of the gas as confined in a box T^3 with periodic boundary conditions, which can be identified, after rescaling, with the usual three-dimensional torus R^3/Z^3. We also remark that $n(t)$ is a constant, due to mass conservation.

The main results we are going to prove are Theorem 3.7, concerning the inversion of Eq. (2.23), and Eq. (3.51) on the behavior of the pair correlation function g_2 when the density approaches its maximum allowed value.

Lemma 3.5. If, for a given t; $n(\mathbf{r}; t) \equiv n(t)$ and it is in $L^1_+(T^3, d\mathbf{r})$, then there exists an N' such that the series given by Eqs. (2.7), (2.11), and (2.18) are truncated at N'.

Proof. If we let $B = \frac{4}{3}\pi(a/2)^3$ be the measure of a single sphere and $N' = [V/B]$, then we easily obtain

$$\prod_{i>j=1}^{N} \Theta_{ij} \equiv 0 \qquad \forall N > N' \tag{3.20}$$

(Here, for $x \in R$, $[x]$ denotes the largest integer $< x$.) ∎

Remark. The same property is true for Résibois' H-function given by

$$H(t) = \sum_{N=0}^{\infty} \int_{T^{3N} \times R^{3N}} d\Gamma^N \rho_N(t) \ln[N! \rho_N(t)] \tag{3.21}$$

because the external system T^3 is explicitly considered to be *finite.*[5]

Lemma 3.6. There exists an $\tilde{N} \leqslant N'$ such that $\forall N > \tilde{N}$ we have

$$\alpha_N = 0 \tag{3.22}$$

$$\beta_{N-1}(\mathbf{r}_1) \equiv 0 \tag{3.23}$$

$$\eta_{N-2}(\mathbf{r}_1, \mathbf{r}_2) \equiv 0 \tag{3.24}$$

$\forall N \leqslant \tilde{N}$ we have

$$\alpha_N > 0 \tag{3.25}$$

$$\beta_{N-1}(\mathbf{r}_1) > 0 \tag{3.26}$$

$$\eta_{N-2}(\mathbf{r}_1, \mathbf{r}_2) \geqslant 0 \tag{3.27}$$

where the following notations have been introduced:

$$\alpha_N = \int_{T^{3N}} d\gamma^N \prod_{i>j=1}^{N} \Theta_{ij} \tag{3.28}$$

$$\beta_{N-1}(\mathbf{r}_1) = \int_{T^{3(N-1)}} d\gamma^{N-1} \prod_{i>j=1}^{N} \Theta_{ij} \tag{3.29}$$

$$\eta_{N-2}(\mathbf{r}_1, \mathbf{r}_2) = \int_{T^{3(N-2)}} d\gamma^{N-2} \prod_{i>j=1}^{N} \Theta_{ij} \tag{3.30}$$

$$d\gamma^{N-n} = d\mathbf{r}_{n+1} \cdots d\mathbf{r}_N \tag{3.31}$$

and $T^{3(N-n)}$ is the product of $N-n$ copies of T^3, i.e., the usual $3(N-n)$-dimensional torus.

Proof. First of all we notice that the boundary conditions and the translation invariance of the Lebesgue measure imply that

$$\beta_{N-1}(\mathbf{r}_1) \equiv \beta_{N-1} \tag{3.32}$$

$$\eta_{N-2}(\mathbf{r}_1, \mathbf{r}_2) \equiv \eta_{N-2}(|\mathbf{r}_1 - \mathbf{r}_2|) \tag{3.33}$$

Then we observe that

$$\alpha_{N+1} \leqslant V\alpha_N \qquad (N \geqslant 0) \tag{3.34}$$

$$\alpha_N = \int_{T^3} d\mathbf{r}_1\, \beta_{N-1} = V\beta_{N-1} \qquad (N \geqslant 1) \tag{3.35}$$

$$\beta_{N-1} = \int_{T^3} d\mathbf{r}_2\, \eta_{N-2}(|\mathbf{r}_1 - \mathbf{r}_2|) \qquad (N \geqslant 2) \tag{3.36}$$

Now if $\tilde{N}$ is the greatest integer such that $\alpha_{\tilde{N}} > 0$, we have, with the help of Eqs. (3.34)–(3.36), the required properties. ∎

Remark. We observe that Eq. (3.36) only implies

$$\eta_{N-2}(|\mathbf{r}_1 - \mathbf{r}_2|) = 0 \qquad \text{a.e.} \quad (\forall N > \tilde{N}) \tag{3.37}$$

However,

$$\eta_{N-2}(|\mathbf{r}_1-\mathbf{r}_2|)=\Theta_{21}\int_{\Delta^{N-2}} d\gamma^{N-2}\prod_{i>j=3}^{N}\Theta_{ij} \tag{3.38}$$

where Δ is the subset of T^3 defined by

$$\Delta\equiv\Delta(\mathbf{r}_1,\mathbf{r}_2)=\{\mathbf{r}\in T^3\colon |\mathbf{r}-\mathbf{r}_i|\geqslant a \quad \forall i=1,2\} \tag{3.39}$$

Now if we prove that the function $\eta_{N-2}(|\mathbf{r}_1-\mathbf{r}_2|)$ is continuous (and decreasing) when $|\mathbf{r}_1-\mathbf{r}_2|\geqslant a$ and obviously zero if $|\mathbf{r}_1-\mathbf{r}_2|<a$, then Eq. (3.37) holds everywhere.

In order to prove that η_{N-2} is continuous, let $|\mathbf{r}'_1-\mathbf{r}'_2|>|\mathbf{r}_1-\mathbf{r}_2|\geqslant a$ and let μ denote the Lebesgue measure on R^3 (or rather the measure on T^3 induced by the Lebesgue measure on R^3); then

$$\begin{aligned}
&\eta_{N-2}(|\mathbf{r}_1-\mathbf{r}_2|)-\eta_{N-2}(|\mathbf{r}'_1-\mathbf{r}'_2|)\\
&\quad=\int_{\Delta^{N-2}} d\gamma^{N-2}\prod_{i>j=3}^{N}\Theta_{ij}-\int_{(\Delta')^{N-2}} d\gamma^{N-2}\prod_{i>j=3}^{N}\Theta_{ij}\\
&\quad=\sum_{k=1}^{N-2}\binom{N-2}{k}\int_{(\Delta')^{N-2-k}(\Delta\backslash\Delta')^k} d\gamma^{N-2}\prod_{i>j=3}^{N}\Theta_{ij}\\
&\quad\leqslant\sum_{k=1}^{N-2}\binom{N-2}{k}[\mu(\Delta')]^{N-2-k}[\mu(\Delta\backslash\Delta')]^k
\end{aligned} \tag{3.40}$$

so if

$$\mathbf{r}'_1-\mathbf{r}_1\to 0, \qquad \mathbf{r}'_2-\mathbf{r}_2\to 0 \tag{3.41}$$

as also

$$\mu(\Delta\backslash\Delta')\to 0 \tag{3.42}$$

we have

$$\eta_{N-2}(|\mathbf{r}_1-\mathbf{r}_2|)-\eta_{N-2}(|\mathbf{r}'_1-\mathbf{r}'_2|)\to 0 \quad \blacksquare \tag{3.43}$$

Theorem 3.7. If, for a given t, $n(\mathbf{r};t)\equiv n(t)$ is in $L^1_+(T^3,d\mathbf{r})$ and $0\leqslant n(t)<\tilde{N}/V$, then there exists a unique $z(\mathbf{r};t)\equiv z(t)$ in $L^1_+(T^3,d\mathbf{r})$ and $0\leqslant z(t)<\infty$ such that Eq. (2.23) holds.

Proof. We proceed in the opposite direction, i.e., we assume $z(\mathbf{r};t)\equiv z(t)$ and then we show that Eq. (2.23) is, for any t, an ordinary function which is bijective in the assigned interval.

Under these hypotheses [by virtue of Lemma 3.6 and of Eq. (3.35)] Eqs. (2.7), (2.18) ($n=1, 2$), and (2.23) become

$$\Xi(z(t)) = \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \tag{3.44}$$

$$b_1(z(t)) = \frac{1}{V} \left\{ \sum_{N=1}^{\tilde{N}} \frac{\alpha_N}{(N-1)!} [z(t)]^{N-1} \right\} \Big/ \left\{ \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \right\} \tag{3.45}$$

$$b_2(|\mathbf{r}_1 - \mathbf{r}_2| \, |z(t)) = \left\{ \sum_{N=2}^{\tilde{N}} \frac{\eta_{N-2}(|\mathbf{r}_1 - \mathbf{r}_2|)}{(N-2)!} [z(t)]^{N-2} \right\} \Big/ \left\{ \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \right\} \tag{3.46}$$

$$n(z(t)) = \frac{1}{V} \left\{ \sum_{N=1}^{\tilde{N}} \frac{\alpha_N}{(N-1)!} [z(t)]^N \right\} \Big/ \left\{ \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \right\} \tag{3.47}$$

The theorem now follows as soon as we prove that Eq. (3.47) is strictly monotone in the interval $0 \leqslant n(t) < \tilde{N}/V$: as a matter of fact, a simple calculation shows that

$$\begin{aligned} Vz(t) \frac{dn(t)}{dz(t)} &= \left\{ \sum_{N=1}^{\tilde{N}} \frac{N\alpha_N}{(N-1)!} [z(t)]^N \right\} \Big/ \left\{ \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \right\} \\ &\quad - \left(\left\{ \sum_{N=1}^{\tilde{N}} \frac{\alpha_N}{(N-1)!} [z(t)]^N \right\} \Big/ \left\{ \sum_{N=0}^{\tilde{N}} \frac{\alpha_N}{N!} [z(t)]^N \right\} \right)^2 \\ &= (\langle N^2 \rangle_{GC} - \langle N \rangle_{GC}^2) = \langle (N - \langle N \rangle_{GC})^2 \rangle_{GC} \end{aligned} \tag{3.48}$$

and so we get the required property:

$$\frac{dn(t)}{dz(t)} > 0 \quad \blacksquare \tag{3.49}$$

By the same notation [here $\langle \cdots \rangle_{GC}$ stands for the grand canonical mean value, i.e., $\langle \cdots \rangle_{GC} = \sum_{N=0}^{\infty} \int d\Gamma^N (\cdots) \, \rho_N(t)$] we have

$$n(t) = \frac{\langle N \rangle_{GC}}{V} \tag{3.50}$$

In Appendix A a less standard derivation of Eq. (3.49) is given.

Remark. It is simple to prove, with the help of Lemma 3.6 and Lemma 3.5, that $n_{max} =: \tilde{N}/V$ is $< 1/B$ (in fact, $n_{max} = \tilde{N}/V \leqslant N'/V = [V/B]/V < 1/B$); therefore, the necessary condition given by Eq. (3.4) is verified. As stated in the remark after Theorem 3.4, the bound $n(t) < n_{max}$

is, once more, optimal. In fact, assuming without loss of generality that $n_{\max} \to 1/B$ [in the one-dimensional case $0 < 1/a - n_{\max} \leqslant 1/L$, see Eq. (4.4), so that the assumption is true in the thermodynamic limit] we easily see that if $n(t) > 1/B$, then the functional inversion given by Eq. (2.23) is impossible because Eq. (3.4) does not hold. We also remark that $n_{\max}$ corresponds, physically, to the maximum allowed density of the system [including the usual close-packing density as a particular case; see Eq. (4.4)].

Proposition 3.8. If, for a given t, $n(\mathbf{r}; t) \equiv n(t)$ is in $L^1_+(T^3, d\mathbf{r})$ then, in the interval $0 \leqslant n(t) < n_{\max}$, we have $g_2(\mathbf{r}_1, \mathbf{r}_2 \mid z(t)) \equiv g_2(|\mathbf{r}_1 - \mathbf{r}_2| \mid n(t))$ and

$$\lim_{n(t) \to n_{\max}} g_2(|\mathbf{r}_1 - \mathbf{r}_2| \mid n(t)) \leqslant \frac{\tilde{N} - 1}{\tilde{N}} \frac{V^{\tilde{N}}}{\alpha_{\tilde{N}}} \tag{3.51}$$

Proof. By Lemma 3.6, by Theorem 3.7 [see Eqs. (3.45) and (3.46)], and by keeping in mind the correspondence $n(t) \to n_{\max} \Leftrightarrow z(t) \to \infty$, we obtain $g_2(\mathbf{r}_1, \mathbf{r}_2 \mid z(t)) \equiv g_2(|\mathbf{r}_1 - \mathbf{r}_2| \mid n(t))$ and

$$\begin{aligned} \lim_{n(t) \to n_{\max}} & g_2(|\mathbf{r}_1 - \mathbf{r}_2| \mid n(t)) \\ &= \frac{\tilde{N} - 1}{\tilde{N}} \frac{\eta_{\tilde{N}-2}(|\mathbf{r}_1 - \mathbf{r}_2|)\, V^2}{\alpha_{\tilde{N}}} \\ &\leqslant \frac{\tilde{N} - 1}{\tilde{N}} \frac{V^{\tilde{N}}}{\alpha_{\tilde{N}}} \quad \blacksquare \end{aligned} \tag{3.52}$$

Remark. Equation (3.51) is at variance with the typical assumption made on the high-density factor even in the space homogeneous case.[21]

4. THE ONE-DIMENSIONAL CASE

Let us now apply the results obtained in Section 3 in the space homogeneous case to the one-dimensional gas model consisting of interacting particles of length a moving on a periodic line T^1 of length L (identifiable with the one-dimensional torus R/Z).

The great difference is that the integrals given by Eqs. (3.28)–(3.30) can be now carried out exactly because of the linear order which the hard cores impose. The results, as shown in Appendix B, are

$$\alpha_N = \int_{T^N} dy^N \prod_{i > j = 1}^{N} \Theta_{ij} = L(L - Na)^{N-1} \tag{4.1}$$

$$\beta_{N-1} = \int_{T^{N-1}} d\gamma^{N-1} \prod_{i>j=1}^{N} \Theta_{ij} = (L - Na)^{N-1} \tag{4.2}$$

$$\eta_{N-2}(a) = \left(\int_{T^{N-2}} d\gamma^{N-2} \prod_{i>j=1}^{N} \Theta_{ij} \right)_{x_{12}=a} = (L - Na)^{N-2} \tag{4.3}$$

where, in Eqs. (2.8), (3.31), and (3.33), $\mathbf{r}_i$ is replaced by x_i for all i.

In the present case one can also prove that $\tilde{N}$, as given by Lemma 3.6, is equal to N', as given by Lemma 3.5, i.e., is such that

$$\frac{L}{a} - 1 \leqslant \tilde{N} < \frac{L}{a} \tag{4.4}$$

[in fact, $\alpha_{\tilde{N}} > 0 \Leftrightarrow L - \tilde{N}a > 0$ and $\alpha_{\tilde{N}+1} = 0 \Leftrightarrow L - (\tilde{N}+1)a \leqslant 0$] and that the exact vaue of the function g_2 calculated for the maximum allowed density [which includes the usual close-packing density $L = (\tilde{N}+1)a$] at the contact point $x_{12} = a$ [see Eqs. (3.52), (4.1), and (4.3)] is

$$\lim_{n(t) \to n_{\max}} g_2(a \mid n(t)) = \frac{\tilde{N}-1}{\tilde{N}} \frac{L}{L - \tilde{N}a} \tag{4.5}$$

and so, using twice Eq. (4.4), we get

$$\lim_{n(t) \to n_{\max}} g_2(a \mid n(t)) \geqslant \frac{\tilde{N}-1}{\tilde{N}} \frac{L}{a} > \tilde{N} - 1 \tag{4.6}$$

which shows that the usual assumptions made on the high-density factor[19,21] at the close-packing density become true, at least for the one-dimensional model in the space homogeneous case, if we let $\tilde{N}(L, a)$ go to infinity [i.e., if either $L \to \infty$ or $a \to 0$; see Eq. (4.4)].

Four possible limits suggest themselves:

(1) The so-called[5] *strict thermodynamic limit* ($\lim_{\mathrm{T}}$): $L \to \infty$, $\langle N \rangle_{\mathrm{GC}} \to \infty$, and $\langle N \rangle_{\mathrm{GC}}/L < \infty$.

(2) The *thermodynamic limit* ($\lim_{\mathrm{T}_\infty}$): $L \to \infty$.

(3) The *hydrodynamic limit*[2,22] ($\lim_{\mathrm{H}}$): t, x scaled with the diameter a, $a \to 0$, $\langle N \rangle_{\mathrm{GC}} \to \infty$, and $a\langle N \rangle_{\mathrm{GC}} < \infty$.

(4) The *free gas limit* ($\lim_{\mathrm{H}_0}$): t, x scaled with the diameter a and $a \to 0$.

In both cases we get the results

$$\lim_{\mathrm{T}} \left(\lim_{n(t) \to n_{\max}} g_2(a \mid n(t)) \right) = \infty \tag{4.7}$$

$$\lim_{T_\infty}\Big(\lim_{n(t)\to n_{\max}} g_2(a\,|\,n(t))\Big)=\infty \tag{4.8}$$

$$\lim_{H}\Big(\lim_{n(t)\to n_{\max}} g_2(a\,|\,n(t))\Big)=\infty \tag{4.9}$$

$$\lim_{H_0}\Big(\lim_{n(t)\to n_{\max}} g_2(a\,|\,n(t))\Big)=\infty \tag{4.10}$$

Remark. We notice that $\langle N\rangle_{GC}\to\tilde{N}$ when $n(t)\to n_{\max}$ [see Eq. (3.50)]. This implies that if now $L\to\infty$, then $\langle N\rangle_{GC}\to\infty$ and $\langle N\rangle_{GC}/L\to 1/a$ (and, resp., $a\to 0\Rightarrow\langle N\rangle_{GC}\to\infty$ and $a\langle N\rangle_{GC}\to L$). In other words, Eqs. (4.7) and (4.8) [resp. (4.9) and (4.10)] have the same meaning if we take first the maximum allowed density limit. This does not happen if we interchange the order in these limiting processes (in fact, e.g., $\lim_H g_2>1$ and $\lim_{H_0} g_2=1$, see below). Moreover, if this is done, Eqs. (4.7), (4.9), and (4.10) become

$$\lim_{n(t)\to n_{\max}}\Big(\lim_{T} g_2(a\,|\,n(t))\Big)=\infty \tag{4.11}$$

$$\lim_{n(t)\to n_{\max}}\Big(\lim_{H} g_2(a\,|\,n(t))\Big)=\infty \tag{4.12}$$

$$\lim_{n(t)\to n_{\max}}\Big(\lim_{H_0} g_2(a\,|\,n(t))\Big)=1 \tag{4.13}$$

In order to prove Eqs. (4.11) and (4.12), it is sufficient to observe that, by means of the notation introduced after Eq. (3.49), $g_2(a\,|\,n(t))$ may be written as follows:

$$g_2(a\,|\,n(t))=\frac{L}{\langle N\rangle_{GC}^2}\left\langle\frac{N(N-1)}{L-Na}\right\rangle_{GC} \tag{4.14}$$

In Appendix C we show that

$$\left\langle\frac{N(N-1)}{L-Na}\right\rangle_{GC}\geqslant\frac{\langle N(N-1)\rangle_{GC}}{\langle L-Na\rangle_{GC}} \tag{4.15}$$

so that

$$\begin{aligned} g_2(a\,|\,n(t)) &\geqslant \frac{L}{\langle N\rangle_{GC}^2}\,\frac{\langle N(N-1)\rangle_{GC}}{\langle L-Na\rangle_{GC}}\\ &=\frac{\langle N^2\rangle_{GC}-\langle N\rangle_{GC}}{\langle N\rangle_{GC}^2}\,\frac{L}{L-a\langle N\rangle_{GC}}\\ &\geqslant\left(1-\frac{1}{\langle N\rangle_{GC}}\right)\frac{L}{L-a\langle N\rangle_{GC}} \end{aligned} \tag{4.16}$$

[here, as in Eq. (3.49), we have used the fact that $\langle N^2\rangle\geqslant\langle N\rangle^2$].

Taking now the *strict thermodynamic limit* ($\lim_T$) [i.e., $L \to \infty$, $\langle N \rangle_{GC} \to \infty$, $\langle N \rangle_{GC}/L \to 1/a_0(t)$, $a_0(t) > a$] and the *hydrodynamic limit* ($\lim_H$) [i.e., t and x scaled with a, $a \to 0$, $\langle N \rangle_{GC} \to \infty$, $a\langle N \rangle_{GC} \to L_0(t) < L$] we obtain [if these limits exist as in, e.g., the canonical ensemble[6] where Eq. (4.16) holds with the equality signs]

$$\lim_{T} g_2(a \mid n(t)) \geqslant \frac{1}{1 - a/a_0(t)} \tag{4.17}$$

and

$$\lim_{H} g_2(a \mid n(t)) \geqslant \frac{1}{1 - L_0(t)/L} \tag{4.18}$$

so that we finally get

$$\lim_{n(t) \to n_{\max}} (\lim_{T} g_2(a \mid n(t))) = \infty \tag{4.19}$$

and

$$\lim_{n(t) \to n_{\max}} (\lim_{H} g_2(a \mid n(t))) = \infty \tag{4.20}$$

(here $\lim_{n(t) \to n_{\max}}$ is the maximum allowed density limit and means, respectively, $\lim_{a_0(t) \to a}$ and $\lim_{L_0(t) \to L}$). ∎

Let us now prove Eq. (4.13). We start from the remark that $\Xi(z(t))$ (and, likewise, b_1 and b_2) may be written in the form

$$\Xi(z(t)) = \sum_{N=0}^{\infty} \tau(L - Na) \frac{L(L-Na)^{N-1} [z(t)]^N}{N!} \tag{4.21}$$

where $\tau(x)$ means zero for $x \leqslant 0$, unity elsewhere [i.e., in terms of the Heaviside step function, $\tau(x) = 1 - \Theta(-x)$] and the series in Eq. (4.21) converges uniformly for any arbitrary $a > 0$, provided that $z(t)$ and L are fixed (in fact, for any $a > 0$, $\Xi(z(t)) < \exp[Lz(t)]$). Hence, by a well-known theorem concerning the order in which limit operations are carried out, we obtain

$$\lim_{a \to 0} \Xi(z(t)) = \sum_{N=0}^{\infty} \lim_{a \to 0} \tau(L - Na) \frac{L(L-Na)^{N-1} [z(t)]^N}{N!} = \exp[Lz(t)] \tag{4.22}$$

and, by the same arguments,

$$\lim_{a \to 0} b_1(z(t)) = \lim_{a \to 0} b_2(a \mid z(t)) = 1 \tag{4.23}$$

which gives

$$\lim_{\mathrm{H}_0} g_2(a \mid n(t)) = 1 \tag{4.24}$$

and finally

$$\lim_{n(t) \to n_{\max}} (\lim_{\mathrm{H}_0} g_2(a \mid n(t))) = 1 \tag{4.25}$$

(here, as in Proposition 3.8, $\lim_{n(t) \to n_{\max}}$ means $\lim_{z(t) \to \infty}$). ∎

Remark. Equation (4.25) is valid in the general space inhomogeneous three-dimensional case, as one can prove using the equalities

$$\lim_{a \to 0} \int_{T^{3N}} dy^N \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=1}^{N} z_i(t) = (\|z(t)\|_1)^N, \qquad N \geqslant 0 \tag{4.26}$$

$$\lim_{a \to 0} \int_{T^{3(N-1)}} dy^{N-1} \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=2}^{N} z_i(t) = (\|z(t)\|_1)^{N-1}, \qquad N \geqslant 1 \tag{4.27}$$

$$\lim_{a \to 0} \int_{T^{3(N-2)}} dy^{N-2} \prod_{i>j=1}^{N} \Theta_{ij} \prod_{i=3}^{N} z_i(t) = (\|z(t)\|_1)^{N-2}, \qquad N \geqslant 2 \tag{4.28}$$

(which follow from Lebesgue's monotone convergence theorem) together with the identity $\sum_{N=0}^{\bar{N}} f_N = \sum_{N=0}^{\infty} \tau(f_N) f_N$.

Concerning the *thermodynamic limit* (i.e., $L \to \infty$), at this time, we can only prove that

$$\frac{1 + 2az(n(t)) + a^2[z(n(t))]^2}{1 + 3az(n(t)) + \frac{3}{2}a^2[z(n(t))]^2} \leqslant \lim_{\mathrm{T}_\infty} g_2(a \mid n(t)) \leqslant 1 + 2az(n(t)) \tag{4.29}$$

(if this limit exists; see, e.g., refs. 23 and 24), which gives the trivial inequality

$$\tfrac{2}{3} \leqslant \lim_{n(t) \to n_{\max}} (\lim_{\mathrm{T}_\infty} g_2(a \mid n(t))) \leqslant \infty \tag{4.30}$$

[we know in fact that, for $L \in R_+$ and $z(t) \in R_+$ fixed, $g_2(a \mid z(t)) \geqslant 1$]. In order to prove Eq. (4.29), we observe that Hôpital's rule implies that

$$\frac{1}{1 + 2az(t)} \leqslant \lim_{\mathrm{T}_\infty} b_1(z(t)) \leqslant \frac{1}{1 + az(t)} \tag{4.31}$$

and

$$\frac{1}{1+3az(t)+\frac{3}{2}a^2[z(t)]^2} \leqslant \lim_{T_\infty} b_2(a\,|\,z(t)) \leqslant \frac{1}{1+2az(t)} \tag{4.32}$$

In fact, deriving k times with respect to L the numerator and the denominator of $b_1(z(t))$, we obtain

$$b_1^k(z(t)) = \frac{\left\{ \sum_{N=k+1}^{\tilde{N}} \frac{(L-Na)^{N-1-k}}{(N-1-k)!} [z(t)]^{N-1} \right\}}{\left\{ \sum_{N=k}^{\tilde{N}} \frac{(L-ka)(L-Na)^{N-1-k}}{(N-k)!} [z(t)]^N \right\}} \tag{4.33}$$

so that, letting $k=\tilde{N}-1$ and taking $\liminf b_1^k(z(t))$ and $\limsup b_1^k(z(t))$ as L goes to infinity, we finally get Eq. (4.31) and, by means of the same arguments, Eq. (4.32). ∎

5. DISCUSSION

In the present paper the functional dependence on the local density of the pair correlation function g_2 has been studied from a mathematical viewpoint with the purpose of showing how many details have to be spelled out before one can start talking about existence and uniqueness theorems for the REE.

In particular, the usual[4] *formal* Mayer cluster expansion

$$g_2(\mathbf{r}_1, \mathbf{r}_2\,|\,n(t)) = \Theta_{12} \sum_{k=2}^{\infty} \frac{1}{(k-2)!} \int_{\Lambda^{k-2}} d\gamma^{k-2} \prod_{i=3}^{k} n_i(t)\, V_k(12\,|\,3\cdots k) \tag{5.1}$$

[here $n_k(t)=n(\mathbf{r}_k;t)$ and $V_k(12\,|\,3\cdots k)$ is the sum of all graphs of k labeled points which are biconnected when the Mayer factor $f_{12}=\Theta_{12}-1$ is added; see ref. 20] has been shown to be not defined when the local density does not satisfy Eq. (3.4) (the latter bound, in the space homogeneous case, corresponds, physically, to maximum allowed density).

Another difficulty presented here is that one cannot write the high-density factor in RET in a sufficiently self-contained way even in the space homogeneous case; one should take either the thermodynamic or the hydrodynamic limit (but this has never been said explicitly in many places, to the best of our knowledge). As a matter of fact, it has been proved that the high-density factor for a finite system ($V<\infty$) of interacting particles of finite diameter ($a>0$) is bounded at the maximum allowed density, contrary to a well-known assumption.[19,21]

Concerning the first point in this section, we briefly discuss the derivation of a new possible form for the REE without making use of the *inverse conjecture.*

The idea is to write Eq. (2.2) with the collision operator given by Eq. (2.5) for the new function $W(\mathbf{r}_1, \mathbf{v}_1; t)$; in fact, now the pair correlation function is correctly written as a functional of the local "fugacity" $z(\mathbf{r}_1; t)$.

Equation (2.2) now becomes

$$\frac{\partial Wb_1(\cdot\,|\,z)}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial Wb_1(\cdot\,|\,z)}{\partial \mathbf{r}_1} + \mathbf{F} \cdot \frac{\partial Wb_1(\cdot\,|\,z)}{\partial \mathbf{v}_1} = J^{\mathrm{E}}(Wb_1(\cdot\,|\,z), Wb_1(\cdot\,|\,z)) \tag{5.2}$$

In general,

$$f_1(\mathbf{r}_1, \mathbf{v}_1\,|\,W(t)) \in L^1_+(\Lambda \times R^3, d\Gamma) \nRightarrow W(\mathbf{r}_1, \mathbf{v}_1, t) \in L^1_+(\Lambda \times R^3, d\Gamma) \tag{5.3}$$

but, recalling Eqs. (2.16) and (2.17),

$$W(\mathbf{r}_1, \mathbf{v}_1, t) \in L^1_+(\Lambda \times R^3, d\Gamma) \Leftrightarrow 1 \leqslant \Xi(W(t)) < \infty \tag{5.4}$$

and

$$W(\mathbf{r}_1, \mathbf{v}_1, t) \in L^1_+(\Lambda \times R^3, d\Gamma) \Rightarrow f_1(\mathbf{r}_1, \mathbf{v}_1\,|\,W(t)) \in L^1_+(\Lambda \times R^3, d\Gamma) \tag{5.5}$$

As a consequence, it seems natural to take $L^1_+(\Lambda \times R^3, d\Gamma)$ as the functional space for this REE.

In closing, we present some open questions raised by our analysis:

(1) Is Eq. (3.4) a sufficient condition in Theorem 3.1 (see refs. 17 and 18)? Is Eq. (3.4) a necessary and sufficient condition for the convergence of the *formal* sum given by Eq. (5.1)? What condition replaces Eq. (3.4) in the thermodynamic and hydrodynamic limits?

(2) Is it possible to extend the results obtained in Section 4 to the space inhomogeneous (or homogeneous) three (or two)-dimensional case? To this end, we notice that one of the difficulties is to calculate exactly α_N and $\eta_{N-2}(a)$ [as in Eqs. (3.28) and (3.30)] for an arbitrary integer N. Of course if $N = 0, 1, 2$ (resp. $N = 2, 3$) the integrals given by α_N [resp. $\eta_{N-2}(a)$] can be easily carried out, with the results

$$\alpha_0 = 1 \tag{5.6}$$

$$\alpha_1 = V \tag{5.7}$$

$$\alpha_2 = V(V - v(a)) \tag{5.8}$$

$$\eta_{2-2}(a) = 1 \tag{5.9}$$

$$\eta_{3-2}(a) = V - \tfrac{19}{12} v(a) \tag{5.10}$$

[where $v(a)=\frac{4}{3}\pi a^3$ is the volume of the protection sphere[2] and $(19/12)\, v(a)$ is the total volume of two protection spheres whose centers are at a distance equal to a]; in the two-dimensional case, Eqs. (5.6)–(5.10) are still valid once the replacements

$$V \rightleftharpoons S=\mu(T^2), \qquad v(a) \rightleftharpoons s(a)=\pi a^2, \qquad \frac{19}{12} \rightleftharpoons \frac{4}{3}+\frac{\sqrt{3}}{2\pi} \tag{5.11}$$

are made.

(3) Is it possible to interchange the limit processes in Eq. (4.8)? (See ref. 23 and, for the one-dimensional case, ref. 24).

(4) Does $g_2(x_{12} \mid n(t))$ become, at the maximum allowed density, a *Dirac distribution* concentrated at $x_{12}=a^+$ in the thermodynamic and hydrodynamic limits?

APPENDIX A

In this Appendix we present an equivalent derivation of Eq. (3.49). By a direct calculation we get

$$\frac{dn(t)}{dz(t)}=\frac{\alpha_1\alpha_0+\sum_{K=1}^{2\tilde{N}-1} s_K[z(t)]^K}{V(\Xi(z(t))^2} \tag{A.1}$$

where $\Xi(z(t))$ is given by Eq. (3.44) and s_K is defined by

$$s_K=\sum_{N=0}^{K-1}\frac{2N-K+1}{N!\,(K-N)!}\,\alpha_{N+1}\alpha_{K-N}+\frac{K+1}{K!}\,\alpha_{K+1}\alpha_0 \tag{A.2}$$

Equation (3.49) now follows as soon as we prove that $\forall K=1, 2,..., 2\tilde{N}-1$

$$\sum_{N=0}^{K-1}\frac{2N-K+1}{N!\,(K-N)!}\,\alpha_{N+1}\alpha_{K-N}\geqslant 0 \tag{A.3}$$

In order to prove Eq. (A.3), we have only to take its symmetric part, i.e., we let $M=K-1-N$ and thus

$$\begin{aligned}
&\sum_{N=0}^{K-1}\frac{2N-K+1}{N!\,(K-N)!}\,\alpha_{N+1}\alpha_{K-N}\\
&\quad=\sum_{M=0}^{K-1}\frac{-2M+K-1}{(K-1-M)!\,(M+1)!}\,\alpha_{K-M}\alpha_{M+1}\\
&\quad=\frac{1}{2}\sum_{N=0}^{K-1}\frac{(2N-K+1)^2}{(N+1)!\,(K-N)!}\,\alpha_{N+1}\alpha_{K-N}\geqslant 0 \quad \blacksquare
\end{aligned} \tag{A.4}$$

APPENDIX B

In this Appendix we prove the identities (3.53)–(3.55). We start with Eq. (3.54): because of the translation invariance of the Lebesgue measure on R^{N-1} and because of the linear order $x_2 < x_3 < \cdots < x_N$ which the hard cores impose we get

$$\beta_{N-1} = \beta_{N-1}|_{x_1=0} = (N-1)! \int_{\Omega} d\gamma^{N-1} \tag{B.1}$$

where Ω is the subset of R^{N-1} defined by

$$\begin{aligned}\Omega = \{(x_2, x_3,..., x_N) \in R^{N-1}: a < x_2, x_N < L-a,\\ a < x_{i+1} - x_i < L-a \quad \forall i = 2, 3,..., N-1\}\end{aligned} \tag{B.2}$$

and so we obtain

$$\begin{aligned}\beta_{N-1} &= (N-1)! \int_{(N-1)a}^{L-a} dx_N \int_{(N-2)a}^{x_N-a} dx_{N-1} \cdots \int_a^{x_3-a} dx_2\\ &= (L-Na)^{N-1}\end{aligned} \tag{B.3}$$

If we now let $N \geqslant 1$, then Eq. (3.53) follows from Eq. (3.35) [of course Eq. (3.53) is still valid if $N = 0$].

Let us now prove Eq. (3.55): once more the translation invariance of the Lebesgue measure on R^{N-2} and the linear order $x_3 < x_4 < \cdots < x_N$ imply that

$$\begin{aligned}\eta_{N-2}(a) &= \eta_{N-2}|_{\substack{x_1=0\\ x_2=a}}\\ &= (N-2)! \int_{(N-1)a}^{L-a} dx_N \int_{(N-2)a}^{x_N-a} dx_{N-1} \cdots \int_{2a}^{x_4-a} dx_3\\ &= (L-Na)^{N-2}\end{aligned} \tag{B.4}$$

This completes the proof. ▮

Remark. We note that Ω is a subset of R^{N-1} *without* periodic boundary conditions but including these conditions implicitly [see Eq. (B.2)]. For example, the function Θ_{ij} regarded on $[0, L]$ means zero for $0 \leqslant x_{ij} < a$ and $L - a < x_{ij} \leqslant L$, unity elsewhere, to take explicitly into account the correspondence $[0, L] \rightleftharpoons T^1$, i.e., the fact that the position variables must be understood *modulo L*; Δ [see Eq. (3.39)] is, on the contrary, a subset of T^3 *with* periodic boundary conditions.

We also remark that the most general method used for evaluating multiple integrals of this type [Eqs. (3.53)–(3.55)] is that attributable to Gürsey.[25] However, in Gürsey's paper the integration is not performed on the one-dimensional torus T^1, but on the real interval $[0, L]$ under the boundary assumption that the walls behave like particles, identical with those of the system, fixed at $x=0$ and $x=L$, so that the integration domain actually reduces to $[a, L-a]$ *without* periodic boundary conditions [this implies, among other things, that $\alpha_N=[L-(N+1)a]^N$ and that $\beta_{N-1}(x_1)$ is no longer constant, contrary to an explicit statement of Résibois[5]].

APPENDIX C

In this Appendix we prove the inequality

$$\left\langle \frac{N(N-1)}{L-Na} \right\rangle_{\mathrm{GC}} \geqslant \frac{\langle N(N-1)\rangle_{\mathrm{GC}}}{\langle L-Na\rangle_{\mathrm{GC}}} \tag{C.1}$$

where

$$\left\langle \frac{N(N-1)}{L-Na} \right\rangle_{\mathrm{GC}} = \left\{ \sum_{N=0}^{\tilde{N}} \frac{N(N-1)}{L-Na} C_N \right\} \Big/ \sum_{N=0}^{\tilde{N}} C_N \tag{C.2}$$

$$\frac{\langle N(N-1)\rangle_{\mathrm{GC}}}{\langle L-Na\rangle_{\mathrm{GC}}} = \frac{\sum_{N=0}^{\tilde{N}} N(N-1)\, C_N}{\sum_{N=0}^{\tilde{N}} (L-Na)\, C_N} \tag{C.3}$$

and C_N is given by

$$C_N = \frac{L(L-Na)^{N-1}\,[z(t)]^N}{N!} \tag{C.4}$$

As we will prove, Eq. (C.1) is valid in the general case, i.e., when C_N is, for any N, an arbitrary positive constant.

A simple calculation shows that Eq. (C.1) holds $\Leftrightarrow$

$$\sum_{N=0}^{\tilde{N}} \sum_{j=0}^{N} \frac{j(j-1)}{L-ja} C_j [L-(N-j)a]\, C_{N-j} \geqslant \sum_{N=0}^{\tilde{N}} \sum_{j=0}^{N} j(j-1)\, C_j C_{N-j} \tag{C.5}$$

i.e., $\Leftrightarrow$

$$\sum_{N=0}^{\tilde{N}} \sum_{j=0}^{N} a C_j C_{N-j} \frac{j(j-1)(2j-N)}{L-ja} \geqslant 0 \tag{C.6}$$

In order to prove Eq. (C.6), it is sufficient to show that

$$S_N = \sum_{j=0}^{N} C_j C_{N-j} \frac{j(j-1)(2j-N)}{L-ja} \geqslant 0 \qquad \forall N = 0, 1, \ldots, \tilde{N} \tag{C.7}$$

In fact, taking the symmetric part of S_N, we obtain

$$S_N = \frac{1}{2} \sum_{j=0}^{N} C_j C_{N-j} \left[\frac{j(j-1)(2j-N)}{L-ja} + \frac{(N-j)(N-j-1)(N-2j)}{L-(N-j)a} \right] \tag{C.8}$$

and

$$\frac{j(j-1)(2j-N)}{L-ja} + \frac{(N-j)(N-j-1)(N-2j)}{L-(N-j)a} = \frac{(2j-N)^2 \, [(L-ja)(N-j) + L(j-1)]}{(L-ja)[L-(N-j)a]} \geqslant 0 \tag{C.9}$$

which completes the proof. ▮

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