Regularity and resilience of short-range order in uniformly randomized lattices

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Abstract
Randomly perturbed lattice models play a vital role in the exploration of novel quasi-disordered structures such as disordered photonic crystals that combine the coherent optical effects of crystals and the broadband, isotropic power spectra of disordered media. Recent studies have shown that the Bragg scattering peaks of uniformly randomized lattices can be switch-on and -off by increasing the perturbation strength while preserving the long-range order of the underlying lattice. In this work, we investigate the pair correlation statistics of uniformly randomized lattices focusing on the impact of the perturbations on the system’s short-range order. We find that locally isotropic perturbations generate disordered structures with resilient hyperuniformity and short-range order. The interplay of these two properties has been discovered to be critical in the design of disordered materials with enhanced photonic band gaps and light absorption. The present study provides an alternative approach for designing partially disordered hyperuniform structures.

1. Introduction

Perturbed lattices play a crucial role in the search of novel quasi-disordered materials exhibiting desirable properties such as large isotropic photonic band gaps [1, 2], enhanced sunlight absorption [3–6], and high temperature superconductivity [7, 8]. Randomly perturbed lattices (RPLs) are also used as toy-models for studying structure formation in a wide range of physical systems found in astronomy [9–12], biology [13, 14], wireless communication [15, 16], and material science [17, 18]. Perturbed lattice models are also used in statistical physics to quantify the impact of imperfections in ordered systems [19–21].

RPLs are generated by randomly displacing each lattice point of a perfect lattice. As the random perturbation strength increases, the translational order of the underlying lattice vanishes at short distances. Since the ensemble average of the RPLs remains periodic, positional order at large distances is preserved in a hidden form. It is now established that RPLs are hyperuniform or super-homogenous since they retain positional order at large distances [9–12, 20]. Hyperuniformity is characterized by the number variance \( \sigma_N^2(R) \), of point particles inside a randomly placed observation window of radius \( R \). The number variance grows slower in the large-\( R \) limit, \( \sigma_N^2 \sim R^{d-3} \), compared to a Poisson point process where \( \sigma_N^2 \sim R^d \) in a \( d \)-dimensional system. The impact of random perturbations on the short-range order of the underlying lattice can be characterized by \( n \)-body distribution functions. One common quantity is the pair correlation function \( g_2(r) \), where \( r \) is the translational vector between a pair of point particles. In a system without long-range order, \( g_2(r) \to 1 \) [23]. On the other hand, in a perfect crystal, the pair correlation is defined by multiple Dirac spikes corresponding to the discrete separation distances of point particles in a lattice. The pair correlation function is related to the structure factor \( S(k) \) that is observed in scattering experiments as [22, 23]:

\[
S(k) = 1 + \rho \tilde{h}(k),
\]

where \( \rho \) is the number density, \( \tilde{h}(k) \) is the Fourier transform of \( g_2(r) - 1 \) and \( k \) is the wave vector.

In this work, we focus on uniformly randomized lattices (URL) that are a subset of RPLs [20]. In a URL each lattice point is displaced by a random vector that is uniformly distributed over a given region. Recent studies
have shown that the structural order of URLs can be manipulated to produce disordered hyperuniform structures with vanishing Bragg peaks [20]. It is anticipated that such URL models would be used to simulate disordered hyperuniform materials. The ability to tune structural order of perturbed lattices is essential in engineering spectral responses of photonic crystals with enhanced optical properties [3–6].

Here, we consider URLs generated with isotropic stochastic displacements applied to each lattice site of Bravais lattice. In particular, we investigate the impact of these random perturbations on a square lattice under two cases: (i) when the displacement vectors have the same length but are randomly oriented and (ii) when both the length and angle of the displacement vectors are randomized. Under these two protocols the resultant randomly perturbed lattice retains some structural order of the underlying lattice since the perturbations cannot cover the entire space without overlapping. This is different from recent studies where the stochastic displacements were uniformly distributed over cells congruent to the unit cell of the underlying lattice [3, 20]. In these cases the perturbations can cover the whole space without overlapping, leading to structure with vanishing Bragg peaks [20].

The rest of the paper is organized as follows. In section 2 the basic statistical properties of URLs are briefly presented. This include the measures utilized in the study to quantify structural order of the URLs. In section 3 numerical results demonstrating the impact of the random perturbation at short and large length-scales are given. Conclusions and future considerations are presented in section 4.

2. Methods

2.1. Statistical properties of uniformly randomly perturbed lattices

We begin by demonstrating that the two URL models generate hyperuniform point patterns following well-established arguments about the inherent long-range order of stochastic lattices [9–12, 20]. We first consider a URL model where the lattice points are displaced by the same distances in uniformly randomized directions. We henceforth refer to distorted lattices generated from this model as 'perturbed I' lattices. In these lattices the displacement vector \( \mathbf{u} \), of the \( i \)th lattice point is defined by a statistically isotropic probability distribution function (PDF) \( F(\mathbf{u}) = F(u) \), where \( u = |\mathbf{u}| \). Precisely the single displacement vector PDF can be given as

\[
F_i(u) = \frac{\delta(|\mathbf{u}|-s)}{A_d},
\]

(2)

where \( \delta(\ldots) \) denotes a Dirac delta function, \( s \) is the magnitude of the displacement vectors, and \( A_d = 2, 2\pi s \) and \( 4\pi s^2 \), in \( d = 1, 2, \) and 3 dimensions, respectively.

In the second URL model, each lattice point is displaced from its initial position a random vector uniformly distributed inside the volume of a \( d \)-dimensional sphere of radius \( s \) centered on the initial site. We henceforth refer to distorted lattices generated by this model as 'perturbed II' lattices. Following similar arguments as the previous case, the single displacement vector PDF for perturbed II lattices can be given as

\[
F_{II}(u) = \begin{cases} \frac{1}{V_d}, & |\mathbf{u}| \leq s \\ 0, & |\mathbf{u}| > s \end{cases},
\]

(3)

where \( V_d \) is the volume of \( d \)-dimensional sphere of radius \( s \), i.e., \( V_d = 2s, 2\pi s^2 \), and \( 4\pi s^3 / 3 \), respectively. The so-called characteristic functions of the PDF can be then determined from their Fourier Transforms

\[
\widehat{F}_i(q) = \int_{-\infty}^{+\infty} d^d u \ F_i(u)e^{-iq\cdot u},
\]

(4)

where \( n = I \) or \( II \) and \( q \) is the wavenumber. In two-dimensions, for an example, equation (4) corresponds to the Fourier transform of a ring delta function\(\mathcal{F}(F_i)\) or circular disk step function \(\mathcal{F}(F_{II})\), which leads to [24]

\[
\begin{align*}
\mathcal{F}(F_I(q)) &= J_0(\mathbf{q}) \\
\mathcal{F}(F_{II}(q)) &= \frac{2}{\pi} \frac{J_1(qs)}{qs},
\end{align*}
\]

(5)

where \( J_m(z) \) is the \( m \)-th order Bessel function.

A hyperuniform point pattern is characterized in scattering experiments by a structure function \( S(\mathbf{q}) \) that tends to zero as the wave vector \( \mathbf{q} \) tends to zero [9, 22]

\[
\lim_{|\mathbf{q}| \to 0} S(\mathbf{q}) = 0.
\]

(6)

It follows that an unperturbed lattice (e.g. a Bravais lattice) is hyperuniform since the structure factor of a distribution of point particles of unitary mass in lattice is given as [25, 26]:
in \( d \)-dimensions, where \( \mathbf{G} \) is a reciprocal lattice vector. Applying random perturbations to the lattice points, the structure factor of the perturbed lattice is then given as \([11, 20, 27]\)

\[
S_{\text{per}}(\mathbf{q}) = 1 - |E_0(\mathbf{q})|^2 + |E_0(\mathbf{q})|^2 S_\mathcal{C}(\mathbf{q}), 
\]

where the subscript \( n = 1, \, II \) and \( S_\mathcal{C} \) is defined in equation (7). Therefore, the structure factor of the perturbed lattice consists of two contributions: a background field characterising density fluctuations [first two terms in equation (8)] and the Bragg peaks of the underlying lattices [the third term in equation (8)]. The Bragg peaks are modulated by a multiplicative factor that reduces their amplitude at large-\( q \) more than at small-\( q \) i.e., \( |E_0(\mathbf{q})|^2 \) as given in equation (3) decays to zero at large-\( q \). The random perturbation induced density fluctuations provide a background to the Bragg peaks that decays as \( q^2 \) at small-\( q \) and converges to one at large-\( q \). This can be confirmed by substituting equation (5) into equation (8) to obtain that for small-\( q \)

\[
S_{\text{per}}(\mathbf{q}) = c q^2 + O(q^4),
\]

where \( c \) is a constant and \( q = |\mathbf{q}| \) for both perturbed I and II lattices. This means both URL models produce distorted lattices that are always hyperuniform.

### 2.2. Generating perturbed lattices

We also explored numerically the structural properties of URL in two-dimensions. We considered a square lattice with a lattice spacing \( a \) such that the position vectors \((x_i, y_j) = (i, j)a\) with the index integers \( i, j \in [1, N] \). We applied periodic boundary conditions. The URL was then given as

\[
(x', y') = (x_i, y_j) + (\xi_i, \eta_j),
\]

where \((\xi_i, \eta_j)\) was the displacement vector of the lattice point at \((x_i, y_j)\). Perturbed I lattices were generated with

\[
(\xi_i, \eta_j) = s \cos \theta \sin \theta,
\]

where \( \theta \) was an angle chosen randomly from a uniform distribution in the interval \([0, 2\pi]\). Likewise perturbed II lattices were generated with

\[
(\xi_i, \eta_j) = s \sqrt{\eta} \cos \theta \sin \theta,
\]

where \( \eta \in [0, 1] \) was a random number drawn from a uniform distribution. The square-root function ensures that each displacement vector was uniformly distributed within a circle centred at each lattice site.

### 2.3. Statistical measures of regularity and hyperuniformity

To characterize the uniformly randomized square lattices we generated configurations of \( N = 500^2 \) point particles and monitored three statistical measures namely, the pair correlation function \( g_2(r) \), particle number variance \( \sigma_N^2(R) \), and the nearest neighbor distance metric \( O_N(s) \). Specifically the pair correlation functions was computed via the relation \([21]\)

\[
g_2(r) = \frac{\langle N(r) \rangle}{4\pi r^2 \Delta r} \rho \rho \rho
\]

with \( \langle N(r) \rangle \) being the number particles that fall into the circular ring with an inner and outer radius \( r - \Delta r \) and \( r + \Delta r \), respectively from a central particle, \( \Delta r \) an infinitesimal distance, \( \rho \) the number density \( (\rho = L/\sqrt{N}) \), \( L \) the system length, and \( \langle \ldots \rangle \) denoting an ensemble average, which corresponded to \( 10 \, 000 \) ensembles in our case.

We also characterized the regularity of the perturbed lattices using the nearest neighbor distance (NND) metric that was computed as \([28]\)

\[
O_N = \frac{\langle r \rangle_D}{\langle r \rangle_E} - 1
\]

with \( \langle r \rangle_D \) being the observed average nearest neighbor and \( \langle r \rangle_E = 0.5 \sqrt{L^2/N} \) the expected nearest neighbor distance in a Poisson-like point process \([28]\). For a set of \( N \) points where the positions of the \( i \)th and \( j \)th point particles are \( r_i \) and \( r_j \):

\[
\langle r \rangle_D = \frac{1}{N} \sum_{i=1}^{N} \min(|r_i - r_j|).
\]

where the minimization is over \( j \) not equal to \( i \) to obtain the nearest neighbour distance to the \( i \)th particle. The NND metric takes the following values \( O_N = 1, \, 0, \) and \(-1\) in a perfect square lattice, Poisson point process, and in a cluster, respectively.
Lastly, we computed the number variance of point particles inside an ensemble of windows with the same volume (radius R) to quantify the long-range positional order of the perturbed lattices,

\[
\sigma_N^2(R) = \langle N^2(R) \rangle - \langle N(R) \rangle^2,
\]

where \(N(R)\) is the number of particles enclosed in the circular window and \(\langle \ldots \rangle\). The scaling behavior of \(\sigma_N^2(R)\) was used as measure for hyperuniformity [9, 10, 22].

3. Results

3.1. Manipulating lattice regularity

In this section we present the results from the numerical simulation of the perturbed lattices. The point patterns configurations of the perturbed lattices are shown in figure 1. For the same perturbation strength, perturbed I lattices appear more disordered than perturbed II [compare figure 1(c) and (e)]. The corresponding pair correlation functions exhibits sharp peaks (inverse square-root divergences) in perturbed I lattices while for perturbed-II lattices the peaks are diffuse, indicating a stronger structural correlations in the former. A closer look of the pair correlation functions for the two URL models is given figure 2. The square lattice symmetry of the underlying Bravais lattice dictates that sharp peaks must be positioned at \(r/a = 1, \sqrt{2}, 2, \sqrt{5}\), etc. A comparison between the pair correlation functions indicate that perturbed-I lattices possess robust structural correlation of the underlying lattice. In perturbed-I lattices, these peaks in \(g_2(r)\) persist into the limit of maximal disorder where neighboring lattice sites can overlap, i.e., when \(s \geq 0.5a\). This is a signature of robust structural correlations (short-range ordering) in perturbed I lattices.

Interestingly, the structural order in these lattices is not visually apparent. This can be confirmed from observing that \(O_2\) decays faster in perturbed I lattices as the perturbation strength is increased as shown in figure 3. For an example, the irregularity of the nearest neighbor distances in perturbed-I at \(s = 0.45\) is achieved at \(s = 0.75\) in perturbed II lattices. The irregularity of point particles in perturbed-I lattices approaches that of a Poisson point process for \(s \geq 0.5\) indicating that the short-range ordering in these lattices is hidden beyond this threshold.

3.2. Hidden order on large lengthscales

To confirm that both URL models produce hyperuniform point patterns, we computed \(\sigma_N^2(R)\) as given in figure 4 (a) and (b). Both perturbed lattices are hyperuniform with \(\sigma_N^2(R) \sim R\). We also tested the impact of lattice vacancies on the long range ordering of the URL. We introduced vacancies via a two step process: (i) in a square lattice with \(N\) lattice points and \(N_p\) points were removed, leaving square lattice with a fraction \(p = N_p/N\) of vacancies. (ii) the vacancy riddled square lattice was perturbed according to the two protocols. We generated 500 configurations for each set of parameters to determine \(\sigma_N^2(R)\) from the ensemble average. Figure 4(c) shows that even though it is hard to visually distinguish between a vacancy-free and vacancy riddled URL, the former is hyperuniform and the later is nonhyperuniform with \(\sigma_N^2(R) \sim R^2\). Figure 4(d) demonstrates that uncorrelated vacancies destroy hyperuniformity in perturbed or unperturbed lattices as expected [18, 19]. This is characterized by the scaled number variance \(\sigma_N^2(R)/R^2\) converging to constant value at large \(R\).

4. Discussions and conclusions

In this work, we have presented a URL model that produces hyperuniform point patterns that are locally disordered but exhibiting robust structural correlations. The pair particle statistics of these patterns is characterized by sharp Bragg peaks and significant oscillations in the \(g_2(r)\) even at large perturbation strengths, a
manifestation of resilient short-range order. While Bragg peaks appear in thermalized crystals or crystals containing uncorrelated vacancies (see for example [17]), such structures are nonhyperuniform. The manifestations of robust short-range order in perturbed I lattices is analogous to one observed in amorphous graphene samples containing Stone-Wales defects [18]. This work, therefore, provides another example of an algorithm that preserves hyperuniformity and short-range correlations, in addition to the bond-flipping algorithm utilized in [18].

The interplay of hyperuniformity and short-range order has been found to be critical in the optimization of spectral responses in disordered photonic materials. The co-existence of the two properties has been shown to enhance the photonic bandgap of disordered dielectric structures [29] and light absorption in disorder media.

Figure 2. Pair correlation function $g_2(r)$ versus $r/a$ for the two perturbation schemes lattices at different perturbation levels: $s = 0.1$, 0.2, 0.5, and 0.7 for (a)—(d), respectively.

Figure 3. Nearest neighbor distance metric $O_N$ versus $s$ for the two URL types. Point patterns: (a)—(f) corresponds to systems at different perturbation levels.
[30]. Partially disordered patterns similar to the URLs in this work are anticipated to exhibit superior optical properties because they combine the coherent optical effects of crystals and the broadband, isotropic power spectra of disordered media. A number studies have focused on developing algorithms that generate partially disordered photonic crystals films and they sublattice randomization [3], quasi-periodic structure generation [31, 32], and quasi-crystalline formation [33].

The results presented here do not consider pattern formation expected in systems consisting of interacting particles. In a future work we would explore pattern formation disordered crystals using the phase field crystal model formalism [34–36] that incorporate elastic interactions. We anticipate that pattern formation process would lead to the self-assemble of defective crystals characterized by a network of hyperuniformity-preserving topological defects [18].

**Data availability statement**

No new data were created or analysed in this study.

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