Correlation functions in statistical mechanics and astrophysics

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A general review of distribution functions reveals that the two- and three-point correlation functions familiar to galaxy studies may be identified with the total correlation functions relevant to the study of liquids. In this context a discussion is included of the Peebles-Groth three-point correlation function. A recently derived two-point correlation function in polynomial form is reviewed. Renormalization of this expression is found to bring it into very good agreement with the well-established $r^{-\gamma}$ form (where r is intergalaxy displacement and γ is a constant).

I. INTRODUCTION

The principal spatial correlation functions in the study of liquids are the radial distribution function and the total correlation function.[1–4] Such functions describe the spatial correlations between sets of two or more particles in a material. Spatial correlation functions in galaxy correlation work are called the two-point correlation function, three-point correlation function, etc.[5–8]

In the present work these two formalisms are compared and it is concluded that the s-point correlation function of astrophysics may be identified with the s-particle total correlation function of statistical mechanics. The disparity between the Peebles-Groth[6] three-point correlation and the Kirkwood superposition relevant to fluids is reviewed. An alternative form of the three-particle radial distribution is illustrated which is shown to imply the Peebles-Groth function. A discussion is included of a recently derived two-point correlation function[8] which, in the present work, is brought into agreement with empirical results through proper normalization.

II. ANALYSIS

A. Correlation functions

1. Definitions

Let $F_N(1,\ldots,N)$ represent the N-body joint probability distribution relevant to an aggregate of N identical bodies of mass m which occupy a volume V. The variable "1" represents phase coordinates $\mathbf{x}_1$ and $\mathbf{v}_1$ where $\mathbf{x}$ is displacement and $\mathbf{v}$ is velocity.

Correlation functions $\{C_2(1,2),C_3(1,2,3),\ldots\}$ are defined through the mapping[4]

$$F_2(1,2)=F_1(1)F_1(2)+C_2(1,2)\ ,$$
$$F_3(1,2,3)=F_1(1)F_1(2)F_1(3)+\sum_{P(1,2,3)}F_1(1)C_2(2,3)+C_3(1,2,3)\ , \tag{1}$$
$$\ldots .$$

The sum in the second equation is over the permutations of the phase variables 1,2,3. Note in particular that if bodies are uncorrelated then $F_2=F_1F_1$, etc., and all correlation functions vanish.

2. Equilibrium distributions

In the absence of external potentials, the equilibrium one-body distribution is given by the Maxwellian

$$F_0(v)=\frac{n}{(2\pi)^{3/2}C^3}\exp\left[-\frac{v^2}{2C^2}\right]\ , \tag{2}$$

where $n=N/V$ is number density and C is thermal speed,

$$C^2\equiv\tfrac{1}{3}\langle(v-\langle v\rangle)^2\rangle=\frac{k_BT}{m}\ . \tag{3}$$

In astrophysics this variance is called the rms proper peculiar speed.[8]

The distribution (2) has the normalization

$$\int_0^\infty F_0(v)4\pi v^2dv=n\ . \tag{4}$$

The key spatial correlation functions of statistical mechanics are defined as follows. The total correlation function $h_2(r)$ is given by

$$F_2(1,2)=F_0(1)F_0(2)[1+h_2(r)]\ , \tag{5}$$

where r is written for interparticle displacement

$$\mathbf{r}\equiv|\mathbf{x}_1-\mathbf{x}_2|\ . \tag{5a}$$

Note that with (1) we may write

$$C_2(1,2)=F_0(1)F_0(2)h_2(r)\ . \tag{6}$$

If particles are uncorrelated then $h_2(r)=0$. The radial distribution $g_2(r)$ is given by

$$F_2(1,2)=F_0(1)F_0(2)g_2(r) . \tag{7}$$

If particles are uncorrelated, $g_2(r)=1$. With (5) and (6) we may write[9]

$$h_2(r)=g_2(r)-1 . \tag{8}$$

For liquids, $g_2(r)$ is constructed from neutron scattering data in conjunction with the structure factor.[2]

3. *Limiting values*

In fluids, boundary values of these functions are given by

$$\begin{aligned} &g_2(0)=0, \quad h_2(0)=-1 , \\ &g_2(\infty)=1, \quad h_2(\infty)=0 . \end{aligned} \tag{9}$$

The first two equations reflect the impenetrability of constituents in the fluid. The latter two equations assume that constituent particles grow uncorrelated with separation.

4. *Higher-order correlations*

Three-particle correlations are defined as follows. The three-body total correlation function is given by

$$F_3(1,2,3)=F_0(1)F_0(2)F_0(3) \times \left[1+\sum_{\substack{i,j\\ i\neq j}} h_2(r_{ij})+h_3(r_{12},r_{23},r_{31})\right] , \tag{10}$$

where i and j run from 1 to 3. The three-particle radial distribution is given by

$$F_0(1,2,3)=F_0(1)F_0(2)F_0(3)g_3(r_{12},r_{23},r_{13}) . \tag{11}$$

It follows that

$$g_3(r_{12}r_{23}r_{31})=1+\sum_{\substack{i,j\\ i\neq j}} h_2(r_{ij})+h_3(r_{12},r_{23},r_{31}) . \tag{12}$$

The dependence of spatial distributions on interparticle displacements r_{ij}, as in (5) *et seq.*, is relevant to a fluid invariant under translation and rotation.[10]

B. Kirkwood superposition and canonical forms

In obtaining closed equations for correlation functions for liquids assorted approximations are introduced.[1,2] Thus, for example, in the Kirkwood superposition one sets

$$g_3^K(r_{12},r_{23},r_{13})=g_2(r_{12})g_2(r_{23})g_2(r_{13}) . \tag{13}$$

This decomposition may be related to the canonical distribution,

$$F_N^{(0)}(1,\ldots,N)=A_N e^{-\beta K}G_N(\mathbf{x}_1,\ldots,\mathbf{x}_N) , \tag{14}$$

as follows. In (14), K represents kinetic energy, $\beta\equiv 1/k_BT$, A_N is a normalization constant, G_N is the configuration term

$$G_N=\exp\left[-\beta\sum_{\substack{i,j\\ i\neq j}}\varphi(r_{ij})\right] , \tag{15}$$

and $\varphi(r_{ij})$ represents the two-body potential. Integrating (14) we find

$$\begin{aligned} \int F_N^0(d\mathbf{v})^N d\mathbf{x}_4 d\mathbf{x}_5\cdots d\mathbf{x}_N &= A_3\exp\{-\beta[\varphi(r_{12})+\varphi(r_{23})+\varphi(r_{13})]\} \\ &=g_3(r_{12},r_{23},r_{13}) , \end{aligned} \tag{16}$$

where the second equality in (16) follows from (11). The relation (16) strongly motivates the decomposition (13) as well as the low-density approximation[1,2]

$$g_2(r)\propto e^{-\beta\varphi(r)} . \tag{17}$$

For further reference the Kirkwood superposition is written in terms of total correlations. With (12) and (13) we obtain

$$\begin{aligned} h_3^K(r_{12},r_{23},r_{13})=&h_2(r_{12})h_2(r_{23})h_2(r_{13}) \\ &+\sum_{P(i,j,k)} h_2(r_{ij})h_2(r_{jk}) . \end{aligned} \tag{18}$$

In the sum over permutations, terms like ijk and kji are counted once. The relation (18) is returned to below.

C. Correlation functions in astrophysics

Integrating (5) over velocity and recalling the normalization (4) gives

$$\int F_2(1,2)d\mathbf{v}_1 d\mathbf{v}_2=n^2[1+h_2(r)] . \tag{19}$$

Let δV_1 and δV_2 denote volume elements so that

$$\delta V_1\delta V_2\int F_2 d\mathbf{v}_1 d\mathbf{v}_2=\delta P \tag{20}$$

represents the probability of finding galaxies in δV_1 and δV_2 separated by the distance r. Relabeling

$$h_2(r)\rightarrow\xi(r) , \tag{21}$$

(19) and (20) give

$$\delta P=n^2[1+\xi(r)]\delta V_1\delta V_2 . \tag{22}$$

This equation is found in most works on galaxy correlations,[5–8] and $\xi(r)$ is called the two-point correlation function. We see that it is identical to the total correlation function familiar to statistical mechanics. The function $\xi(r)$ is determined from measured values of the angular galaxy correlation function in conjunction with Limber's rule[11,5]

Continuing in this manner, integrating (10) over velocities and multiplying by $\delta V_1\delta V_2\delta V_3$ we obtain

$$\delta V_1\delta V_2\delta V_3\int F_3 d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{v}_3 =n^3\left[1+\sum_{\substack{i,j\\ i\neq j}} h_2(r_{ij})+h_3(r_{12},r_{23},r_{13})\right] . \tag{23}$$

Calling the left-hand side of this equation δP and setting

TABLE I. List of nomenclature for correlation functions in statistical mechanics and astrophysics.

Name	Statistical Mechanics	Astrophysics	Name
Radial distribution	$g(r)$ or $g_2(r)$		
Total correlation	$h(r)$ or $h_2(r)$	$\xi(r)$	Two-point correlation
Three-particle total correlation	$h_3(r_{12},r_{23},r_{13})$	$\zeta(r_{12},r_{23},r_{13})$	Three-point correlation
s-particle total correlation	$h_s(r_{12},r_{23},\ldots)$	$\zeta_s(r_{12},r_{23},\ldots)$	s-point correlation

$$h_3 \rightarrow \zeta \tag{24}$$

together with (21) gives

$$\delta P = n^3 \left[1+\sum_{i,j}\xi(r_{ij})+\zeta(r_{12},r_{23},r_{13})\right]\delta V_1 \delta V_2 \delta V_3 \ . \tag{25}$$

Here δP represents the probability of finding galaxies in each of the volumes δV_1, δV_2, and δV_3 with separations r_{12}, r_{23}, and r_{13}. The relation (25) is the form popular to galaxy correlation functions. With (23) we see that the three-point correlation function ζ of astrophysics may be identified with the three-particle total correlation function of statistical mechanics, h_3. A list of these comparisons is given in Table I.

D. Peebles-Groth superposition

The Pebbles-Groth[6] approximation of the three-point correlation function is given by

$$\zeta^P(r_{12},r_{23},r_{13}) = Q \sum_{P(i,j,k)} \xi(r_{ij})\xi(r_{jk}) \ . \tag{26}$$

The constant Q has the value

$$Q = 1.3 \pm 0.2 \ . \tag{26a}$$

Comparing the form (26) with the Kirkwood relation (18) reveals that the Peebles-Groth superposition ignores the three-body product form in (18). Nonetheless it has been noted[5] that (26) gives good agreement with measured angular galaxy correlations.

We wish to illustrate the three-particle radial distribution that implies (26). It is given by the symmetric form

$$g_3^P = Q\{g_2(r_{12})[g_2(r_{23})-1]+g_2(r_{23})[g_2(r_{13})-1] + g_2(r_{13})[g_2(r_{12})-1]\}+1 \tag{27}$$

or, equivalently,

$$g_3^P(r_{12},r_{23},r_{13}) = Q \sum_{P(i,j,k)} g_2(r_{ij})h_2(r_{jk})+1 \ . \tag{27a}$$

The $g_2(r_{ij})$ factor of each product on the right-hand side of (27a) gives the probability of finding galaxies i and j separated by r_{ij}, whereas the $h_2(r_{jk})$ factor gives the correlation of galaxy j with galaxy k separated by r_{jk}.

The validity that (27) implies (26) rests on the assumption that $Q \simeq 1$ which, with (26), is seen to be a reasonable assumption. Let us derive this result. Comparing g_3^P (27) with the generic form (12) gives (in astrophysical terminology)

$$\begin{aligned} \sum\xi+\zeta &= Q\sum(1+\xi)\xi \ , \\ \zeta &= Q\sum\xi\xi+(Q-1)\sum\xi \ . \end{aligned} \tag{28}$$

With the said assumption concerning Q, (28) establishes the equivalence of (27) to (26). It is also noted that the two-point galaxy correlation function ξ is typically greater than 1, in which case products of ξ may be assumed to be somewhat larger than linear terms in ξ.

III. TWO-POINT GALAXY CORRELATIONS

A. Previous results

For galaxy interactions, the two-body potential is given by

$$\varphi(r) = -\frac{Gm_1 m_2}{r} \ , \tag{29}$$

where m_1 and m_2 are galaxy masses and G is the gravitational constant. A distinct difference between molecular correlation in liquids and galaxy correlation in the universe is obtained by substituting the potential (29) into the approximate form (17). For small r one finds that $\xi(r) \rightarrow \infty$ in dramatic difference with the boundary value given in (9). For large r, we see that correlations vanish in agreement with the result for liquids. See Table II.

A number of calculations and observations have suggested the following form[12–14] for the two-point correlation function:

$$\xi_P(r) = (r_0/r)^\gamma \ . \tag{30}$$

In 1974 Peebles[15] obtained the values

$$\gamma = 1.77 \pm 0.44, \quad r_0 = (4.3 \pm 0.3)h^{-1} \text{ Mpc}$$

relevant to the domain

$$0.1h^{-1} \text{ Mpc} \le r \le 9h^{-1} \text{ Mpc} \ . \tag{31}$$

For purposes of comparison, the form (30) is labeled $\xi_P(r)$. The nondimensional factor h^{-1} in (31) is included

TABLE II. Limiting values of correlation functions for molecular and galactic media. In the present discussion, for galaxies, r lies in the domain given by (30). The scale length $a \simeq n^{-1/3}$, where n is the molecule or galaxy number density.

Medium	$r \ll a$	$r \gg a$
Liquids	$h \sim -1$	$h \sim 0$
Galaxies	$\xi \sim \infty$	$\xi \sim 0$

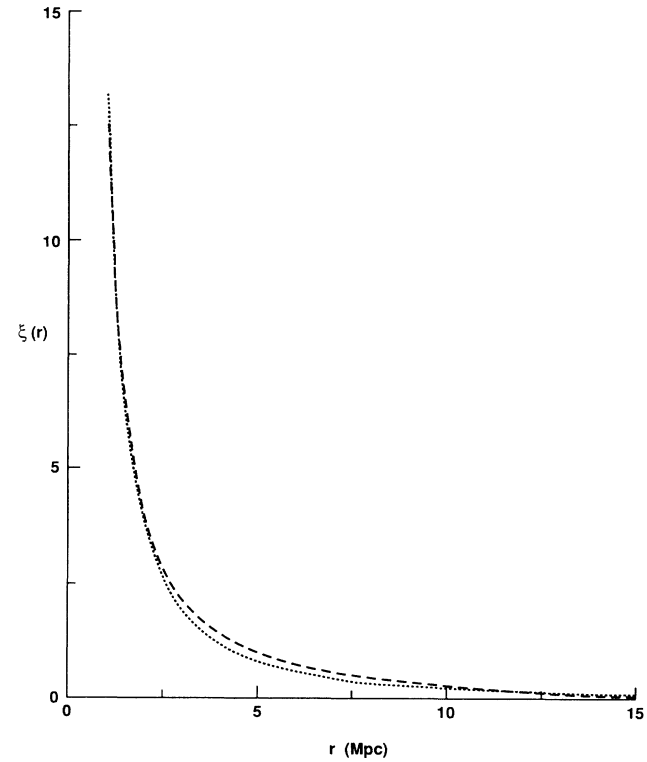

FIG. 1. Graphs of $\xi_{GL}(r)$ as given by (32) with $D=0.61$ and $R_{THS}=13$ Mpc vs $\xi_P(r)$ as given by (30) with $\gamma=1.77$ and $r_0=4.3$ Mpc. Correlation functions are labeled as follows: ξ_{GL}, — — —; ξ_P, · · · · ·.

as an expression of uncertainty in astronomical distances and is given by

$$h=H_0/[100\ (\text{km/sec})/\text{Mpc}]\ ,$$

where H_0 is Hubble's constant, which lies between 40 and 100 (km/sec)/Mpc.[16]

B. New two-point correlation functions

In a more recent work[8] stemming from the Bogolivbov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy,[4] and angular correlation data, and taking into account strong coupling between galaxies, the following two-point correlation function was obtained:

$$\xi_{GL}(r)=D(0.09\bar{r}^{\,-2}+0.42\bar{r}^{\,-1}-0.31\bar{r})\ , \qquad (32)$$

where D is a constant $\simeq 1$ and

$$\bar{r}\equiv r/R_{THS}\ . \qquad (32a)$$

The parameter R_{THS} (radius of the "thermal Hubble sphere") is given by

$$R_{THS}\equiv H_0^{-1}C\ , \qquad (32b)$$

which was taken to be $\simeq 13$ Mpc. In the present work, a mean-square fit of (32) to $\xi_P(r)$ (see the Appendix) given by (30) reveals the value $D\simeq 0.61$. See Fig. 1. It should be noted that both $\xi_P(r)$ and $\xi_{GL}(r)$ give good agreement with measured angular galaxy correlations. The sharper decrease of $\xi_{GL}(r)$ for large r (i.e., $r \gtrsim 10$ Mpc) may be a precursor of oscillatory behavior of the total correlation function familiar to the study of strongly coupled fluids.[2,17]

IV. CONCLUSIONS

Correlation functions familiar to liquid and galaxy studies were compared. It was noted that the form relevant to galaxy work is commonly labeled the total correlation function in the study of liquids. Asymptotic values of these functions in liquid and galaxy theory were compared and found to agree at large two-body separation but to be vastly different at small values of displacement. A symmetric form of the three-particle radial distribution was presented which was found to return the Peebles-Groth three-point correlation approximation. Lastly, a new polynomial form for the two-point correlation function was reviewed which, through simple renormalization, was brought into good agreement with the well-established $r^{-\gamma}$ form.

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APPENDIX

Here is an outline of the mean-square fit of ξ_{GL} to ξ_P. First we divide the $r \gtrsim 0$ axis into segments of equal length. The ith segment is labeled r_i. The program then seeks to minimize the net square difference

$$R\equiv\sum_{i=1}^{N}[\xi_P(r_i)-\xi_{GL}(r_i)]^2\ . \qquad (A1)$$

Setting

$$\xi_{GL}(r_i)\equiv Df_{GL}(r_i) \qquad (A2)$$

and differentiating (A1) with respect to D gives

$$R'=-2\sum(\xi_P-Df_{GL})f_{GL}\ . \qquad (A3)$$

Setting $R'=0$ we obtain

$$D=\frac{\sum\xi_P f_{GL}}{\sum f_{GL}^2}\ .$$

This expression was used to obtain the cited value of D.

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