Fractals and Cosmological Large-Scale Structure

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Observations of galaxy-galaxy and cluster-cluster correlations as well as other large-scale structure can be fit with a "limited" fractal with dimension $D \approx 1.2$. This is not a "pure" fractal out to the horizon: the distribution shifts from power law to random behavior at some large scale. If the observed patterns and structures are formed through an aggregation growth process, the fractal dimension D can serve as an interesting constraint on the properties of the stochastic motion responsible for limiting the fractal structure. In particular, it is found that the observed fractal should have grown from two-dimensional sheetlike objects such as pancakes, domain walls, or string wakes. This result is generic and does not depend on the details of the growth process.

The origin of cosmological large-scale structure is probably the most pressing problem in physical cosmology today. Understanding the observed structure requires the use of quantitative methods to describe it. The measurement of the two-point galaxy-galaxy correlation function, that is, $\xi_{gg} \approx (r)^{-1.8}$, for separations r up to ~10 Mpc, marked the beginning of quantitative attempts to understand the large-scale structure of the universe (*1*). The two-point correlation function for clusters of galaxies appears to have similar behavior, but with higher amplitude (*2, 3*). Initial worries about projection effects biasing the results have been minimized somewhat by the result of West and Van den Bergh (*4*) for cD galaxies (cD's are associated with the core of rich clusters) and that of Lahav *et al.* (*5*) for x-ray clusters; these show the same behavior as the clusters. Several years ago, Szalay and Schramm (*6*) showed that the correlation functions could be written in a unified way by using a dimensionless variable r/L, where L is the average separation of objects in the catalog being examined: $\xi(r) = \beta(L)(r/L)^{-1.8}$. They found the correlation amplitude β (≈ 0.35) is a constant for all clusters of galaxies and is unity for galaxies. The slightly larger correlation for the galaxies in this scale-free approach is probably an indication of gravitational clustering.

The near constant behavior of β for clusters indicates that the clustering process may be roughly scale invariant or, in other words, that the structure is a fractal. But it is not a true fractal because it does not show power law behavior to infinite scale. Statements about a so-called "fractal universe" are therefore excessive. At scales $\gtrsim 100$ Mpc, the data are sufficiently poor that the power law correlation is not evident, and at very large scales we know that the universe is isotropic and not fractal from microwave observations and the relatively smooth distribution of objects on large scales (*7*). Thus, at best, the fractal is a limited fractal.

It is interesting that as the sampling of the universe gets larger and deeper, more observations appear to continue to support this limited-fractal hypothesis. As was shown in Bahcall and Chokshi [in (*9*)], Fig. 1 shows a summary of the current situation and our error bar estimates, with data points for correlation of superclusters (*8*), quasars (*9*), x-ray clusters (*5*), and the cD's at the center of superclusters (*4*), as well as recent work by Efstathiou [in (*10*)] with the Automated Plate Measuring (APM) survey that has supported this basic clustering behavior. For $10 \lesssim L \lesssim 100$ Mpc/h, $\beta(L)$ is nearly constant; the current best fit value is $\beta \approx 0.26$. Note that a power law correlation function with index 1.8 corresponds in three-dimensional (3-D) space to a fractal with $D = 1.2$.

The following questions arise when we discuss the possible fractal structures in the universe: How far out does the fractal correlation extend? What can we learn from the fractal dimension $D = 1.2$? What physical process can give rise to a fractal structure in the distribution of observable objects? At present these questions have ambiguous answers. Most researchers of fractal large-scale cosmological structure have either tried to assume a pure fractal structure (*11, 12*) or to emphasize how a pure fractal cannot explain the structure of the universe because of the isotropy of microwave radiation and the relatively uniform distribution of objects at large distances (*7*). A point that can be lost in such arguments is that if the universe is fractal-like for some range of scale, then some insight might be gained by looking at how such fractals can develop, even though the fractal is eventually truncated.

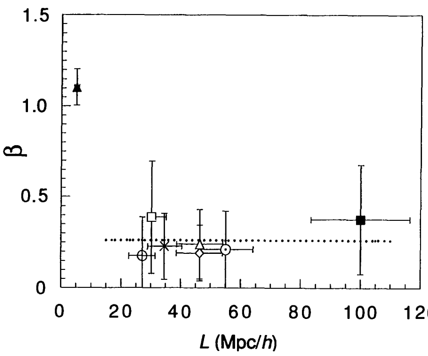

Fig. 1. The two-point correlation function can be expressed in the scale-invariant form: $\xi(r) = \beta(r/L)^{-1.8}$, where $L = n^{-1/3}$ is the mean distance between objects in a catalog, n is the mean density, and β is the dimensionless correlation amplitude. The best fit (broken line) to the updated observational data gives $\beta \approx 0.26$. The error bars represent ±50% uncertainty in the density, ±50% uncertainty in the correlation amplitude, and ±20% uncertainty in determining the power law index. (▲), Galaxies; (○), quasi-stellar objects; (□), Schectman; (◇), cDs; (×), APM; (△), x-ray; (⊙), Bahcall-Soniera ($R \geq 1$); and (■), supercluster.

If the fractal behavior is real, gravity alone cannot be used to explain it because the clustering amplitude of clusters would then not be higher than that of galaxies. Although some form of biasing (*13*) may be useful here, we instead see if accepting the fractal interpretation offers any useful insights. In particular, let us assume that some sort of fractal seed or growth process provides the fractal correlation while gravity enhances correlation amplitude on small scales. We find that applying fractal analysis techniques to large-scale matter distribution in the universe yields some interesting results.

There are two basic requirements to form large-scale structure: (i) primordial seeds or fluctuations (density perturbations) and (ii) the aggregation of matter to the seed (growth process). The correlation of seeds or density perturbations and the scaling behavior of growth processes are all responsible for any fractal structure we observe today, and it is interesting to find that most structure formation theories can be fitted in the category of emphasizing one or the other.

In a continuous clustering model (*14*)—for example, the variant of Mandelbrot (*11*), in which galaxies are placed on each step of a Levy flight (*11*)—the correlation between seeds is fully responsible for the fractal distribution of observed objects. The model is simple and successful in reproducing the observed correlation functions. For the Mandelbrot model the fractal dimension D enters the program through the ansatz of the probability distribution of Levy flight: for a random walk with step size l, $P(l) = 0$ for $l < l_0$; and $P(l) = Dl_0^D/l^{D+1}$ for $l > l_0$. Thus the model is more an empirical computational device than a true physically motivated growth process. It also has the problem of no natural truncation of the fractal at large scales. On the other hand, in the random Gaussian fluctuation model (*15*), the seeds are randomly distributed in a Gaussian manner. If the ampli-

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tude of the fluctuations is scale invariant, the model is able to reproduce the two-point correlation on a small scale ($\lesssim$10 Mpc). When the scale gets larger, some problems appear, as illustrated by the excess power observed on larger scales relative to the falloff in the model (*10*). (If biasing is invoked to fit the cluster correlations from the galaxy correlations, then the cluster correlation function is directly proportional to the galaxy correlation function. If the galaxy function should unambiguously be negative, then so should the cluster function on that scale. As of this time, the data are too ambiguous for this test to be made.)

Numerical modeling with N-body simulations has become the prime tool used in cosmology for exploring the aggregation of matter to seeds beyond linear gravitational perturbation theory [see (*16*)]. In general, matter undergoes a stochastic motion in space until it is gravitationally bound by seeds to form clumps, and the growth rate of the clump is controlled by the diffusing flux of matter onto the seed. The underlying physics of this kind of growth process can be modeled by DLA (diffusion-limited aggregation), and studies with the model show that the resulting aggregate has a well-defined scaling behavior (*17*).

In particular, the two assumptions used by Ball and Witten (*18*) in deriving their causality limits are that the aggregate grows by absorbing particles doing a random walk and that the aggregate is limited by diffusion. Both of these assumptions seem well justified in the cosmological case. In the growth of a traditional DLA fractal, the interaction of the diffusing particles with the aggregate is short ranged, and the aggregate does not grow until the diffusing particles are attached, so the aggregate is connected. In the cosmological case, because gravity is long ranged, the star cluster is more loosely bound. In this report we do not go into the details of a particular growth model but rather show that based on the growth process, the fractal dimension D can serve as an interesting constraint on the growth space, which is defined as the possible trajectories of the stochastic motion of matter clumps. The overall space is 3-D, but the stochastic motion is not necessarily 3-D.

The aggregate grows by absorbing particles that are randomly moving in d-dimensional growth space and the outer radius R of the aggregate grows with time, but dR/dt is limited by some value v, which is proportional to the density u of moving particles, because of the "shadow" effect, in which parts of a cluster begin to block the interior sites. In our case, the "shadow" effect also occurs for a different reason—when the material is used up, the sites adjacent to the "void" cannot grow. So, $dR/dt < v \approx u$. The quantity dR/dt is related to the change of mass M ($\approx R^D$) of the aggregate by $dR/dt = (dM/dt)/(dM/dR)$. The quantity dM/dt is also the rate at which the diffusing particles are first bounded by the aggregate:

$$\frac{dM}{dt} \approx uR^{d-2} \quad (1)$$

So

$$\frac{dR}{dt} \approx uR^{d-1-D} < v \approx u \quad (2)$$

thus

$$d - 1 - D \leq 0 \quad (3)$$

or

$$D \geq d - 1 \quad (4)$$

This is Ball and Witten's causality bound (*18*) on the fractal grown from a diffusion-limited process. The observed fractal dimension $D = 1.2$ implies that the dimension d of the growth space is less than 2.2. In other words, the growth space should involve a two-dimensional sheetlike object. This fact can constrain the properties of topological defects that might serve as seeds for large-scale structure. This result favors light domain walls (*19*), wakes of string (*20*), superconducting strings (the explosive model) (*21*), the pancake model (*22*), or collapsing textures (*23*). (Of course it says nothing about other problems these models may have, such as the microwave background y-parameter constraint on the explosive models, and so on.)

One consequence of embedding a fractal structure generation mechanism into the well-established big bang framework (*7*) is the prediction that the fractal correlation should break down at some scale. As pointed out by Peebles (*1*), a pure fractal contradicts the observed large-scale angular correlation function. It also has problems with microwave background isotropy. Because the growth process is limited by the diffusion of particles onto the aggregate, it can drop below the expansion rate of the universe. Furthermore, when the random motion of the matter is not constrained, the growth will be 3-D. From Eq. 4 we know that it is impossible to grow a $D = 1.2$ pure fractal in three dimensions with any kinematic growth process.

The breakdown scale of the fractal correlation can be estimated from the constraint of microwave background anistropy $\delta T/T \lesssim 10^{-5}$ in the extreme case of a sheetlike seed model, for example, light domain walls from a late-time phase transition. In the late time phase transition scenario, the cosmological seed and density perturbation is generated after the decoupling of the microwave background, which minimizes the cosmic blackbody radiation (CBR) anisotropy (*17, 24, 25*). However, significant non-Gaussian fluctuations can be produced, which may have large amplitudes (*24*). To grow a fractal extending to scale L, the aggregation of matter onto the seeds will perturb the cosmic microwave background (*24*),

$$\delta T/T \approx (9/32)(3\pi)^{1/2}(H_0L)^3\Omega_{\text{wall}} \quad (5)$$

where H_0 is the Hubble constant and Ω_{wall} is the ratio of present density of walls to the critical density, and the density perturbation $\delta\rho/\rho$ induced by a wall is estimated to be

$$\delta\rho/\rho \approx (3\pi^2/20)\Omega_{\text{wall}} \quad (6)$$

The fractal growth process can only proceed when $\delta\rho/\rho > 1$ or $\delta T/T \gtrsim (H_0L)^3$. So $\delta T/T < 10^{-5}$ implies $L \gtrsim 100h^{-1}$ Mpc, where the normalized Hubble constant is $h \equiv H_0/(100$ km s^{-1} Mpc$^{-1})$. This is a natural result because the horizon size at the time of structure formation serves as a cutoff for the fractal correlation. The horizon size R at the time of a late-time phase transition ($z \approx 1000$), $R \approx 3000$ Mpc $(h\sqrt{1+z})^{-1} \approx 100h^{-1}$ Mpc ≈ 200 Mpc, with $h = 0.5$. This agrees reasonably well with the previous argument.

The fractal argument not only casts further doubt on the 3-D–filling Gaussian fluctuation model with cold dark matter, but it also helps point the way toward plausible solutions.

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Metallo-Carbohedrenes [$M_8C_{12}^+$ (M = V, Zr, Hf, and Ti)]: A Class of Stable Molecular Cluster Ions

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Findings of magic peaks corresponding to $M_8C_{12}^+$ (M = V, Zr, and Hf) formed from reactions of the respective metals with various small hydrocarbons, in conjunction with recent findings for the titanium system, establish metallo-carbohedrenes as a stable general class of molecular cluster ions. A dodecahedral structure of T_h point symmetry accounts for the stability of these ionic clusters.

We report findings of magic peaks corresponding to $M_8C_{12}^+$ (where M is V, Zr, and Hf) which, along with prior observations for $Ti_8C_{12}^+$, now establish metallo-carbohedrenes as a class of stable molecular cluster ions. The question of whether a general class of such species exists was raised following recent reporting (*1*) of a prominent (magic) peak in the distributions of titanium-carbon clusters generated through reactions of the metal with hydrocarbons using a laser vaporization source. In view of the nature of the species, we raised the issue of whether $Ti_8C_{12}^+$ might be the first observed member of a new class of molecular clusters comprised of a cage-like network of carbon and metal atoms, possibly arranged in the form of a pentagonal dodecahedron. If metallo-carbohedrenes do exist, it is expected that other early transition metals should be capable of forming molecules of a similar type which would also display an unusual stability. A short while after the observation of $Ti_8C_{12}^+$, we extended our work to other transition metal systems, with particular attention to vanadium, and thereafter zirconium and hafnium. Like $Ti_8C_{12}^+$, all $M_8C_{12}^+$ (M is V, Zr, or Hf elements) also are found to display an enhanced stability.

The experiments were conducted with both a double mass spectrometer (MS/MS) system (*2*) and a time-of-flight (TOF) mass spectrometer (*3*) coupled with a laser vaporization source. Ionic species comprised of transition metal atoms and carbons are produced with a versatile laser-induced plasma reaction concept (*1*). Employing a simple laser vaporization device (*4*, *5*), the methodology enables the generation of pure metal-carbon and metal-nitrogen clusters in either neutral or ionized form. The details of the technique will be given elsewhere (*6*, *7*). Briefly, a high power laser is used to irradiate the surface of the metal. In the presence of a plasma containing both neutral and ionic metal species, fast dehydrogenation reactions with hydrocarbons occur. As a result, in many cases the hydrocarbons lose all hydrogens and pure metal-carbon clusters are generated. The distribution of the ionic species are analyzed with a quadrupole or TOF mass spectrometer.

Figure 1 shows a typical mass spectrum of vanadium-carbon cationic clusters produced from reactions with CH_4. Other small hydrocarbons yield a similar cluster distribution. The TOF spectrum was obtained with an electric pulser to attract the ionic clusters from the source and analyze them via TOF mass spectrometry. It is evident in this spectrum that the peak at a mass of 552 atomic mass units (amu) (magic peak) displays enhanced abundance compared to proximate clusters. Because the reactions involve three elements, the molecule corresponding to the magic peak could, in principle, have the molecular formula $V_aC_bH_c$, where *a*, *b*, and *c* are the number of vanadium, carbon, and hydrogen atoms contained in the molecule, respectively. However, the isotope-labeling experiments made with hydrocarbons containing deuterium and ^{13}C establish that the molecule has no hydrogen atoms at all and contains exactly 12 carbon atoms. Based on these facts and its mass position, the molecule is assigned as V_8C_{12}.

Figures 2 and 3 display the mass spectra of zirconium and hafnium-carbon cluster cations, respectively. These spectra were obtained under the same experimental conditions used to obtain Fig. 1, except the use of the zirconium or hafnium rods instead of the vanadium rod. Interestingly, the two spectra are seen to truncate at $Zr_8C_{12}^+$ and $Hf_8C_{12}^+$. It is well established that the intensity anomalies (magic numbers) observed in a mass spectrum of clusters reflect the stability of the corresponding cluster (*8*). Magic numbers do not always become manifested as prominent peaks, but more typically as a discontinuity, namely truncation in the present case, in an otherwise smoothly varying distribution, indicating the formation of geometric structures of special stability. Hence, the truncation seen in Figs. 2 and 3 indicates that $Zr_8C_{12}^+$ and $Hf_8C_{12}^+$ also display magic behavior.

Because Zr and Hf have a similar electronic structure to that of Ti, it is expected that the dodecahedron model proposed for $Ti_8C_{12}^+$ can rationalize the magic nature of the corresponding species, $M_8C_{12}^+$. As for the ionic form of V_8C_{12}, although the vanadium atom has one more electron than Ti, we believe that its geometric structure should also be dodecahedral, in which the vanadium atoms occupy eight unique positions. In order to gain supporting evidence for the proposed structure, we conducted titration experiments with ND_3 under thermal reaction conditions. In conducting

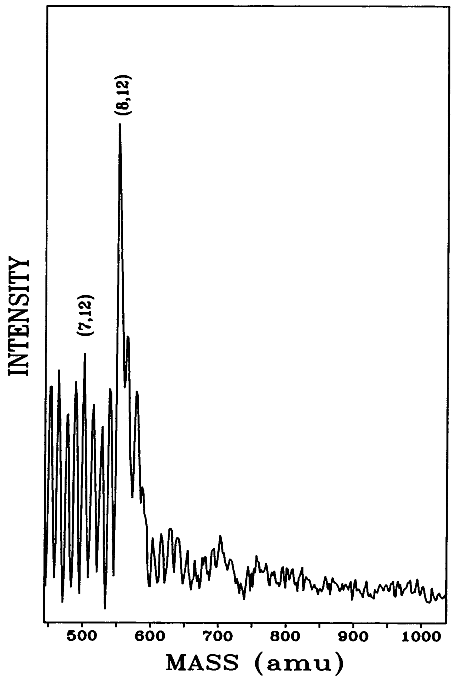

Fig. 1. Time-of-flight mass spectrum of vanadium-carbon cluster cations. The labeled magic peak is $V_8C_{12}^+$. Note that there are other prominent peaks proceeding the magic $M_8C_{12}^+$ which are precursors involved in the mechanism of formation of the cage-like metallo-carbohedrenes. Species with one- and two-carbon atoms attached to $M_8C_{12}^+$ are also visible, where some carbons remain on the magic structure upon its closing (*9*). Other precursors to the magic peak are seen, such as (7, 12).

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