The Number of Structures Compatible with any Specified Correlation Function

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Many experimental methods for the analysis of nanometer-scaled structures, most notably scattering methods, provide data in the form of correlation functions. However, a correlation function is an incomplete characterization because distinctly different microstructures may have the same correlation function. Patterson coined the word "homometric" to describe different structures having identical correlation functions [1].

We address the question of the enumeration of homometric structures. In other words: what is the number of microstructures compatible with a specified correlation function? We compute this in the framework of reconstruction methods. In this context, any microstructure having a two-point correlation function $S_2(r)$ is assigned an energy-like functional E defined as

$$E = \sum_r \left[S_2(r) - \hat{S}_2(r) \right]^2$$

where the sum is over all distances and $\hat{S}_2(r)$ is a target correlation function. This definition of E enables us to map the problem of the enumeration of all structures compatible with $\hat{S}_2(r)$ to the determination of a ground-state degeneracy [2]. A general Monte-Carlo algorithm is them used to calculate the ground-state degeneracy of a variety of microstructures such as realizations of hard disks and Poisson point processes with various densities. A few examples are given in Fig. 1.

The Monte Carlo results are explained in terms of the roughness of the energy landscape associated with the reconstruction problem. Since the configuration space of discrete microstructures is a hypercube on which a Hamming distance is defined, we can calculate analytically the energy profile of any reconstruction problem, corresponding to the average energy of all microstructures at a given Hamming distance from a ground state. The steepness of the energy profile is a measure of the roughness of the energy landscape. We show that this roughness metric - which is calculated analytically with no size or dimensionality restriction - can be used as a proxy for the ground-state degeneracy.

Finally, we show that the degeneracy can be expressed in terms of the information content of the two-point correlation functions [3]. From this perspective, the condition for a reconstruction to be accurate is that the information content, expressed in bits, should be comparable to the number of pixels in the unknown microstructure.

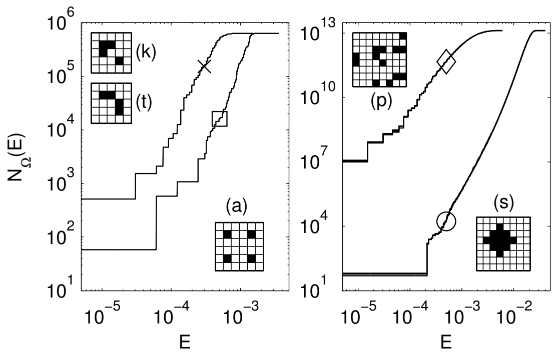

FIG. 1. Cumulative densities of states of various correlation functions, determined by the Monte-Carlo algorithm. structures (a) and (s) are uniquely determined by their correlation functions (□ and ◦); (k) and (t) have identical correlation functions (×); (p) is a realization of a Poisson process (⋄).

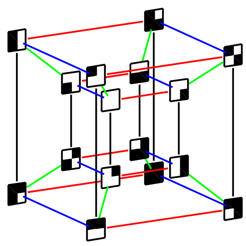

FIG. 2. The configuration space of discrete microstructures is a hypercube on which a Hamming distance is defined.

CJG is a Research Associate at the Funds for Scientific Research, Belgium. This work was done during a stay in the Department of Chemistry of Princeton University, in collaboration with Prof. S. Torquato and Dr. Y. Jiao.

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[3] C.J. Gommes, Y. Jiao and S. Torquato, Microstructural degeneracy associated with a two-point correlation function and its information content, Phys. Rev. E 85, 051140 (2012)

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