Point configurations have been widely used as model systems in condensed-matter physics, materials science, and biology. Statistical descriptors, such as the $n$-body distribution function $g_n$, are usually employed to characterize point configurations, among which the most extensively used is the pair distribution function $g_2$. An intriguing inverse problem of practical importance that has been receiving considerable attention is the degree to which a point configuration can be reconstructed from the pair distribution function of a target configuration. Although it is known that the pair-distance information contained in $g_2$ is, in general, insufficient to uniquely determine a point configuration, this concept does not seem to be widely appreciated and general claims of uniqueness of the reconstructions using pair information have been made based on numerical studies. In this paper, we present the idea of the distance space called the $D$ space. The pair distances of a specific point configuration are then represented by a single point in the $D$ space. We derive the conditions on the pair distances that can be associated with a point configuration, which are equivalent to the realizability conditions of the pair distribution function $g_2$. Moreover, we derive the conditions on the pair distances that can be assembled into distinct configurations, i.e., with structural degeneracy. These conditions define a bounded region in the $D$ space. By explicitly constructing a variety of degenerate point configurations using the $D$ space, we show that pair information is indeed insufficient to uniquely determine the configuration in general. We also discuss several important problems in statistical physics based on the $D$ space, including the reconstruction of atomic structures from experimentally obtained $g_2$ and a recently proposed “decorrelation” principle. The degenerate configurations have relevance to open questions involving the famous traveling salesman problem.

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I. INTRODUCTION

A collection of a finite or infinite number of points in $d$-dimensional Euclidean space $\mathbb{R}^d$ is called a point configuration. Point configurations are one of the most popular and widely used models for many-particle systems in various branches of modern science, including condensed-matter physics and materials science [1–5], statistical mechanics [6–8], discrete mathematics (packing problems) [9], astrophysics (distribution of galaxy clusters) [10,11], ecology (tree distributions in forests) [12], and biology (various cellular structures) [13]. Point configurations can exhibit a variety of degrees of disorder, from the most random Poisson distribution [2] to a perfectly ordered Bravais lattice [1]. The degrees of disorder can be quantified by discriminating order metrics [1,14], which, in their simplest forms, are scalars and normalized such that the most disordered system is associated with zero and the most ordered ones with unity.

In this paper, we focus on individual point configurations. In most circumstance, it is impossible and even unnecessary to acquire detailed knowledge of all positions of the points in a single configuration. Instead, statistical descriptors, such as distribution functions, are typically employed to characterize point configurations. In particular, the $n$-body distribution function $g_n(x_1,x_2,\ldots,x_n)$ is related to the probability of finding a generic configuration of $n$ points at positions $x_1,x_2,\ldots,x_n$. It is well known that a set of $n$-body distribution functions $g_1,g_2,\ldots,g_n$ [2] is required to statistically characterize an $n$-point configuration completely. As $n \to \infty$ in the thermodynamic limit (e.g., the volume $V$ which the $n$ points occupy also increases to infinity such that the number of points per volume—number density $\rho=\mathcal{N}/V$—is a well-defined finite number), the set contains an infinite number of correlation functions. For statistically homogeneous systems, which are the focus of this paper, $g_n$ is translationally invariant and hence depends only on the relative displacements of the positions with respect to some chosen origin, say $x_1$, i.e., $g_n(x_1,x_2,\ldots,x_n)=g_n(x_{12},x_{13},\ldots,x_{1n})$ with $x_{ij}=x_j-x_i$. Thus, the one-body distribution function $g_1$ is just equal to the number density $\rho$. The important two-body quantity $g_2(x_{12})$ is usually referred to as the pair distribution function. In the statistically isotropic case, $g_2$ is a radial function, i.e., $g_2(x_{12})=g_2(|x_{12}|)$ and it is also called the radial distribution function. The radial distribution function, which is one of the

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most widely used structural descriptors, essentially provides the distribution of the point-pair separation distances and can be obtained experimentally via scattering of radiation [1]. The three-body function $g_3$ contains information about how the pair separations involved in $g_2$ are linked into triangles.

It is worth noting that by decorating the points in the system (e.g., letting equal-sized spheres be centered at each point), one can construct a two-phase random texture from a given point configuration. In general, there is an infinite number of ways to decorate a point configuration. In the characterization of random textures, the analog of the $n$-body distribution functions are the $n$-point correlation functions $S_n(x_1, x_2, \ldots, x_n)$ [2], which give the probability of finding $n$ points at positions $x_1, x_2, \ldots, x_n$ in the phase of interest. In general, a complete statistical characterization of a continuum random texture requires an infinite set of $S_n$. Though under certain conditions, $g_2$ of a point configuration and $S_2^*$ of the associated decorated random texture might convey the same level of structural information (in fact the associated $S_2^*$ can expressed as functional of $g_2$, given the details of the decorating phase [2]), the former evidently reflects the essential geometrical features of the point configuration more directly.

An intriguing inverse problem that has been receiving considerable attention is the reconstruction (or construction) of configurations of a many-body system (essentially point configurations) that match the prescribed structural information of the system in the form of $g_2$ or $S_2$ obtained from either experiments or theoretical considerations. Examples include the reconstruction of random media [15–23] and colloidal suspensions [24], investigation of the iso-$g_2$ process [25] or $g_2$-invariant processes, and the realizability conditions of $g_2$ [26] as well as the more recent discovery of unusual disordered classical ground states [27]. X-ray scattering techniques have been an indispensable tool historically in the study of the structures of crystalline matter, and it has been generalized to probing disordered media [1]. In particular, the pair distribution function $g_2(r)$ is obtainable from the Fourier transform of the structure factor $S(k)$ [1], which is proportional to the scattering intensity (with the atomic structure function removed) and can be directly measured in experiments. With the obtained $g_2$, one can then employ various reconstruction techniques to generate realizations of the system of interest. Another related family of inverse problems is the reconstruction of pair interaction potential from a given radial distribution function $g_2(r)$ between particles, i.e., the inverse Monte Carlo problems [28]. It is worth mentioning that in quantum mechanics, the analog of the $g_2$-realizability condition is the representability condition for the two-body density matrix, i.e., the conditions the density matrix must satisfy in order to correspond to a physical state [29–32].

It is known that though the information contained in $g_2$ can be sufficient to completely characterize ordered point configurations in very special circumstances [33], it is generally devoid of crucial structural information to uniquely determine a disordered point configuration [34–36]. However, it seems that this aspect has not been widely appreciated and general claims of uniqueness of the reconstructions using $g_2$ or $S_2$ have been made based on numerical studies

[18,23]. One aim of this paper is to show via a variety of examples the existence of distinct point configurations with identical pair-distance distributions (e.g., $g_2$), which implies the nonuniqueness of the reconstructions involving $g_2$ of these point configurations. Besides, general mathematical formalism to characterize the structural ambiguity of pair information is also devised.

Figure 1 shows two distinct configurations of four points in two dimensions with identical pair distances. In particular, one configuration (with the pair distances shown) resembles a “kite” and the other resembles a “trapezoid.” In order to provide an in-depth presentation of the ambiguity of pair-distance distributions, it is necessary to examine the problem mathematically first and then discuss the physical implications. Some definitions are in order here. Two $d$-dimensional statistically homogeneous and isotropic $n$-point configurations $\Gamma_{d,n}$ and $\Gamma'_{d,n}$ are identical if and only if they possess identical sets of $k$-body distribution functions $g_k$ for $k=1,2,\ldots,n$. The configurations $\Gamma'_{d,n}$ and $\Gamma_{d,n}$ are $d$-fold distinct if and only if they process distinct $n$-body distribution functions for all $n\equiv k$. A $d$-dimensional $n$-point configuration $\Gamma^i_{d,n}$ is $k$-fold degenerate if and only if there exist additional $(k-1)$-dimensional $n$-point configurations $\Gamma^i_{d,n}$ ($i=2,\ldots,k$) that are mutually $g_2$ distinct and also $g_3$ distinct from $\Gamma^i_{d,n}$, all of which possess the same two-body distribution function $g_2$. This definition of structural degeneracy rules out the possibility that two degenerate point configurations are trivially connected by translation, rotation, mirror reflection, or any of their combinations. Moreover, we consider that two-point configurations are equivalent (i.e., do not form a degenerate pair) if they are related by a trivial isotropic rescaling, which does not change the internal structure of the configuration. Thus, we see that the kite and the trapezoid are associated with the same set of pair distances (i.e., they are twofold degenerate), but the triangle information of the two is distinguishable [37]. It is worth noting the historically prominent Kirkwood superposition approximation of $g_3$, which replaces the three-body distribution function with a product of three pair distribution functions [38]. Because the separate members of our pair-distance degeneracy examples present distinct triangle (i.e., three-body) distributions, the conclusion must be that no functional of $g_2$ (Kirkwood or otherwise) can uniquely specify $g_3$.

It is clear that given $g_2$ associated with the degenerate point configurations, it is impossible even in principle to obtain a unique reconstruction, and each degenerate configuration should be recovered with equal probability. Therefore, an outstanding problem is to determine under what conditions the pair-distance information contained in $g_2$ could
uniquely determine a point configuration, i.e., there is no associated structural degeneracy. A question with more practical importance is that how the point configurations would change when the measurement of $g_2$ is subject to slight imprecision, a common situation in experiments and numerical simulations.

In addition to their physical relevance, degenerate point configurations are also of mathematical interest. For example, open questions connected to the famous traveling salesmen problem [39] can be raised. Given the degenerate configurations associated with the same set of pair distances, what are the optimal solutions of the traveling salesman problem for each configuration and are they unique? Are there special degenerate configurations whose solutions are associated with the same set of pair distances, i.e., triangles? And two distinguishable circuits for the kite collapse onto a line segment, and in that limiting case all circuits have the same length. For more general and complicated degenerate configurations, such questions are notoriously difficult to solve; the problem belongs to the NP-complete class.

In this paper, we present the idea of the distance space (i.e., the $D$ space), in which each dimension is associated with the separation distance between a given point pair. The pair-distance distribution of a particular point configuration is then presented by a single point in the $D$ space. It is clear that not all the points in $D$ space correspond to realizable configurations, i.e., the separation distances have to satisfy certain conditions such that they could be assembled into a point configuration. These conditions together define a (partially) bounded region in the $D$ space. For example, for three-point configurations in $R^2$ (i.e., triangles), the region of the feasible distances is an open "pyramid" in the three-dimensional $D$ space, as shown in Fig. 3. When degeneracy exists, the region of the feasible distances is generally a complicated closed intersection of several such simple curved pyramids in high dimensions. The determination of the region of feasible distances is equivalent to obtaining the conditions of a realizable $g_2$, i.e., a pair distribution function that can be associated with a point configuration. We emphasize that our focus here is the pair-distance distribution of a single point configuration (or a single realization of a point process). Thus, the function $g_2$ we examine should be interpreted as the volume-averaged pair distribution [14]. Although in the infinite-volume limit, volume averaging is equivalent to ensemble averaging for ergodic systems, we do not explicitly consider this limiting case here. Discussions of the realizability conditions and the nonuniqueness issue for ensemble-averaged pair distributions can be found in Refs. [25, 26, 40, 41]. Using the $D$ space, we will answer various aspects of the aforementioned questions concerning the degenerate point configurations and the nonuniqueness issue of the reconstruction. We will show that the utility of the $D$ space also improves our understanding of various important problems in statistical physics such as the recently proposed decorrelation principle in high-dimensional Euclidean space [42]. In a sequel to this paper, we will extend the present analysis to understand degeneracy issues pertaining to two-phase random media which is a larger classification than point configurations [43].

The rest of the paper is organized as follows. In Sec. II, we discuss the $D$ space in detail and derive the conditions for feasible distances and for the occurrence of degeneracy, through which we show that in general degeneracy is rare. In Sec. III, we provide a variety of examples of degenerate point configurations and illustrate how the conditions derived in Sec. II could be employed to construct point configurations with specific degeneracy. In Sec. IV, we discuss several problems in statistical physics such as the reconstruction of atomic structures from experimentally obtained $g_2$ and the decorrelation principle, based on the idea of the $D$ space. Finally, we make concluding remarks.

II. DISTANCE SPACE $D$

In this section, we will discuss in detail the $D$ space. In particular, we will derive the conditions under which the pair distances could be assembled into a point configuration, i.e., the feasibility conditions as well as the conditions under which the pair distances correspond to degenerate point configurations. We will first study a four-point configuration in $R^2$ to illustrate the idea and then consider the general $n$-point configurations in $R^d$.

A. Simple example: Four-point configuration in $R^2$

Consider a four-point configuration $\Gamma_{2,4}$ in $R^2$ (see Fig. 4) and the associated six-dimensional $D$ space. We would like
FIG. 4. A four-point configuration in \( \mathbb{R}^2 \).

to know the answers to the following two questions:

(i) What are the conditions the six pair separation distances must satisfy so that they correspond to a four-point configuration in \( \mathbb{R}^2 \)?

(ii) What are the conditions the pair distances must satisfy so that they correspond to \( k \)-fold degenerate four-point configurations in \( \mathbb{R}^2 \)?

To answer these questions, we consider a particular construction as follows. Suppose the six pair distances are elements of the set \( \Omega=\{d_1, d_2, \ldots, d_6\} \), which can be further partitioned as \( \Omega=\{\Omega_1, \Omega_2, \Omega_3, \Omega_4\} \), where \( \Omega_i=\{\emptyset\} \) (\( \emptyset \) is the null set), \( \Omega_2=\{d_1\} \), \( \Omega_3=\{d_2, d_3\} \), and \( \Omega_4=\{d_4, d_5, d_6\} \). We will see that such a partition enables us to associate the pair distances with the corresponding points in a convenient way. Recall that from our definition (Sec. I), point configurations are considered identical if they are connected by translation, rotation, mirror reflection, and any of their combinations. Thus, we can put point \( P_1 \) at the origin of a Cartesian coordinate system and put point \( P_2 \) on one of the two orthogonal axes of the coordinate system separated from the origin (i.e., \( P_1 \)) by a distance \( d_1 \). Note different choices of the position of \( P_1 \) and the orientation of the line segment \( P_1P_2 \) lead to point configurations that are identical up to translations and rotations. For point \( P_3 \), we can either let \( P_1P_3=d_2, P_2P_3=d_3 \) or \( P_1P_3=d_3, P_2P_3=d_2 \). The two choices correspond to two configurations connected by a mirror reflection, which are considered identical and either choice is acceptable. Without loss of generality, we choose \( P_1P_3=d_2, P_2P_3=d_3 \). Finally, we choose \( P_1P_4=d_4, P_2P_4=d_5, P_3P_4=d_6 \) for point \( P_4 \).

We see from the above construction that the positions of points \( P_1 \) and \( P_2 \) are determined with respect to the line segment defined by points \( P_1 \) and \( P_2 \) as a “reference” structure. Note that the line segment is a one-dimensional simplex. In \( \mathbb{R}^2 \), the position of a point is completely determined by a distance \( d \) in the direction of the point of interest, the free dimension is five, which leads to an upper bound on the order of the degeneracy, i.e., \( k_{\text{max}}=5 \). This condition is only a necessary one because there are certain permutations that lead to identical configurations, such as those that correspond to the permutations among the point indices, which do not change the structure of the configuration, since the points are indistinguishable. For example, \( \Omega_1=\{d_1, d_2, d_3, d_4, d_5, d_6\} \) and \( \Omega_2=\{d_1, d_4, d_5, d_6, d_2, d_3\} \) correspond to an exchange of \( P_1 \) and \( P_2 \), which possess the identical feasible regions and thus do not contribute to the degeneracy. No further conclusions can be made without knowing the details of how the distances are permuted. In

\[
\begin{align*}
d_1^2 + d_2^2 + d_3^2 - 2d_1d_2 - 2d_1d_3 - 2d_2d_3 > 0, \\
d_1^2 + d_2^2 + d_3^2 - 2d_1d_2 - 2d_1d_3 - 2d_2d_3 > 0.
\end{align*}
\]
Sec. III, we will construct concrete examples of degenerate $\Gamma_{2,a}$, where the details of permutations are considered.

B. General formulation: Feasibility conditions

The generalization of the above formulation is straightforward. Note in the following discussion in this section, we assume $n>(d+1)$; the case when $n=d+1$ (i.e., the simplex configurations) is discussed in detail in Sec. III A and the case when $n<(d+1)$ is trivial. Consider an $n$-point configuration $\Gamma_{d,n}$ in $\mathbb{R}^d$, which possesses $m=n(n-1)/2$ pair distances $\Omega=\{d_1, d_2, \ldots, d_m\}$. The distances can be further partitioned, i.e., $\Omega=\{\Omega_1, \Omega_2, \ldots, \Omega_n\}$, where $\Omega_1=\{d_1\}$, $\Omega_2=\{d_2\}$, $\Omega_3=\{d_3\}$, $\Omega_4=\{d_4\}$, ... $\Omega_5=\{d_{15}\}$, $\Omega_6=\{d_{16}\}$, ..., $\Omega_7=\{d_{21}\}$, $\Omega_8=\{d_{22}\}$, ..., $\Omega_{n-1}=\{d_{n(n-1)/2}\}$. Following the same construction procedure prescribed in Sec. II A, the distances associated with the first $d$ points, i.e., $\Omega_1, \Omega_2, \ldots, \Omega_d$, are assembled into a $(d-1)$-dimensional simplex as the reference structure. Each point $P_i (i>d)$ is associated with $(i-1)$ distances and the position of point $P_i$ is completely determined by specifying the $d$ distances from $P_i$ to the vertices of the reference structure, given that the $d$-dimensional simplex formed by $P_i$ and the vertices of the reference structure possesses a non-negative volume. In particular, denote the $(d+1)$ vertices of the $d$-dimensional simplex by $v_i (i=1, \ldots, d+1)$, we can define a $(d+1) \times (d+1)$ distance matrix $M$, i.e.,

$$M_{ij} = M_{ji} = ||v_i - v_j||^2,$$  

(5)

where $\| \cdot \|$ denotes the $L^2$ norm of a $d$-dimensional vector and $M_{ij}$ ($M_{ji}$) is the squared distance between vertices $i$ and $j$. The volume $\Delta$ of the simplex is then given by the Cayley-Menger determinant, i.e.,

$$\Delta^2 = \frac{(-1)^{d+1}}{2^d (d-1)!} |M| \geq 0,$$  

(6)

where $\hat{M}$ is a $(d+2) \times (d+2)$ matrix obtained from $M$ by bordering $M$ with a top row $(0,1,\ldots,1)$ and a left column $(0,1,\ldots,1)^T$. For example, Eq. (6) reduces to Eq. (1) in $\mathbb{R}^2$, and in $\mathbb{R}^3$ we obtain

$$\Delta^2 = \frac{1}{288} \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & M_{12} & M_{13} & M_{14} \\ 1 & M_{21} & 0 & M_{23} & M_{24} \\ 1 & M_{31} & M_{32} & 0 & M_{34} \\ 1 & M_{41} & M_{42} & M_{43} & 0 \end{vmatrix}.$$  

(7)

The requirement that the constructed $d$-dimensional simplex possesses non-negative volume leads to higher-dimensional analogs of the well-known triangle inequalities in two dimensions, which we will refer to as simplex inequalities. In general, each set of the simplex inequalities associated with a point $P_i$ ($i>d$) defines a partially bounded region in the $D$ space, the intersection of which is a high-dimensional analog of the open pyramid shown in Fig. 3(b).

It is clear from the above construction that a point configuration $\Gamma_{d,n}$ can be completely determined by only specifying $f=[\frac{1}{2}d(d-1)+(n-d)d]$ distances (e.g., “free” distances), satisfying the simplex inequalities. Thus, the free dimension of the $D$ space is $f$ and the remaining $(m-f)$ pair distances (e.g., “constrained” distances) cannot be chosen freely but instead are completely determined by the $f$ free distances. To obtain the relations between the constrained and free distances, we will employ the following theorem [36].

**Theorem 1.** For a set of $n$ vectors $v_1, v_2, \ldots, v_n$ in $\mathbb{R}^d$ ($n>d$), let the Gram matrix be defined by $\hat{G}_{ij} = \langle v_i, v_j \rangle$, where $\langle \cdot \rangle$ denotes the inner product. Then all $(d+1) \times (d+1)$ minors of $G$ must have zero determinant.

The proof of the theorem is given in Ref. [36]. It is essentially another way of stating the fact that there are at most $d$ linearly independent vectors among $v_1, v_2, \ldots, v_n$ in a $d$-dimensional Euclidean space. Without loss of generality, we can choose the origin at $v_1$ and obtain

$$\hat{G}_{ij} = \langle \hat{v}_i, \hat{v}_j \rangle = \langle v_i - v_1, v_j - v_1 \rangle.$$  

(8)

Consider the identity [36],

$$\langle v_i - v_1, v_j - v_1 \rangle = \frac{1}{2} [\langle v_i - v_1, v_j - v_1 \rangle + \langle v_j - v_1, v_i - v_1 \rangle - \langle v_i - v_j, v_j - v_i \rangle],$$  

(9)

we obtain that

$$\hat{G}_{ij} = \frac{1}{2} (\hat{d}_{ij}^2 + \hat{d}_{ji}^2 - \hat{d}_{ij}^2),$$  

(10)

where $\hat{d}_{ij}$ is the distance between the two points $i$ and $j$. Thus, we see the requirement that all $(d+1) \times (d+1)$ minors of $\hat{G}$ have zero determinant (denoted by $M_{(d+1)}$, i.e.,

$$|M_{(d+1)}(\hat{G})| = 0$$  

(11)

leads to fourth-order algebraic equations, involving the $(m-f)$ constrained distances. It is clear that each constrained distance can be explicitly expressed as a function of the free distances alone. For four-point configuration in $\mathbb{R}^2$, Eq. (11) gives Eq. (4). Note these inequalities define curved hypersurfaces in the $D$ space. The intersection of these curved hypersurfaces as well as the partially bounded regions defined by Eq. (6) gives the feasible region of the $D$ space, i.e., when any permutation of the $m=n(n-1)/2$ pair distances lies within the feasible region, these distances can be assembled into an $n$-point configuration in $\mathbb{R}^d$.

C. General formulation: Necessary conditions of degeneracy

For the distances $\Omega$ to correspond to k-fold degenerate point configurations $\Gamma_{a_{k,n}}$, $\Gamma_{a_{k,n}}$, $\ldots$, $\Gamma_{a_{k,n}}$ ($k \leq f$), the feasibility conditions for $k$ distinct permutations of $\Omega$ should be satisfied simultaneously. The feasibility conditions associated with any particular permutation of $\Omega$ include a set of equalities, which would reduce the dimension of the feasible region in the $D$ space. Suppose that for each distinct permutation, only one additional equality constraint is introduced. Then we can obtain an upper bound on the order of the degeneracy, i.e., $k_{\text{max}} = f$, which corresponds to a feasible region that has been reduced to a single curve (with one free...
dimension). That is, only one distance can be chosen arbitrarily. However, different choices of the single free distance correspond to trivial isotropic rescaling of the entire configuration, which leads to no degeneracy based on our definition. Note that if the permutation does not introduce new feasibility conditions, it corresponds to a permutation of the point indices, which does not affect the structure of the configuration.

The properties of the feasible regions have important implications. As we have seen, the structural degeneracy would reduce the dimension of the feasible regions, the volume of which is proportional to the number of feasible distance sets. For a particular \(n\)-point configuration, we could in principle identify all feasible distance sets by exploring the whole feasible region in the \(D\) space point by point. However, the distance sets associated with degeneracies can only lie on a hypersurface with lower dimensions than the feasible region. The volume ratio of the hypersurface to the feasible region, which is also the number ratio of the distance sets associated with degeneracies to those without degeneracies, is vanishingly small. In other words, although degeneracies exist they are extremely rare. This might explain why perfect reconstructions (identical match of the pair distances and the configurations up to translations, rotations and mirror reflections) can be obtained numerically [18,23]. However, the general conclusion that pair statistics alone would uniquely determine the configurations could not be made only based on those numerical results, as we will show in the next section via a variety of examples of degeneracy.

### III. EXAMPLES OF DEGENERATE POINT CONFIGURATIONS

In this section, we construct a variety of degenerate point configurations using the general scheme developed in Sec. II. In particular, we study the degeneracies of simplices in \(R^d\), four-point configurations in \(R^2\), and specific \(n\)-point configurations in \(R^d\) possessing twofold degeneracy.

#### A. Degenerate \(d\)-dimensional simplices

A simplex in \(R^d\) is the convex hull of a set of \((d+1)\) points \(\Gamma_{d+1}\) that do not all lie on the same theta-dimensional hyperplane. A simplex in \(R^2\) is a triangle and in \(R^3\) it is a tetrahedron. Simplices in \(R^d\) \((d \geq 4)\) can be considered to be \(d\)-dimensional generalizations of the three-dimensional tetrahedron. The simplex is so named because it represents the simplest possible polyhedron in the given dimension. The volume a \(d\)-dimensional simplex is given by Cayley-Menger determinant \((6)\).

A unique feature of simplex configurations \(\Gamma_{d+1}\) is that their feasibility conditions only include the simplex inequalities. These inequalities define a partially bounded region possessing the same dimensions as the \(D\) space. In other words, the free dimension of the feasible region is not reduced due to degeneracy. Thus, one should expect that it is much easier to obtain highly degenerate simplices than other point configurations.

Suppose we have a distance set \(\Omega = \{d_1, d_2, \ldots, d_m\}\) \((m = d(d+1)/2)\). It is clear that if we choose \(d_i = \delta + \delta_i\), where \(\delta_i\) \((i=1, 2, \ldots, m)\) are mutually distinct small numbers, they will satisfy all the simplex inequalities and correspond to a point in the vicinity of the centroid of the feasible region. The maximum magnitude of the \(\delta\)'s depends on the boundaries of the feasible region, which we need not to worry about for the moment, as long as the \(\delta\)'s are sufficiently small and mutually distinct.

In \(R^2\) \((d=2)\), the three distances can be assembled into a unique triangle, i.e., we have \(k_{\max} = 1\). This can also be seen from the following argument. Since configurations connected by translations and rotations are considered identical, we could pick any one of the three distances along one of the coordinate axes starting from the origin and require the same for the corresponding distance of all possible degenerate configurations. In this way, we rule out translations and rotations in a plane. There are only two distances left, which can be assembled into a triangle in two ways. However, the two resulting triangles are mirror image of each other. Thus, we have \(k_{\max}^{(2)} = 2!/2 = 1\). where "!" indicates factorial.

In \(R^3\) \((d=3)\), we similarly choose one of the six distances as the reference distance, and the remaining five are assigned to different edges of a tetrahedron, which results in \(5!\) tetrahedra. However, among these tetrahedra there are pairs that are connected by mirror reflection, which has to be excluded. Two mirror reflection plane can be identified: one perpendicular to the reference distance and the other contains the reference distance. This further reduces the number of distinct tetrahedra by a factor of \(1/4\). Thus, we obtain \(k_{\max}^{(3)} = 5!(2 \times 2) = 30\).

Generally, in \(d\) dimensions when one of the \(m = d(d+1)/2\) distances is chosen as the reference distance, there are \((m-1)!\) ways to assemble the remaining \((m-1)\) distances into a simplex in \(R^d\). However, \((d-1)!\) hyperplanes (among which one contains the reference distance and the others are perpendicular to it) can be identified that are mirror reflection hyperplanes of the simplex. Each mirror reflection reduces the number of distinct simplices by a factor of \(1/2\). Thus, we have

\[
k_{\max}^{(d)} = \frac{(m-1)!}{2(d-1)} = \frac{d(d+1)/2 - 1)!}{2(d-1)}.
\]

We can see that for simplex configurations in \(R^d\) with \(d \geq 3\), \(k_{\max}^{(d)}\) is significantly larger than the dimension of the feasible region \(f = d(d+1)/2\), which indeed implies a high level of degeneracies associated with these configurations.

#### B. Two-dimensional four-point configurations

We show here how the conditions determining the feasible region in \(D\) space can be employed to construct four-point configurations \(\Gamma_{2,4}\) in \(R^2\) with \(k\)-fold degeneracy. As pointed out in Sec. II, the feasibility conditions are only necessary and the details of how the distances are permuted must be considered.

The relations of the six distances of \(\Gamma_{2,4}\) are given by Eq. (4) for the particular order \(\Omega = (d_1, d_2, d_3, d_4, d_5, d_6)\). For a permutation \(\Omega^*\), the variable \(d_i\) in Eq. (4) should be replaced by the \(i\)th element of \(\Omega^*\), which generally would lead to a different equation for the six distances. As mentioned in the
last section, we could choose \( d_1 \) as the reference distance to rule out translation and rotation and only consider the permutations of the remaining five distances, which gives 5! = 120 distinct equations. Without loss of generality, we could also choose \( d_1 = 1 \), which corresponds to a trivial isotropic rescaling of the entire point configuration.

In principle, a \( k \)-fold degeneracy (\( k \leq k_{\text{max}} = 5 \)) could be constructed by requiring that the \( k \) equations for the five distances corresponding to \( k \) distinct permutations hold simultaneously. However, we find that high level degeneracies (those with \( k \) close to \( k_{\text{max}} \)) are difficult to realize. In particular, when \( k \) is large the equations for the distances possess roots that are algebraically multiple, i.e., \( \Omega \) contains two or more equal valued distances, which leads to configurations connected by rotations and mirror reflections. Thus, the number of distinct configurations associated with the distances is smaller than \( k \). For \( n \)-point configurations, the largest \( k \) that we have realized is \( k = n - 1 \). Due to space limitation, we could not exhaust all degeneracies for each \( k \) (i.e., about \( \binom{6}{n} \times 120 \) cases) in this paper and only provide a few specific examples.

For \( k = 2 \), requiring the distance permutations \( \Omega_1 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \) and \( \Omega_2 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \) to hold simultaneously yields

\[
D(\Omega_1) = D(d_1, d_2, d_3, d_4, d_5, d_6) = 0,
\]

\[
D(\Omega_2) = D(d_1, d_2, d_3, d_4, d_5, d_6) = 0,
\]

where \( D(x_1, x_2, x_3, x_4, x_5, x_6) \) is the multinomial given by

\[
D(x_1, \ldots, x_6) = \sum_{\pi} \frac{x_1^{p_1} x_2^{p_2} x_3^{p_3} x_4^{p_4} x_5^{p_5} x_6^{p_6}}{p_1! p_2! p_3! p_4! p_5! p_6!}
\]

Equations (13) reduce the free dimensions of the 6-space from five to four. Without loss of generality, we choose \( d_1 = 1 \), \( d_2 = 1.581141 \ldots \), \( d_3 = 0.70710 \ldots \), \( d_4 = 0.87228 \ldots \), and solve Eqs. (13) to obtain \( d_5 = 1.32698 \ldots \), and \( d_6 = 1.54551 \ldots \). The twofold-degenerate configurations are shown in Fig. 5. It should be noted in passing that the kite-trapezoid example shown earlier in Fig. 1 is a special case of this four-point twofold degeneracy, for which the shapes each have a reflection symmetry. If we require the permutations \( \Omega_3 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \) and \( \Omega_4 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \) to hold simultaneously, the same degeneracy can be obtained because the apparently different groups of distance permutations \( (\Omega_1, \Omega_2) \) and \( (\Omega_3, \Omega_4) \) correspond to the permutation of indistinguishable points.

Similarly, for \( k = 3 \), we choose \( \Omega_1 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \), \( \Omega_2 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \), and \( \Omega_3 = \{d_1, d_2, d_3, d_4, d_5, d_6\} \) to hold simultaneously, which reduces the free dimensions to three. By choosing \( d_1 = 1 \), \( d_2 = 1.581144 \ldots \), \( d_3 = 0.70710 \ldots \), equations \( D(\Omega_i) = 0 \) \( (i = 1, 2, 3) \) can be solved to yield \( d_4 = 1.34371 \ldots \), \( d_5 = 0.37267 \ldots \), and \( d_6 = 0.68718 \ldots \). The threefold degenerate configurations are shown in Fig. 6.

C. \( d \)-dimensional \( n \)-point configurations with twofold degeneracy

In general, the feasible region of \( k \)-fold degenerate \( n \)-point configurations in \( \mathbb{R}^d \) can be obtained by carrying out a similar calculation used in the previous section, which would be extremely tedious. However, when the point configurations possess certain symmetries, particular degeneracies can readily be constructed. Here we provide constructions of twofold-degenerate \( n \)-point configurations in \( \mathbb{R}^d \) by taking advantage of their symmetries.

Consider a centrally symmetric \( n_1 \)-point configuration \( \Gamma_{d_{n_1}}^{(1)} \) in \( \mathbb{R}^d \), i.e., there exists a center \( O_1 \) such that for every point \( P^{(i)} \) in \( \Gamma_{d_{n_1}}^{(1)} \) there exists a point \( P^{(j)} \) for which the line segment \( P^{(i)} P^{(j)} \) passing \( O_1 \) is bisected by \( O_1 \) (note that \( i \neq j \) is allowed), i.e., \( P_i^{(1)} \) and \( P_j^{(1)} \) are points of inversion symmetry about \( O_1 \). Consider another centrally symmetric point configuration \( \Gamma_{d_{n_2}}^{(2)} \) in which all the \( n_2 \) points are distributed symmetrically on a one-dimensional line \( l^{(2)} \) embedded in \( \mathbb{R}^d \). Denote the symmetry center of \( \Gamma_{d_{n_2}}^{(2)} \) by \( O_2 \). We require that the line segment \( O_1 O_2 \) is perpendicular to \( l^{(2)} \). Finally, consider the centrally symmetric point configuration \( \Gamma_{d_{n_3}}^{(3)} \) in \( \mathbb{R}^d \) the \( 2n_3 \) points of which are also distributed symmetrically on a one-dimensional line \( l^{(3)} \) that is parallel to \( l^{(2)} \) with the symmetry center coinciding with \( O_1 \). \( \Gamma_{d_{n_3}}^{(3)} \) can be further partitioned into two subsets: \( A_{d_{n_3}}^p \) which contains \( n_3 \) points in \( \Gamma_{d_{n_3}}^{(3)} \) such that no two points in \( A_{d_{n_3}}^p \) are symmetric about \( O_1 \) (i.e., they are “primary” points), and \( A_{d_{n_3}}^d \) which contains the remaining \( n_3 \) points of \( \Gamma_{d_{n_3}}^{(3)} \) (i.e., the “dual” points). It is clear that

\[
\Gamma_{d_{n_1} + n_2 + n_3}^{d} \subset \Gamma_{d_{n_1}}^{(1)} \cup \Gamma_{d_{n_2}}^{(2)} \cup A_{d_{n_3}}^p \cup A_{d_{n_3}}^d.
\]

form a degenerate pair, i.e., the distances from the \( n_3 \) primary points to the remaining \((n_1 + n_2)\) points in \( \Gamma_{d_{n_1} + n_2 + n_3}^{d} \) are
IV. DISCUSSION

The D space concept can be applied to reconcile a variety of problems in statistical physics, such as the reconstruction of atomic structures from experimentally obtained \( g_2 \), and the decorrelation principle, which we will discuss in the ensuing subsections.

A. Reconstruction of atomic structures from experimentally obtained \( g_2 \)

As mentioned in Sec. I, a knowledge of atomic structures of condensed matter can be obtained via x-ray scattering experiments. In particular, the two-body distribution function \( g_2(r) \) is related to the Fourier transform of the structure factor \( S(k) \), which is proportional to the scattering intensities (with the atomic structure function removed). For ideal crystalline structures (without any thermal agitation of the atomic centers), \( g_2 \) consists of a series of Dirac delta functions at specific distances. For disordered structures (lack of long-range order), \( g_2 \) is generally a continuous damped oscillating function that decays to its long-range value very quickly. Interestingly, it seems that though the pair information contained in \( g_2 \) of the crystalline matter would determine the structures to high accuracy, it is not the case for disordered structures.

The reason can be easily seen if we consider the D space. For an ordered point configuration (i.e., a lattice), there are strong dependencies among the distances besides those required by the feasibility conditions. For example, consider a \( d \)-dimensional Bravais lattice whose basis vectors are \( a_1, a_2, \ldots, a_d \). The vector connecting any two points in the lattice can then be expressed as

\[
d = n_1 a_1 + n_2 a_2 + \cdots + n_d a_d, \tag{16}
\]

where \( n_i (i = 1, \ldots, d) \) are integers. Thus, the distance \( d \) between any two lattice points is given by

\[
d^2 = \sum_{i=1}^{n} n_i^2 \langle a_i, a_i \rangle + \sum_{i<j} n_i n_j \langle a_i, a_j \rangle, \tag{17}
\]

where \( \langle \cdot, \cdot \rangle \) denotes the inner product of two vectors. Note that \( \langle a_i, a_j \rangle = \frac{1}{2}(\langle a_i, a_j \rangle + \langle a_j, a_i \rangle - \langle a_i - a_j, a_j - a_i \rangle) \). Thus, Eq. (17) implies that every distance of an ordered point configuration can be obtained if the lengths of the basis lattice vectors and the distances between the end points of different basis lattice vectors are specified. In other words, Eq. (17) further reduces the free dimensions of the D space of the ordered point configuration in \( \mathbb{R}^d \) to \( f = d(d+1)/2 \). The additional conditions given by Eq. (17) significantly reduce the number of feasible permutations of the distances. A unique feature of the distances for lattices is that the basis lattice vectors are associated with the smallest distances. To completely reconstruct the lattice configuration, the smallest \( d(d+1)/2 \) distances are selected to be assembled into a simplex in \( \mathbb{R}^d \) defined by the common origin and the end points of all the lattice vectors, which in turn determines the fundamental cell of the lattice. In \( \mathbb{R}^2 \), three feasible distances uniquely determine a triangle and, thus, the rhomboidal fundamental cell. In \( \mathbb{R}^3 \), there are maximally 30 ways that the six distances could be assembled into a tetrahedron. However, even for a twofold degeneracy, the number of equality constraints introduced by Eq. (17) [i.e., for two permutations of the 6 distances, Eq. (17) should hold simultaneously] is much larger than the free dimensions of the system, which generally rules out all nontrivial solutions. Indeed, it is known that for \( d \leq 3 \), pair distances are sufficient to uniquely determine Bravais lattices. However, in high dimensions, degeneracies of Bravais lattices can be constructed [9].

For a disordered structure, Eq. (17) does not hold and the values of distances would form a continuous spectrum in the infinite-volume limit. We consider the idealized case that there are a finite number of well-defined distances and try to reconstruct the configuration from them. An important point is that no matter how carefully experiments might be carried out, there would still be small but finite errors associated with the distances, i.e., \( d = d^\prime + \epsilon \), where \( d^\prime \) denotes the real value of the distance and \( \epsilon \) denotes the error. Thus, instead of a single point in the D space, the distances correspond to a small uncertainty region with same dimensions as the D space. As we have pointed out, the presence of degeneracies corresponds to a feasible region with reduced free dimension and thus has vanishing “volume” compared with the feasible region free of degeneracies, which leads us to the conclusion.
that degeneracies are rare in general. However, due to the uncertainties of the measured distances, we see that the feasible regions now are “finite” in size compared with those free of degeneracies. This explains why in the reconstructions it is hard to exactly recover the target configurations, i.e., all configurations associated with the distances corresponding to the points in the feasible region should be considered with equal probability for a “fair” reconstruction procedure.

B. Decorrelation principle

Recently, Torquato and Stillinger [42] proposed a decorrelation principle concerning the disordered hard-sphere packings in high-dimensional Euclidean space \( \mathbb{R}^d \). In particular, the decorrelation principle states that unconstrained spatial correlations vanish for disordered packings as the spatial dimension becomes large. In other words, as \( d \) increases, the short-ranged order beyond contact that exists in low dimensions must diminish. This principle has been explicitly observed in a variety of disordered packings in high dimensions [45].

The centroids of the hard spheres completely determine a packing, which can be considered as a point configuration in \( \mathbb{R}^d \), in which there is a minimum value of pair separation distances \( D \) (i.e., the diameter of the spheres) due to the nonoverlapping condition. The decorrelation principle amounts to the following statement concerning the \( \mathbb{D} \) space of the configuration: the requirement that the distances cannot be smaller than \( D \) does not affect the occurrence frequency of distances with values greater than \( D \) in very high dimensions. Note the above should be true for any disordered packings, including both dilute and jammed packings. It is known that in low dimensions, \( g_2 = H(r - D) \) can only be maintained for packings with densities less than a critical value [26] and for disordered jammed packings \( g_2 \) shows strong short-ranged oscillations [46], which is the manifestation of local spatial correlations due to the nonoverlapping constraint. In other words, for the jammed disordered packings, the requirement that a desired number of distances of value \( D \) must be realized in the configuration strongly constrains the possible values of other distances in low dimensions, especially those on the same magnitude of \( D \). In high dimensions, the above requirement becomes less significant in determining the local arrangements of points. Consider the construction used in deriving the feasibility conditions to completely determine the position of a point in \( \mathbb{R}^d \), a “reference” structure containing at least \( d \) points is used. The positions of the points in the reference structure can be chosen almost freely subject to the mild constraint that no two points can be closer than \( D \). As \( d \) increases, larger local structures (containing more points) can be constructed before the constraints on the separation distances between the points begin to play an important role. In addition, there are \( (d - m) \) ways to arrange a point that has fixed distances to \( m \) \((m < d)\) points in \( \mathbb{R}^d \). Thus, as \( d \to \infty \), the constraints on the pair-distance values imposed by the requirement that a desired number of distances with value \( D \) must be realized become insignificant, which is consistent with the decorrelation principle.

C. Additional structural information

As we have shown, pair-distance statistics in general is not sufficient information to completely determine the point configuration. A natural question is what additional information could be used to further reduce the compatible configurations associated with identical radial distribution functions. A conventional choice is the three-body correlation function \( g_3 \) [6,8], which provides information how the pair distances should be linked into triangles. Though in certain circumstances \( g_3 \) could provide additional information on the point configuration, its determination requires additional effort either theoretically or computationally.

It has been suggested in Ref. [47] that instead of incorporating information contained higher-order versions of \( g_2 \), namely, \( g_3, g_4, \) etc., one might be better served to seek other descriptors at the two-point level, which can be both manageably measured and yet reflect nontrivial higher-order structural information. One such quantity is the pair-connectedness function \( P_2 \) [2], i.e., the connectedness contribution to \( g_2 \), which contains nontrivial topological connectedness information of the point configuration. Note the “connectedness” in a point configuration can be defined in many ways, e.g., one could circumscribe spheres around each of the points and then define that two points are connected if the two associated spheres are either contacting or overlapping, for example. Connectedness information contained in \( P_2 \) is distinct from the “triangular” information embodied in \( g_3 \), e.g., \( P_2 \) is sensitive to clustering effects, whereas \( g_3 \) is not.

D. Generalization to two-phase media

As pointed out in Sec. I, two-phase media can be constructed by decorating point configurations. For example, one can construct sphere packings by assigning to each point a sphere centered at the point with diameter equal to the minimal distance in the configuration. In this sense, two-phase media are more general than point configurations. The degeneracy of discrete point configurations implies the existence of degenerate two-phase media. The corresponding pair-distance information for two-phase media is the two-point correlation functions \( S_2 \) [2]. The degeneracy of two-phase media and the nonuniqueness issue of their reconstruction will be discussed in a sequel (Part II). Here we only provide an example of a twofold-degenerate two-phase medium constructed from the kite-trapezoid example given in Sec. I.

As shown in Fig. 9, suppose we have two large solid circles, in which small circular holes are made. One large circle contains the kite holes and the other contains the trap-

V. CONCLUDING REMARKS

In this paper, we discussed various aspects of the geometrical ambiguity of pair-distance statistics associated with
though degeneracies are rare, one could not exclude their existence merely based on numerical reconstruction studies. We also applied the $D$ space to problems in statistical physics, such as the reconstruction of atomic structures from experimentally obtained $g_2$, and the decorrelation principle.

As pointed out in Sec. IV D, the degeneracy of point configurations implies the existence of degenerate random media and a simple example is provided there. In a sequel to this paper [43], we will study the structural degeneracy of general random media and the nonuniqueness issue in the reconstruction of heterogeneous materials [2,3,5,48].

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