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Sum Rules and Perfect Screening Conditions for the One-Component Plasma

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First we show, from the BBGKY hierarchy and under exponential clustering assumption, that the three-dimensional one-component plasma obeys the compressibility sum rule which links the compressibility to the fourth moment of the two-point correlation function. Then it is proved that the first equation of the hierarchy is equivalent to the known value of the correlation function of momentum current and density. Finally we are concerned with the energy density, its definition, and its correlation with the numerical density and with itself.

KEY WORDS: One-component plasma; sum rules; screening.

1. INTRODUCTION

Over the last few years, the study of the one-component plasma has attracted renewed interest because of rigorous results which have been obtained. Let us recall that the model is a fluid of classical ions which interact via a purely Coulombic potential and which are immersed in a uniform and rigid background of opposite charge in order to ensure charge neutrality.

Some properties, like the perfect screening condition of the two-point correlation function (Stillinger–Lovett condition), were traditionally accepted on the basis of arguments which are intuitively appealing but not rigorous.

Recent works[1-5] have been devoted to rigorous proofs of these perfect-screening conditions for the density correlation functions, using the BBGKY hierarchy of equations. The proof is based on the only assumption that the Ursell correlation functions have a spatial decay faster than some power of the distance (clustering hypothesis).

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In this work, we present a systematic (but not exhaustive) study of the properties, of the two-, three-, and four-point correlation functions, which can be deduced from the hierarchy and the clustering hypothesis (we make the assumption of a decay faster than any power of the distance).

After having described, in Section 2, the general framework of this study, we show in Section 3 the perfect screening conditions (PSC) and the sum rules satisfied by the Ursell functions u_2, u_3, and u_4. This section does not contain any new results compared to Refs. 1–5 but is presented with a pedagogical aim. From the hierarchy equation for u_n, which gives the gradient of u_n in terms of the functions $u_2, u_3, \ldots, u_{n+1}$, we deduce the PSC for u_n and the sum rules for u_{n+1}. The compatibility of the PSC and the sum rules for u_3 defines the second moment of u_2, giving thus the ratio of the structure factor $S(q)$ over q^2 as the wave vector q tends to zero. Applying the same calculation for u_4 does not lead to any new condition. By using the symmetries of u_3 and u_4, some other new relations between two-, three-, and four-point integrals are derived (Section 4). In Section 5 we are concerned with the temperature derivative of the two-point integrals which are, *a priori*, four point integrals. These are generally expressed in terms of three-point integrals because of the sum rules for u_4 and in a few cases these three-point integrals are reduced to two-point integrals. Thus the q^4 term of $S(q)$ at small q values, is linked to the compressibility.

In Section 6 we show that the hierarchy for u_2 is equivalent to the known value of the correlation function of momentum current and density. In Sections 7 and 8 we examine the problem concerning, the definition of the energy density, and its correlation with the density and with itself. In fact it is necessary to take some care with this definition in order to avoid long-range correlation (and unusual behavior at small wave vectors).

Finally we present, in an appendix, a list of relations between the moments of $u_2(r)$ and those of the structure factor.

2. GENERAL FRAMEWORK

We consider a set of N-point ions of mass m, charge e in a volume V. The numerical density is $\rho = N/V$. These ions are classical and interact via purely Coulombic forces. A uniform and rigid background ensures the electrical neutrality as it is necessary for the thermodynamical limit. Periodic boundary conditions are taken. Then the Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} v(r_{ij}), \qquad v(r) = \frac{1}{V} \sum_{k \neq 0} \frac{4\pi e^2}{k^2} e^{ik \cdot r} \tag{1}$$

where p_i is the momentum of particle i and $r_{ij} = r_j - r_i$ is the vector which defines the relative position of ions i and j. The potential $v(r)$ is equal to e^2/r as long as r is small compared to $L = V^{1/3}$.

The mean distance between ions, r_0, and the coupling parameter, Γ, are defined, as usual, by

$$\frac{4}{3}\pi\rho r_0^3 = 1, \qquad \Gamma = \beta\frac{e^2}{r_0}, \qquad \beta = \frac{1}{T} \tag{2}$$

T is the temperature measured in energy units. Frequently, dimensionless quantities will be used; the distances r, s, t will be denoted by x, y, z ($x = r/r_0$, etc.) and the wave vectors k, by $q = kr_0$.

The n-point correlation functions are defined by

$$\begin{gathered}\rho_n(r_1, r_2, ..., r_n) = \rho^n g_n(r_1, r_2, ..., r_n) = \langle [\rho(r_1)\,\rho(r_2)\cdots\rho(r_n)]_{\mathrm{SL}}\rangle \\ \rho(r) = \sum_i \delta(r - r_i)\end{gathered} \tag{3}$$

$\rho(r)$ is the one-point density, as a function of the ion positions; the symbol $[\ \ ]_{\mathrm{SL}}$ indicates that the self-terms are left out, that is, in the n sums only the terms where all the particles are different, are taken into account; and the symbol $\langle\ \ \rangle$ stands for the canonical average.

Finally, the Ursell functions[6] are introduced:

$$\begin{aligned} g_2(r_1, r_2) &= u_2(r_1, r_2) + 1 \\ g_3(r_1, r_2, r_3) &= u_3(r_1, r_2, r_3) + u_2(r_1, r_2) + u_2(r_1, r_3) + u_2(r_2, r_3) + 1 \\ g_4(r_1, r_2, r_3, r_4) &= u_4(r_1, r_2, r_3, r_4) + u_3(r_1, r_2, r_3) + u_3(r_1, r_2, r_4) \\ &\quad + u_3(r_1, r_3, r_4) + u_3(r_2, r_3, r_4) \\ &\quad + u_2(r_1, r_2)\, u_2(r_3, r_4) + u_2(r_1, r_3)\, u_2(r_2, r_4) \\ &\quad + u_2(r_1, r_4)\, u_2(r_2, r_3) + u_2(r_1, r_2) \\ &\quad + u_2(r_1, r_3) + u_2(r_1, r_4) \\ &\quad + u_2(r_2, r_3) + u_2(r_2, r_4) + u_2(r_3, r_4) + 1 \end{aligned} \tag{4}$$

We assume that these functions (i) depend only on the shape of the figure formed by the various points (and not on its space orientation), (ii) are symmetrical in any permutation of the particles, and (iii) tend to zero faster than any power of the distance when a particle is removed to infinity (exponential clustering hypothesis).

The BBGKY hierarchy is then written

$$\frac{\partial}{\partial r_1}\rho_n(r_1, r_2,..., r_n)$$
$$= -\beta\rho_n(r_1, r_2,..., r_n)\sum_{j=2}^{n}\frac{\partial}{\partial r_1}v(r_1 - r_j)$$
$$-\beta\int d^3r_{n+1}\rho_{n+1}(r_1, r_2,..., r_{n+1})\frac{\partial}{\partial r_1}v(r_1 - r_{n+1}) \qquad (n\geqslant 2) \quad (5)$$

3. PERFECT SCREENING CONDITIONS AND SUM RULES FOR u_2, u_3, AND u_4

3.1. Hierarchy for $n=2$

Expressing ρ_2 and ρ_3 as functions of u_2 and u_3 and taking their properties into account, we obtain from the hierarchy ($n=2$) a PSC for u_2 and a sum rule for u_3. The triangle, formed by the three points of u_3, is defined by $x=x_2-x_1$ and $y=x_3-x_1$ in dimensionless units. It follows from (5) that

$$3\int\frac{d^3y}{4\pi}\frac{\hat{x}\cdot\hat{y}}{y^2}u_3(x, y)$$
$$=\frac{1}{\Gamma}\frac{d}{dx}u_2(x)-\frac{1}{x^2}u_2(x)-\frac{1}{x^2}-\frac{3}{x^2}\int_0^x y^2\,dy\,u_2(y) \qquad (6)$$

where the symbol $\hat{}$ indicates unit vectors ($\hat{x}=x/\|x\|$).

If the left-hand side of (6) tends to zero faster than any power of x as x tends to infinity, the sum of the last two terms on the right-hand side must vanish in the same way in this limit. From this, the well-known PSC for u_2 follows[1]:

$$I_2 = -1/3 \qquad (7)$$

with the following definition of the integrals I_n:

$$I_n=\int_0^{+\infty}dx\,x^n u_2(x) \quad (n\geqslant 0), \qquad I_n=\int_0^{+\infty}dx\,x^n g_2(x) \quad (n\leqslant -2)$$

$$I_{-1}=\lim_{\varepsilon\to 0}\left[\int_\varepsilon^{+\infty}\frac{dx}{x}u_2(x)-\log\varepsilon\right] \qquad (8)$$

$$I_{Ln}=\int_0^{+\infty}dx\,x^n\log x\,u_2(x) \quad (n\geqslant 0)$$

By taking (7) into account. the Eq. (6) is then written

$$3\int \frac{d^3y}{4\pi}\frac{\hat{x}\cdot\hat{y}}{y^2}u_3(x, y)=\frac{1}{\Gamma}\frac{d}{dx}u_2(x)-\frac{1}{x^2}u_2(x)+\frac{3}{x^2}\int_x^{+\infty} y^2\,dy\,u_2(y) \qquad (6')$$

After multiplying (6′) by a function $w(x)=w(\|x\|)$, which is assumed to be integrable at the origin [$\int_0 dy\,w(y)$ does exist] and integrating over x, we obtain the relation

$$L\left[\frac{w(x)}{y^2}\hat{x}\cdot\hat{y}\right]=-\frac{1}{3\Gamma}I\left[\frac{1}{x^2}\frac{d}{dx}(x^2w(x))\right]-\frac{1}{3}I\left[\frac{w(x)}{x^2}\right]$$
$$+I\left[\int_0^x dy\,w(y)\right] \qquad (9)$$

where the two- and three-point integrals I and L are defined by

$$I[a(x)]=3\int\frac{dx}{4\pi}a(x)\,u_2(x), \qquad I[x^n]=3I_{n+2}$$
$$L[b(x, y)]=3\int\frac{d^3x\,d^3y}{(4\pi)^2}b(x, y)\,u_3(x, y) \qquad (10)$$

$a(x)$ and $b(x, y)$ are arbitrary functions subjected to the only condition that the integrals (10) exist.

For $w(x)=x^n$ $(n>0)$, (9) leads to

$$L\left[\frac{x^n}{y^2}\hat{x}\cdot\hat{y}\right]=-\frac{n+2}{\Gamma}I_{n+1}-I_n+\frac{3}{n+1}I_{n+3} \qquad (n\geqslant 0) \qquad (11)$$

When negative values of n are considered, it is better to start from (6′):

$$L\left[\frac{1}{xy^2}\hat{x}\cdot\hat{y}\right]=-\frac{I_0}{\Gamma}-I_{-1}+3IL_2$$
$$L\left[\frac{1}{x^2y^2}\hat{x}\cdot\hat{y}\right]=-\frac{1}{\Gamma}-I_{-2}-3I_1 \qquad (12)$$

3.2. Hierarchy for $n=3$

In the same way, we will obtain PSC for u_3 and sum rules for u_4. The four points of u_4 are located by taking one of them as the origin: $x=x_2-x_1$, $y=x_3-x_1$, and $z=x_4-x_1$. $\hat{n}$ stands for an arbitrary unit vector in the plane of x and y. We get from the hierarchy

$$
\begin{aligned}
3\int \frac{d^3z}{4\pi} u_4(x, y, z)\frac{\hat{z}\cdot\hat{n}}{z^2} \\
&= \frac{1}{\Gamma}\hat{n}\cdot\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)u_3(x, y)-\left(\frac{\hat{x}\cdot\hat{n}}{x^2}+\frac{\hat{y}\cdot\hat{n}}{y^2}\right)u_3(x, y) && \text{(A)} \\
&\quad -3u_2(x)\int\frac{d^3z}{4\pi}u_2(z-y)\frac{\hat{z}\cdot\hat{n}}{z^2}-u_2(x)\frac{\hat{y}\cdot\hat{n}}{y^2} && \text{(B)} \\
&\quad -3u_2(y)\int\frac{d^3z}{4\pi}u_2(z-x)\frac{\hat{z}\cdot\hat{n}}{z^2}-u_2(y)\frac{\hat{x}\cdot\hat{n}}{x^2} && \text{(C)} \\
&\quad -3\int\frac{d^3z}{4\pi}u_3(z-x, z-y)\frac{\hat{z}\cdot\hat{n}}{z^2}-u_2(x-y)\left(\frac{\hat{x}\cdot\hat{n}}{x^2}+\frac{\hat{y}\cdot\hat{n}}{y^2}\right) && \text{(D)}
\end{aligned} \tag{13}
$$

The terms (A), (B), and (C) tend to zero faster than any power of the distances x or y; for example (B) is written in the following form by taking the PSC (7) into account:

$$3u_2(x)\int_y^{+\infty} z^2\,dz\,u_2(z)\frac{\hat{y}\cdot\hat{n}}{y^2}$$

After some transformation, we obtain for the last term (D):

$$
\begin{aligned}
-\hat{n}\cdot\frac{\partial}{\partial x_1}\Bigg[3\int\frac{d^3x_4}{4\pi}u_3(x_2, x_3, x_4)\frac{1}{\|x_4-x_1\|} \\
+\, u_2(x_2-x_3)\left(\frac{1}{\|x_2-x_1\|}+\frac{1}{\|x_3-x_1\|}\right)\Bigg]
\end{aligned} \tag{14}
$$

which has to tend to zero faster than any power of the distance $\|x_1-x_2\|$ [as the left-hand side of (13)] when the latter tends to infinity. Expanding (14) in power of $1/\|x_1-x_2\|$ in this limit, we deduce the PSC for $u_3{}^{(3)}$:

$$
\begin{aligned}
3\int\frac{d^3y}{4\pi}u_3(x, y) &= -2u_2(x) \\
3\int\frac{d^3y}{4\pi}u_3(x, y)\,y^lP_l(\hat{x}\cdot\hat{y}) &= -x^lu_2(x) \qquad (l\geqslant 1)
\end{aligned} \tag{15}
$$

The P_l are the Legendre polynomials. These conditions are not independent as will seen later. Integrating these equations with some function w of $\|x\|$, we get

$$
\begin{aligned}
L[w(x)] &= -\tfrac{2}{3}I[w(x)] \\
L[w(x)\,y^lP_l(\hat{x}\cdot\hat{y})] &= -\tfrac{1}{3}I[x^lw(x)] \qquad (l\geqslant 1)
\end{aligned} \tag{16}
$$

Taking (15) into account, the term (D) in (13) is written in the form

$$-3\int \frac{d^3z}{4\pi} u_3(z-x, z-y)\left[\frac{\hat{z}\cdot\hat{n}}{z^2}-\frac{1}{2}\left(\frac{\hat{x}\cdot\hat{n}}{x^2}+\frac{\hat{y}\cdot\hat{n}}{y^2}\right)\right] \tag{17}$$

As well as the PSC for u_3, we can obtain from (13) sum rules for u_4 by integrating (13) with some functions of x and y. These four-point integrals will be defined in the following way:

$$M[f(x, y, z)] = 3\int \frac{d^3x\, d^3y\, d^3z}{(4\pi)^3} u_4(x, y, z)\, f(x, y, z) \tag{18}$$

where x, y, and z are, respectively, the vectors x_{12}, x_{13}, and x_{14}. Integrating (13) leads to

$$M\left[\frac{z\cdot y}{z^3} w(x)\right] = \frac{1}{9\Gamma} I\left[x\frac{d}{dx} w(x)\right] + \frac{1}{3\Gamma} I[w(x)] + \frac{1}{9} I\left[\frac{w(x)}{x}\right]$$
$$-\frac{1}{3} I\left[\int_0^x dy\, yw(y)\right] - \frac{1}{3} L\left[\frac{w(x)}{y}\right] \tag{19}$$

3.3. PSC for u_4

We could deduce the PSC for u_4 and sum rules for u_5 from the hierarchy (5) with $n=4$. But the number of terms becomes considerable and the sum rules for u_5 present less importance than those for u_4. Another, probably equivalent, way to obtain the PSC for u_4, is to write that the mean potential around three fixed ions decreases faster than any power of the distance far away from these ions. When applied to u_2 and u_3, that argument is right. The mean density at a point 4 around three charges fixed at 1, 2, and 3 is equal to $\rho g_4(1, 2, 3, 4)/g_3(1, 2, 3)$. We conclude that the quantity

$$u_3(x, y)\left(\frac{1}{X}+\frac{1}{\|X-x\|}+\frac{1}{\|X-y\|}\right) + 3\int \frac{d^3z}{4\pi} u_4(x, y, z)\frac{1}{\|X-z\|} \tag{20}$$

has to decrease faster than any power of $1/\|X\|$ when $\|X\|$ tends to infinity. The other terms of the mean potential behave well in this limit and thus are not written. That leads to the PSC for $u_4{}^{(3)}$:

$$3\int \frac{d^3z}{4\pi} u_4(x, y, z) = -3u_3(x, y)$$
$$3\int \frac{d^3z}{4\pi} u_4(x, y, z)\, z^l P_l(\hat{z}\cdot\hat{X}) = -u_3(x, y)\{x^l P_l(\hat{x}\cdot\hat{X}) + y^l P_l(\hat{y}\cdot\hat{X})\} \quad (l \geq 1) \tag{21}$$

where $\hat{X}$ is an arbitrary unit vector.

3.4. Compatibility of the Sum Rules with the PSC

Sum rules for u_n and PSC follow, respectively, from the hierarchy (5) with n and $n+1$. Therefore it is natural to see if these two kinds of integrals are compatible and this allows us to hope for new conditions on integrals with u_{n-1} which occur in both cases.

Let us first look at u_3. We deduce from the sum rules (11),

$$L\left[\frac{x}{y^2}\hat{x}\cdot\hat{y}\right] = -\frac{3}{\Gamma}I_2 - I_1 + \frac{3}{2}I_4 \tag{22}$$

and from the PSC (16),

$$L\left[\frac{y}{x^2}\,\hat{x}\cdot\hat{y}\right] = L\left[\frac{x}{y^2}\hat{x}\cdot\hat{y}\right] = -I_1 \tag{23}$$

That leads to the well-known condition of Stillinger and Lovett[7]:

$$I_4 = \frac{2}{\Gamma}I_2 = -\frac{2}{3\Gamma} \tag{24}$$

which gives the behavior of the structure factor $S(q)$ at small wave vector

$$S(q) = 1 + I\left[\frac{\sin qx}{qx}\right] \underset{q\to 0}{\simeq} 1 + 3I_2 - \frac{q^2}{2}I_4 = \frac{q^2}{3\Gamma} \tag{25}$$

The proof of the Stillinger–Lovett second-moment condition has been first given by Martin and Gruber.[4]

Applying the same method for u_4, we did not obtain any new condition. As a matter of fact, taking the symmetry of u_4 into account, the integral (19) (sum rule) is equal to the integral

$$M\left[\frac{z\cdot y}{y^3}w(x)\right] = \frac{1}{9\Gamma}I\left[x\frac{d}{dx}w(x)\right] + \left(\frac{2}{3\Gamma} + \frac{1}{2}I_4\right)I[w(x)] + \frac{1}{9}I\left[\frac{w(x)}{x}\right] - \frac{1}{3}I\left[\int_0^x dy\,y w(y)\right] - \frac{1}{3}L\left[\frac{w(x)}{y}\right]$$

which follows from the PSC (21). This leads to an identity as soon as (24) is true.

More complicated calculations with $M[(y\cdot z)(y\cdot x)\,w(x)/z^3]$ arrive at the same result.

4. SOME PARTICULAR INTEGRALS OF u_3 AND u_4

The symmetry $u_3(x, y) = u_3(y, x)$ has already been taken into account. There is another symmetry in the exchange of two particles of which one is at the origin:

$$x \to -x, \qquad y \to y - x \tag{26}$$

The following laws of transformation are easily seen to hold:

$$\begin{aligned} x^2 - 2x \cdot y &\to -(x^2 - 2x \cdot y) \\ y^2 - x \cdot y &\to y^2 - x \cdot y \end{aligned} \tag{27}$$

This results in the identity

$$L[w(x)(y^2 - x \cdot y)^p (x^2 - 2x \cdot y)^{2q+1}] = 0 \tag{28}$$

with $w(x) = w(\|x\|)$, p and q are integer ($\geqslant 0$).

For $p = q = 0$ we obtain

$$L[w(x)x] = 2L[w(x)\, y\hat{x} \cdot \hat{y}] \tag{29}$$

That shows that the PSC (16) for $l = 0$ and $l = 1$ are not independent. Moreover, it is easily proved that these two conditions are equivalent (by Fourier transform). The case $p = 1$, $q = 0$ is more interesting. Taking the PSC (16) into account, we obtain

$$\tfrac{5}{3}L[w(x)\, x^2y^2] - 2L[w(x)\, xy^3 P_1(\hat{x} \cdot \hat{y})] = \tfrac{1}{9}I[w(x)\, x^4] \tag{30}$$

which leads for $w(x) = 1$, $1/x^2$, and $1/x^3$ to

$$\begin{gathered} L[x^2y^2] = -I_6, \qquad L\left[\frac{y^3}{x} P_1(\hat{x} \cdot \hat{y})\right] = -\frac{11}{6} I_4 \\ L\left[\frac{y^2}{x}\right] = -\frac{6}{\Gamma} I_4 - I_3 + \frac{9}{10} I_6 \end{gathered} \tag{31}$$

Other new relations concerning three-point integrals can be deduced from (28) with larger values of p and q. Calculations become rather heavy.

The same kind of symmetry for u_4 allows us to deduce from the hierarchy the integral $M[w(x - y)/z]$, which will be useful later. In the exchange of particles 1 and 4, the following quantities are transformed as

$$\begin{aligned} &z \to -z, && y \cdot z \to z^2 - y \cdot z \\ &x \to x - z, && x - y \to x - y \\ &y \to y - z, && \end{aligned} \tag{32}$$

In this way, we obtain the relation

$$M\left[\frac{w(x-y)}{z}\right]=2M\left[\frac{z\cdot y}{z^3}\,w(x-y)\right] \tag{33}$$

It must be noticed that this equation (and what follows) is only true for the Coulombic potential $1/r$ because explicit use is made of

$$r\cdot\frac{\partial}{\partial r}\,v(r)=-v(r)$$

Integrating (13) leads to

$$\begin{aligned} M\left[\frac{w(x-y)}{z}\right] &= -\frac{2}{\Gamma}\,L[w(x)]-\frac{2}{3}\,L\left[\frac{w(y)}{x^3}\,(2x^2-x\cdot y)\right]-\frac{2}{3}\,L[w(x)x\cdot y] \\ &\quad -\frac{1}{6}\,L[w(x)\,x^2]+L[w(x)\,y^2]-6\int\frac{d^3x\,d^3y}{(4\pi)^2}\,u_2(x)\,w(y-x) \\ &\quad \times\left[\int\frac{d^3z}{4\pi}\,u_2(z)\left(\frac{(y+z)\cdot(y+x)}{\|y+z\|^3}-\frac{1}{y}-\frac{y\cdot x}{y^3}\right)\right] \end{aligned} \tag{34}$$

In this relation, some three-point integrals can be reduced to two-point integrals. When necessary, this will be done.

5. TEMPERATURE DERIVATIVES OF THE TWO-POINT INTEGRALS

The temperature derivative of the average value of a quantity f is given in the canonical ensemble by

$$\frac{\partial}{\partial\beta}\,\langle f\rangle=-\langle\delta H\,\delta f\rangle \tag{35}$$

where β is the inverse of the temperature, H is the Hamiltonian, and δf is the fluctuation of the quantity f:

$$\delta f=f-\langle f\rangle \tag{36}$$

Let us consider the two-point integrals

$$\begin{aligned} I[w(x)] &= 3\int\frac{d^3x}{4\pi}\,w(x)\left\langle\frac{1}{\rho^2}\,[\delta\rho(x_1+x)\,\delta\rho(x_1)]_{\mathrm{SL}}\right\rangle \\ &= 3\int\frac{d^3x}{4\pi}\,w(x)\,u_2(x) \end{aligned} \tag{37}$$

Their derivative with respect to Γ are *a priori* functions of two-, three-, and four-point integrals. But the four-point integral, which occurs, can be expressed in terms of two- and three-point integrals. Therefore the derivative $\partial I/\partial\Gamma$ is, in general, a function of two- and three-point integrals and in some cases a function of two-point integrals, when the three-point integrals are reduced to two-point integrals.

It is easily seen that only the potential energy does occur in (35) for the quantities f considered here. Using the expression

$$\begin{aligned}
&\frac{1}{\rho^4}\langle[\delta\rho(r_1)\,\delta\rho(r_2)]_{\mathrm{SL}}[\delta\rho(r_3)\,\delta\rho(r_4)]_{\mathrm{SL}}\rangle \\
&\quad= g_4(r_1, r_2, r_3, r_4) + \frac{1}{\rho}[\delta(r_1 - r_3) + \delta(r_2 - r_3)]\, g_3(r_1, r_2, r_4) \\
&\quad\quad + \frac{1}{\rho}[\delta(r_1 - r_4) + \delta(r_2 - r_4)]\, g_3(r_1, r_2, r_3) \\
&\quad\quad + \frac{1}{\rho^2}[\delta(r_1 - r_3)\,\delta(r_2 - r_4) + \delta(r_2 - r_3)\,\delta(r_1 - r_4)]\, g_2(r_1, r_2) \qquad (38)
\end{aligned}$$

We deduce the derivative of I

$$\begin{aligned}
\frac{\partial}{\partial\Gamma} I[w(x)] = &-\frac{9}{2} M\left[\frac{w(y-z)}{x}\right] - 6L\left[\frac{w(y)}{x}\right] \\
&- 27\int \frac{d^3x\, d^3y\, d^3z}{(4\pi)^3}\frac{w(y-z)}{x}\, u_2(y)\, u_2(x-z) \\
&- 18\int \frac{d^3x\, d^3y}{(4\pi)^2}\frac{w(y)}{x}\, u_2(x-y) - 3\int \frac{d^3x}{4\pi}\frac{w(x)}{x}\, g_2(x) \qquad (39)
\end{aligned}$$

and taking account of the expression (34) of the four-point integrals and of the integrals (9) and (15), we obtain

$$\begin{aligned}
\frac{\partial}{\partial\Gamma} I[w(x)] = &-\frac{3}{\Gamma} I[w(x)] + \frac{1}{\Gamma} I\left[x\frac{dw(x)}{dx}\right] \\
&-\frac{3}{2} I[x^2 w(x)] - \frac{9}{2} L[w(x)\, y^2] \qquad (40)
\end{aligned}$$

with the only condition on $w(x)$ that the integrals do not diverge.

In the particular cases $w(x) = x^{n-2}$ $(n \geqslant 0)$, it follows that

$$\frac{\partial I_n}{\partial\Gamma} = -\frac{6-(n+1)}{\Gamma} I_n - \frac{3}{2} I_{n+2} - \frac{3}{2} L[x^{n-2} y^2] \qquad (n \geqslant 0) \qquad (41)$$

In this equation, the three-point integral is only known for $n=1, 2$, and 4 [Eqs. (16) and (31)]:

$$\begin{aligned}
\frac{dI_1}{d\Gamma} &= -\frac{4}{\Gamma}I_1+\frac{9}{\Gamma}I_4-\frac{27}{20}I_6 \\
\frac{dI_2}{d\Gamma} &= -\frac{3}{\Gamma}I_2+\frac{3}{2}I_4 \\
\frac{dI_4}{d\Gamma} &= -\frac{I_4}{\Gamma}
\end{aligned} \tag{42}$$

As $I_2=-1/3$, the last two equations show only that $I_4=-2/3\Gamma$. More interesting is the first one because it allows to link I_6 to the compressibility. In fact the internal energy per particle is given by

$$\beta e=\beta\frac{\langle H\rangle}{N}=\beta e^K+\beta e^V=\frac{3}{2}(1+\Gamma I_1) \tag{43}$$

and the compressibility by

$$\beta\left.\frac{\partial P}{\partial\rho}\right|_T=1+\frac{4}{9}\beta e^V+\frac{1}{9}\Gamma^2\frac{\partial}{\partial\Gamma}\frac{\beta e^V}{\Gamma}=1+\frac{1}{3}\beta e^V+\frac{1}{9}\Gamma\frac{\partial}{\partial\Gamma}\beta e^V \tag{44}$$

We deduce from (42)

$$I_6=-\frac{40}{9\Gamma^2}\beta\left.\frac{\partial P}{\partial\rho}\right|_T \tag{45}$$

The integral I_6 gives the coefficient of the q^4 term of the structure factor at small q values.

The expansion of $S(q)$ is then

$$S(q)\underset{q\to 0}{=}\frac{q^2}{3\Gamma}-\frac{q^4}{9\Gamma^2}\beta\left.\frac{\partial P}{\partial\rho}\right|_T+O(q^6) \tag{46}$$

This result had been established earlier from various arguments[8–10] but not really proved.

The equation (40) leads to other results; with $w(x)=(\sin qx)/qx$, it follows that

$$\begin{aligned}
\frac{\partial}{\partial\Gamma}[S(q)-1] &= -\frac{3}{\Gamma}[S(q)-1]+\frac{q}{\Gamma}\frac{\partial}{\partial q}[S(q)-1] \\
&\quad +\frac{3}{2}\frac{1}{q^2}\frac{\partial}{\partial q}q^2\frac{\partial}{\partial q}[S(q)-1]-\frac{9}{2}L\left[y^2\frac{\sin qx}{qx}\right]
\end{aligned} \tag{47}$$

and by Fourier transform the temperature derivative of u_2 is then

$$\begin{aligned}\frac{\partial}{\partial \Gamma} u_2(x) &= -\frac{6}{\Gamma} u_2(x) - \frac{x}{\Gamma}\frac{\partial}{\partial x} u_2(x) - \frac{3}{2} x^2 u_2(x) + \frac{3}{2} v_2(x) \\ v_2(x) &= 3 \int \frac{dy}{4\pi} y^2 u_3(x, y)\end{aligned} \tag{48}$$

The ignorance of $v_2(x)$ does not allow to have a differential equation for u_2. On the other hand, this equation can be useful to calculate three-point integrals, which are directly related to v_2, or, which are connected to v_2 by using symmetries of u_3, as it has been considered in Section 4.

6. MOMENTUM CURRENT–DENSITY CORRELATION

Another way to show the q^2 behavior of $S(q)$ and to check the sum rules for u_3 (obtained from the hierarchy), consists in calculating the correlation function of the momentum current and the density. The momentum density $g_\alpha(r)$ and the momentum–current satisfy the conservation equation

$$\partial_t g_\alpha(r) + \partial_\beta \pi_{\alpha\beta}(r) = 0 \tag{49}$$

and are defined by

$$\begin{aligned} g_\alpha(r) &= \sum_i p_{i\alpha} \delta(r - r_i), \qquad \pi_{\alpha\beta}(r) = \pi^K_{\alpha\beta}(r) + \pi^V_{\alpha\beta}(r) \\ \pi^K_{\alpha\beta}(r) &= \sum_i m v_{i\alpha} v_{i\beta} \delta(r - r_i) \\ \partial_\beta \pi^V_{\alpha\beta}(r) &= -f_\alpha(r) = -\sum_i \dot{p}_{i\alpha} \delta(r - r_i) = \sum_{i \neq j} \delta(r - r_i) \frac{\partial}{\partial r_{i\alpha}} v(r_{ij})\end{aligned} \tag{50}$$

Taking the Fourier transform, we obtain

$$\begin{aligned} K_{\pi_l\rho}(k) &= \frac{1}{V} \hat{k}_\alpha \hat{k}_\beta \langle \pi_{\alpha\beta}(k)\, \delta\rho(-k) \rangle \\ &= \rho T S(k) + \frac{ik_\alpha}{k^2} \int dR\, e^{-ik \cdot R} \langle f_\alpha(R + r)\, \delta\rho(r) \rangle \end{aligned} \tag{51}$$

Expressing the correlation function $\langle f_\alpha\, \delta\rho \rangle$ in terms of integrals with u_2 and u_3,

$$\begin{aligned} \langle f_\alpha(R + r)\, \delta\rho(r) \rangle &= \rho^2 e^2 \frac{\hat{R}_\alpha}{R^2} [u_2(R) + 1] + \rho^3 e^2 \int d^3 r_1\, u_2(r_1) \frac{(R - r_1)_\alpha}{\|R - r_1\|^3} \\ &\quad + \rho^3 e^2 \int d^3 r_1 \frac{\hat{r}_{1\alpha}}{r_1^2} u_3(r_1, R) \end{aligned} \tag{52}$$

we deduce (in dimensionless units)

$$\frac{K_{\pi_l\rho}(k)}{\rho T} = S(q)\left(1 + \frac{3\Gamma}{q^2}\right) + \lambda(q) \tag{53}$$

$$\lambda(q) = \Gamma I\left[\frac{j_1(qx)}{qx^2}\right] + 3\Gamma L\left[\frac{j_1(qx)}{qx}\frac{x\cdot y}{y^3}\right] \tag{54}$$

where j_n indicates the spherical Bessel function of order n. Using the sum rules for u_3 (9) leads to

$$\lambda(q) = -I\left[\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{j_1(qx)}{q}\right)\right] + 3\Gamma I\left[\int_0^x dy\,\frac{j_1(qy)}{q}\right] \tag{55}$$

and taking the well-known properties of the Bessel functions into account (55) becomes

$$\lambda(q) = 1 - S(q)\left(1 + \frac{3\Gamma}{q^2}\right) \tag{56}$$

It follows from (53) and (56)

$$K_{\pi_l\rho}(k) = \rho T \tag{57}$$

This relation is well known and can be directly derived[(10,11)] from the conservation equations for momentum (49) and for density $\partial_t\rho + \partial_\alpha(g_\alpha/m) = 0$. Therefore we have shown that (57) is true if the sum rules (9) [which follow from the hierarchy (6)] are true.

Inversely, starting from the relation (57) and the expression (51) of $K_{\pi_l\rho}$, we deduce with the help of the Bessel functions properties that

$$\langle f_\alpha(R+r)\,\delta\rho(r)\rangle = \rho^2 T\frac{\partial}{\partial R_\alpha}u_2(R) \tag{58}$$

and taking account of the expression (52) for that correlation function, it is easily seen that we obtain the hierarchy (6).

That proves that the equation (57) is equivalent to the hierarchy (6) (in the clustering hypothesis) and it must be noticed that the proof fails if the velocities are correlated and not distributed according to the Maxwellian.

7. ENERGY–DENSITY CORRELATION

Here we are dealing with the definition of the energy density and its correlation with the density. It is easily seen that a slow decrease at large distance is to be expected when two potentials $v(R)$ occur in a correlation function. A simple example is the potential–potential correlation which decreases as $1/R$ at infinity.[12] The total Coulombic potential

$$\phi(r) = \frac{1}{e} \int dr_1\, v(r - r_1)\, \rho(r_1) \tag{59}$$

has the following self-correlation function

$$e^2 \langle \phi(R+r)\, \phi(r) \rangle = \rho \int dr_1\, v(R - r_1) \left[v(r_1 + \rho \int dr_2\, u_2(r_2)\, v(r_1 + r_2) \right] \tag{60}$$

which behaves at infinity as

$$\langle \phi(r+R)\, \phi(r) \rangle \underset{R \to \infty}{\simeq} \frac{T}{R} (-3\Gamma I_4) = \frac{T}{R} \tag{61}$$

If we take the following potential energy density,

$$\varepsilon^V(r) = \left[\frac{E^2(r)}{8\pi} \right]_{\mathrm{SL}} \tag{62}$$

where $E_\alpha(r)$ is the electric field, deriving from the potential ϕ (59)

$$E_\alpha(r) = -\partial_\alpha \phi(r) \tag{63}$$

it is easily seen that the correlation function $\langle \delta\varepsilon^V\, \delta\rho \rangle$ decreases at large distance like R^{-6}:

$$\langle \delta\varepsilon^V(r+R)\, \delta\rho(r) \rangle \underset{R \to \infty}{\simeq} \left(\frac{3}{4\pi} \right)^2 \frac{T}{R^6} \Gamma L(x \cdot y) = \frac{3}{8\pi^2} \frac{T}{R^6} \tag{64}$$

The Fourier transform of this function includes a term in k^3 as k tends to zero. That long-range correlation disappears if the self-term is kept in (62) (of course spatially extended charges are then needed in order to avoid divergences at small distances). Only the total field is screened and therefore the exclusion of some terms removes more or less the perfect screening.

Keeping the self-term in ε^V makes the situation more complicated because of the change in the potential $v(r)$ at small distances. It is more interesting to take into account that the energy density is multivalued and to modify the definition of ε^V (and of course the definition of the associated current). The difference with respect to (62) has to be the divergence of a vector. That is true for

$$\varepsilon^V(r) = \frac{1}{2} e[\delta\rho(r)\, \phi(r)]_{\mathrm{SL}} = \frac{1}{2} \int dr_1\, v(r - r_1)[\delta\rho(r)\, \delta\rho(r_1)]_{\mathrm{SL}} \tag{65}$$

because of the following relationship[2]

$$\frac{E^2}{8\pi} = \frac{1}{2} e\delta\rho(r)\, \phi(r) + \operatorname{div}\left(-\frac{\phi E}{8\pi}\right) \tag{66}$$

The correlation of ε^V of (65) with the density is

$$\langle \delta\varepsilon^V(r+R)\, \delta\rho(r) \rangle = \frac{1}{2} \rho^3 \int dr_1\, v(r_1)\, u_3(r_1, R) + \frac{1}{2} \rho^2 \delta(R) \int dr_1\, v(r_1)\, u_2(r_1)$$
$$+ \frac{1}{2} \rho^2 v(R)\, u_2(R) \tag{67}$$

That function decreases faster than any power of the distance as R tends to infinity. Taking the Fourier transform we obtain

$$\frac{1}{V} \langle \delta\varepsilon^V(k)\, \delta\rho(-k) \rangle = \frac{3}{2} \rho T\Gamma \left\{ L\left[\frac{1}{x} \frac{\sin qy}{qy}\right] + I_1 + \frac{1}{3} I\left[\frac{\sin qx}{qx^2}\right]\right\}$$
$$\equiv \frac{3}{2} \rho T S(q)\, \alpha(q) \qquad (q = kr_0) \tag{68}$$

That last equation defines the function $\alpha(q)$.

The kinetic energy is

$$\varepsilon^K(r) = \sum_i \frac{p_i^2}{2m} \delta(r - r_i) \tag{69}$$

[2] This is only possible in the classical (nonrelativistic) limit, where curl $E = 0$. This ε^V has the meaning of potential energy density for the particles and not of field energy density. The radiative effects are excluded out of this framework. The associated current j_ε^V, defined apart from a curl of a vector, is $[c(E \times B/4\pi) - \partial_t(\phi E/8\pi)]_{\mathrm{SL}}$, where B is the magnetic field which is obtained from the Maxwell equations

$$\operatorname{div} B = 0, \qquad \operatorname{curl} B = \frac{1}{c}(\partial_t E + 4\pi e j)$$

j is the particle current. j_ε^V is not confined to the particles, like for the non-Coulombic fluids, because the forces acting on the particles change their energies. In the limit of small wave vector, the two quantities (62) and (65) become identical.

and thus the correlation of the total energy density $\varepsilon = \varepsilon^K + \varepsilon^V$ with the density is given by

$$\frac{1}{V}\langle \delta\varepsilon(k)\,\delta\rho(-k)\rangle = \frac{3}{2}\,\rho T S(q)[1+\alpha(q)] \tag{70}$$

Taking account of (16), (31), and (45), it is easy to show that $\alpha(q)$ tends to a finite limit as q tends to zero:

$$\frac{3}{2}[1+\alpha(0)] = -\frac{3}{2}\left[1+\frac{9\Gamma^2}{20}I_6\right] = \beta\frac{\partial\varepsilon}{\partial\rho}\bigg|_T \qquad (\varepsilon=\rho e) \tag{71}$$

and thus it follows that

$$\langle \delta\varepsilon(k)\,\delta\rho(-k)\rangle \underset{k\to 0}{=} \frac{\partial\varepsilon}{\partial\rho}\bigg|_T \langle \delta\rho(k)\,\delta\rho(-k)\rangle + O(k^4) \tag{72}$$

With the *definition* of the temperature fluctuation

$$\delta\varepsilon(r) = \frac{\partial\varepsilon}{\partial\rho}\bigg|_T \delta\rho(r) + \frac{\partial\varepsilon}{\partial T}\bigg|_\rho \delta T(r) \tag{73}$$

we deduce that the temperature–density correlation tends to zero at least as fast as k^4 at small wave vectors:

$$\lim_{k\to 0}\frac{1}{V}\langle \delta T(k)\,\delta\rho(-k)\rangle\frac{1}{k^4} < \infty \tag{74}$$

8. ENERGY–ENERGY CORRELATION

With the definition (65) of $\varepsilon^V(r)$, the function $\langle \delta\varepsilon^V(r+R)\,\delta\varepsilon^V(r)\rangle$ well exhibits a spatial decay faster than any power of the distance. A direct calculation (with no use of sum rules for the Ursell function) leads to

$$\frac{1}{V}\langle \delta\varepsilon^K(k)\,\delta\varepsilon^K(-k)\rangle = \rho T^2\left[\frac{3}{2}+\frac{9}{4}S(q)\right]$$

$$\frac{1}{V}\langle \delta\varepsilon^K(k)\,\delta\varepsilon^V(-k)\rangle = \frac{3}{2}\mathrm{T}\frac{1}{V}\langle \delta\varepsilon^V(k)\,\delta\rho(-k)\rangle$$

$$\frac{1}{V}\langle \delta\varepsilon^V(k)\,\delta\varepsilon^V(-k)\rangle \equiv \frac{1}{V}\langle \delta\varepsilon^V(k=0)\,\delta\varepsilon^V(k=0)\rangle + \frac{9}{4}\rho T^2 S(q)\,\beta(q)$$

$$\begin{aligned}\frac{1}{V}\langle \delta\varepsilon^V(k=0)\,\delta\varepsilon^V(k=0)\rangle = \rho T^2\frac{\Gamma^2}{2}\bigg\{&\frac{9}{2}M\left[\frac{1}{\|x-y\|}\frac{1}{z}\right] + 6L\left[\frac{1}{xy}\right]\\ &+\frac{3}{\pi}\int_0^{+\infty}\frac{dq}{q^2}S^2(q) - \frac{27}{4}K - \frac{9}{2}I_3 + 3I_0\bigg\}\end{aligned} \tag{75}$$

where K is the integral

$$K=\int \frac{d^3x\, d^3y}{(4\pi)^2}\, u_2(x)\, u_2(y)\, \|x-y\|, \qquad \frac{3}{\pi}\int_0^{+\infty} \frac{dq}{q^2}\, S^2(q) = -\frac{27}{4}K - \frac{9}{2} I_3 \tag{76}$$

The four point integral in (75) can be expressed in term of three-point integrals (34)

$$M\left[\frac{1}{\|x-y\|\, z}\right] = -\frac{2}{\Gamma} L\left[\frac{1}{x}\right] - \frac{4}{3} L\left[\frac{1}{xy}\right] + \frac{2}{3} L\left[\frac{\hat{x}\cdot\hat{y}}{x^2}\right] - \frac{2}{3} L[\hat{x}\cdot y]$$
$$-\frac{1}{6} L[x] + L\left[\frac{x^2}{y}\right] + 3K \tag{77}$$

Substituting this expression in (75), we notice that the unknown integral $L[1/xy]$ disappears and, using the expressions (11) and (16) of the other three-point integrals, we obtain

$$\frac{1}{V}\langle \delta\varepsilon^V(k=0)\, \delta\varepsilon^V(k=0)\rangle = \rho T^2\left[6\Gamma I_1 + 9 + \frac{81}{40}\Gamma^2 I_6\right] \tag{78}$$

which is equal to $\rho T^2 c_v^V$ (45), c_v^V being the potential part of the specific heat per particule at constant volume

$$c_v^V = -\Gamma^2 \frac{\partial}{\partial\Gamma}\frac{\beta e^V}{\Gamma} = \beta e^V - \Gamma\frac{\partial}{\partial\Gamma}\beta e^V = c_v - \frac{3}{2} \tag{79}$$

The energy–energy correlation function follows:

$$\frac{1}{V}\langle \delta\varepsilon(k)\, \delta\varepsilon(-k)\rangle = \rho T^2 c_v + \frac{9}{4}\rho T^2 S(q)[1 + 2\alpha(q) + \beta(q)] \tag{80}$$

When q tends to zero, $\alpha(q)$ and $\beta(q)$ are finite and that function well tends to $\rho T^2 c_v$ as it is expected for the energy fluctuation in the canonical ensemble.

9. CONCLUSION

We have first deduced, from the hierarchy, perfect screening conditions and sum rules for the Ursell functions u_2, u_3, and u_4 (under exponential clustering assumption). By using symmetries of the Ursell functions, some other new three- and four-point integrals have been calculated. In this manner, the temperature derivatives of the two-point integrals can be expressed in terms of three-point integrals (instead of four-point integrals) which reduce to two-point integrals in a few cases. It follows the relationship between I_6 and the compressibility.

Secondly, we have been concerned with the energy density, we have shown that some care has to be taken with the definition of that quantity in order to avoid correlations decreasing as powers of the distance.

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APPENDIX

Until now we have considered the moments of u_2. Sometimes it is more interesting to use the moments of the structure factor $S(q)$. Both sets of moments are related because $S(q)-1$ is the Fourier transform of u_2

$$u_2(x)=g_2(x)-1=\frac{2}{3\pi}\int_0^{+\infty} dq\, q^2\frac{\sin qx}{qx}[S(q)-1] \tag{A1}$$

$$S(q)-1=3\int_0^{+\infty} dx\, x^2\frac{\sin qx}{qx}u_2(x) \tag{A2}$$

We assume that (i) $S(q)-1$ and $u_2(x)$ decrease faster than any negative power of q or x when these quantities tend to infinity, (ii) $x^{-n}g_2(x)$ tend to zero as x goes to zero, whatever integer n is, (iii) I_2 is equal to $-1/3$. The moments of u_2, I_n, are defined in (7) and the moments J_n of $S(q)$ are defined in the following way:

$$\begin{aligned}
J_n&=\int_0^{+\infty} dq\, q^n[S(q)-1] \quad (n\geqslant 0)\\
J_{Ln}&=\int_0^{+\infty} dq\, q^n\log q[S(q)-1] \quad (n\geqslant 0)\\
J_{-2n}&=\int_0^{+\infty}\frac{dq}{q^{2n}}\left[S(q)-1-3\sum_{p=0}^{n-1}\frac{(-1)^p}{(2p+1)!}q^{2p}I_{2p+2}\right] \quad (n\geqslant 1)\\
J_{-(2n+1)}&=\lim_{\varepsilon\to 0}\left\{\int_\varepsilon^{+\infty}\frac{dq}{q^{2n+1}}\left[S(q)-1-3\sum_{p=0}^{n-1}\frac{(-1)^p}{(2p+1)!}q^{2p}I_{2p+2}\right]\right.\\
&\quad\left.+3\frac{(-1)^n}{(2n+1)!}I_{2n+2}\log\varepsilon\right\} \quad (n\geqslant 1)\\
J_{-1}&=\lim_{\varepsilon\to 0}\left[\int_\varepsilon^{+\infty}\frac{dq}{q}[S(q)-1]+3I_2\log\varepsilon\right]
\end{aligned} \tag{A3}$$

A first property follows from the zero value of $g_2(x)$ and all its derivatives at the origin. Expanding $(\sin qx)/qx$ (in power of qx) in (A1) we obtain

$$J_2 = -\frac{3\pi}{2}, \qquad J_{2n} = 0 \quad (n \geqslant 2) \tag{A4}$$

That shows that $S(q) - 1$ always exhibits negative and positive values whatever Γ is.

The odd moments J_{2p+1} $(p \geqslant 1)$ are related to the moments I_{-2p}. We start from

$$I_{-2p} = \lim_{\varepsilon \to 0} \left[\int_\varepsilon^{+\infty} \frac{dx}{x^{2p}} u_2(x) + \frac{\varepsilon^{-(2p-1)}}{2p-1} \right] \qquad (p \geqslant 1) \tag{A5}$$

substitute (A1) for $u_2(x)$ and change the order of integrating. Taking (A4) into account, we obtain

$$I_{-2p} = \frac{1}{3} \frac{(-1)^p}{(2p)!} J_{2p+1} \geqslant 0 \quad (p \geqslant 1), \qquad I_0 = \frac{1}{3} J_1 \tag{A6}$$

The calculation of $I_{-(2p+1)}$ is made in the same way; there appear exponential integral functions $E_n(\varepsilon)$ which are expanded in the limit $\varepsilon \to 0$. It follows that

$$I_{-1} = -(1-\gamma) - \frac{2}{3\pi} J_{L2}, \qquad I_{-(2p+1)} = \frac{(-1)^{p+1}}{(2p+1)!} \frac{2}{3\pi} J_{L2p+2} \geqslant 0 \quad (p \geqslant 1) \tag{A7}$$

where $\gamma = 0.577...$ is Euler's constant.

The moments J_{-n} are related to the moments I by a similar calculation

$$J_0 = \frac{3\pi}{2} I_1, \qquad J_{-2p} = \frac{3\pi}{2} \frac{(-1)^p}{(2p)!} I_{2p+1} \quad (p \geqslant 1)$$

$$J_{-(2p+1)} = 3 \frac{(-1)^{p+1}}{(2p+1)!} [I_{L2p+2} - \psi(2p+2) I_{2p+2}] \qquad (p \geqslant 0) \tag{A8}$$

$$\psi(n+1) = -\gamma + \sum_{m=1}^{n} \frac{1}{m} \qquad (n \geqslant 1)$$

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