Designing spectral bandgaps in phononic networks

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Mechanical and phononic metamaterials with exotic characteristics, including negative elastic moduli, negative effective mass density, and gapped vibrational spectra, enable precise control of mechanical functionality. A promising approach to designing these and other desirable material properties uses network-based techniques, which are also well-suited to describing many naturally occurring and engineered systems such as actin–myosin networks in biological cells or stiff pin–jointed frames used in structural engineering. Here we show that discrete networks allow efficient algorithmic tuning of gaps at almost arbitrary positions in the spectrum, as well as multiple gaps, isolated modes in the center of a gap, and extensions to periodic 2D and 3D crystals. An additional practical advantage of network-based architectures is their ability to accommodate arbitrary topologies and connectivities and the relative ease of fabrication. The proposed spectral network design framework thus offers a direct path towards manufacturing flexible phononic metamaterials.

Phononic metamaterials offer exciting opportunities to precisely control the passage of sound waves in applications ranging from acoustic cloaking and lensing to art. Many of the special properties of such materials are due to gaps in the vibrational spectrum, which prevent or attenuate the conduction of sound over specific frequency ranges. Engineered bandgaps were studied first in optics for the electromagnetic spectrum, with both direct shape-optimization and approaches based on special material properties such as hyperuniformity. The required precision for fabrication was made available through recent advances in additive manufacturing techniques such as 3D printing and lithography. In parallel, acoustic bandgap engineering proceeded through the exploitation of locally resonant units, hierarchical self-similar lattices, gyroscope materials and topologically protected modes, and topology optimization of continuous materials. Resonances and impedance mismatch between different material components are widely understood as the two primary mechanisms underlying bandgap formation. Complementing the prevailing continuum-based approaches to spectral metamaterials design, we introduce here a highly flexible, efficient network-based design framework.

Our approach is based on discrete periodic spring networks, which have shown remarkable tuneability of mechanical properties in the past and are broadly applicable to a diverse range of natural and engineered systems. Direct numerical tuning of spectral bandgaps has been achieved in continuum systems through topology optimization, whereas little comparable work exists for discrete network geometries (although simple networks have been considered, see, e.g., Ref. [28]). Moreover, previous research has focused primarily on low-lying bandgaps realizable in systems with a high degree of symmetry. Overcoming such restrictions, we consider here generic gaps placed anywhere in the spectrum, which is made possible by the absence of finite spatial resolution problems in discrete networks. The results below show that such arbitrary gaps are typically associated to highly asymmetric network structures.

Specifically, we introduce an efficient direct method to control the appearance and number of bandgaps in the vibrational spectrum of an acoustic spring network through numerical optimization of a set of spring stiffnesses either in the unit cell of a periodic crystal or in a finite sample. This flexible approach enables the tuning of bandgaps at almost arbitrary frequencies in the spectrum of the unit cell and can be easily extended to design multiple bandgaps in periodic network-crystals in 2D and 3D. We find that for a generic spectrum with gap between two arbitrary adjacent modes, the resulting networks exhibit a disordered unit cell, not following lattice symmetry; i.e., there is no obvious symmetry-based (or other) way to deduce the spectral properties from network shapes alone. The optimization procedure induces particular correlation patterns in the spring stiffnesses, but these alone are not sufficient for gap formation. Thus, our analysis implies that generic spectral gaps rely on both local and global properties of the networks.

RESULTS

Spectral optimization. We consider point particles of mass connected by a network of springs with stiffnesses \( k_e \), where \( e \) is an edge of the network. For convenience, we assume periodic boundary conditions throughout, but the approach generalizes straightforwardly to non-periodic boundary conditions. To linear
order, the dynamics of this system is given by

\[ m\ddot{u} + K u = 0, \]

(1)

where \( u \) is the vector of mass displacements and the stiffness matrix \( K = Q k Q^\top \) with \( k \) the diagonal matrix of individual spring stiffnesses and \( Q \) the compatibility matrix encoding the relative geometric relationships between the masses (see Ref. [24] and Supplementary Information). The model can be extended to finite spring masses by replacing \( m \) by a non-diagonal mass matrix (Supplementary Information). Equation (1) can be further simplified by expanding into eigenmodes defined by the relation \( K u_i = m \omega_i^2 u_i \), where the set \( \{\omega_i\} \) constitutes the spectrum of possible excitation frequencies. For periodic crystals, taking the spatial Fourier transform [24] of the above relations leads to the eigenmode equation

\[ K(q)u_i(q) = m\omega_i^2(q)u_i(q), \]

where \( q \) is a wavenumber in the first Brillouin zone of the reciprocal crystal lattice.

The appearance of large gaps between consecutive \( \omega_i \) is responsible for reduced acoustic transmission at nearby frequencies, and therefore it is desirable to be able to produce and precisely control these. To optimize for a gap between \( \omega_i \) and \( \omega_{i+1} \) at wavenumber \( q \), we maximize the objective function

\[ \mathcal{L}_i(q) = \frac{\omega_{i+1}^2(q) - \omega_i^2(q)}{\omega_{i+1}^2(q) + \omega_i^2(q)}, \]

(2)

Often, it is sufficient to consider \( q = 0 \) even if the gap is supposed to appear for all wavevectors. For optimization of multiple gaps, one may consider \( \sum w_i \mathcal{L}_i \) with weighting factors \( w_i \) according to the relative importance of the gaps. We always set \( w_i = 1 \). Similarly, if optimization at
FIG. 2. Tuning more complex spectral properties and network topologies. (a) Final state of a triangular lattice network with $10 \times 10$ unit cell and imposed gaps between modes 100, 101, and 102, effectively leading to a single mode separated from the bulk spectrum. Despite tuning only at wavevector $q = 0$, this property persists in the periodic lattice. (b) Final state of a triangular lattice network with $10 \times 10$ unit cell and three imposed gaps at modes 60, 100, 150. Again, the three gaps tuned into the unit cell spectrum survive into the periodic crystal. (c) Final state of a network with disordered unit cell consisting of 45 point masses placed at random and their positions then relaxed (see section Methods). The network was constructed by periodic Delaunay triangulation. The spectral gap survives into the band structure of the associated periodic crystal with square unit cell and high symmetry points $\Gamma = (0, 0)$, $X = (\pi, 0)$, $M = (\pi, \pi)$ in the Brillouin zone. Note that the thresholded networks in (a)–(c) do not exhibit the same properties as the continuous ones, suggesting that complex spectral characteristics are more fragile than simple gaps, and that networks with more than two different spring stiffnesses may be required to realize them.

specific wavevectors $\{q\}$ is desired, we found the summed objective function $\sum_{\{q\}} L_i(q)$ to be effective.

Even though the derivative of the eigengap is ill-defined when there are degenerate states above or below the gap, standard gradient-based optimization methods work well in many cases. In Fig. 1 and the Supplementary Information we compare the result of standard methods to those obtained from more sophisticated techniques first employed for photonic bandgaps [24]. These comparisons show that for many regions of the spectrum, the gradient-based algorithm comes within 10% of the performance of more sophisticated algorithms, at much greater computational speed. We therefore often adopt the faster, less accurate gradient methods below. Although we do not in general find a true local maximum of the objective function, our optimized networks generically possess clear and pronounced spectral gaps.

We fix the possible stiffnesses between two bounds at 0.1 and 1. Since continuous stiffnesses such as those obtained from the optimization can be difficult to fabricate in practice, we also show a thresholded version of the networks where all stiffnesses are fixed to the value of the bound that they are closest to (orange curves in Fig. 2).

2D triangular lattices. During the optimization process, a gap in the prescribed place of the spectrum can be seen to open, creating an amorphous and more or less featureless network on top of the prescribed network topology (Fig. 1(a), (b)). Note that there is also a clear bandgap in the spectrum of the associated periodic crystal, without explicitly tuning this property by using wavevectors other than $q = 0$ (Fig. 1 bottom row). As can be seen from the stiffness histograms (Fig. 1 top row), stiffnesses settle into a roughly binary distribution. The thresholded network still possesses a gap like the original, continuous optimization result (Fig. 1 middle row). Generally, the optimized network structures are ro-
FIG. 3. Tuning bandgaps in 3D materials. (a) $4 \times 4 \times 4$ unit cell of a periodic tetrahedral network with a gap tuned between modes 102 and 103 (edges connecting adjacent unit cells not shown). While the gap is large near the $\Gamma$ point of the associated orthorhombic crystal with lattice vectors $(4, 0, 0), (0, 2\sqrt{3}, 0), (0, 0, 4\sqrt{2}/3)$, the bands almost close in the rest of the Brillouin zone. (b) Unit cell of a similar tetrahedral network with a gap tuned between modes 102 and 103 using the summed objective function $\sum_{\mathbf{q}} L(\mathbf{q})$ with $\{\mathbf{q}\} = \{0, (\pi/8, \pi/4, \pi/8), (\pi/4, \pi/8, \pi/4)\}$. Here, the spectral gap tuned into the spectra at only two points of the Brillouin zone remains open across the entire band structure. (c) Unit cell of a 3D network constructed from the periodic Delaunay triangulation of 45 points with relaxed positions (cf. Fig. 2(c)) in the cubic unit cell $[0, 1] \times [0, 1] \times [0, 1]$. Edges connecting adjacent unit cells not shown. A gap was tuned between modes 81 and 82 with the same objective function as in (b) and $\{\mathbf{q}\} = \{0, (\pi/2, \pi/2, \pi/2)\}$. Again, by tuning the spectrum at only two points in the Brillouin zone, a gap spanning the entire band structure is obtained. For all band structures, the symmetry points were defined as in [26].
more bandgaps in almost arbitrary places in the spectrum poses no problem in principle: three gaps can be produced by appropriately maximizing a objective function consisting of three terms of the form of Eq. (2), see Fig. 2(b). As seen here, the more complicated the engineered gap structure is, the less likely it is to survive into the spectrum of the associated crystal fully intact. Away from the Γ point, the lowest gap begins to partially close. However, adding more terms to the objective function that open the gap at nonzero wavevectors \( \mathbf{q} \) can mitigate this. As can be seen from the thresholded networks in Fig. 2(a) and (b), the more exotic properties tend to be lost when thresholding, suggesting that they may require more than just two different stiffnesses in the networks.

**Random networks.** It is natural to ask whether the underlying topology of the mechanical network has an influence on the ability to shape the spectrum. Going beyond the triangular grids investigated so far, we may consider a network constructed from the periodic Delaunay triangulation of a set of points on the unit square, see Fig. 2(c). Again, a spectral and bandgap can be easily induced in such a randomized topology, and it survives thresholding, and appears in the periodic crystal as well.

**Three-dimensional networks.** In 3D mechanical networks, a gap tuned into the spectrum of the periodic unit cell (i.e., at \( \mathbf{q} = 0 \)) only rarely survives in the band structure of the associated periodic crystal. We demonstrate this in Fig. 3(a) for a \( 4 \times 4 \times 4 \) unit cell composed of points on a tetrahedral lattice (each 2D slice in the \( (x, y) \)-plane is a triangular grid, and triangular grids are connected such that all bond lengths are equal to 1), where the spectral gap in the spectrum of the unit cell is apparent, but the band structure of the associated orthorhombic crystal contains no gap. However, as mentioned earlier, it can be sufficient to add a single gap at a non-zero wavevector to open a gap across the entire spectrum. This is shown in Fig. 3(b), where including one additional gap in the bulk of the first Brillouin zone opens the spectrum everywhere.

**DISCUSSION**

**Correlation structure.** To analyze the statistical properties of the generic gapped networks, we computed statistics over many different, random initial conditions, gap positions, and randomly chosen numbers of gaps in 2D periodic networks at wavevector \( \mathbf{q} = 0 \). In systems with one gap, the position of the lowest gap is strongly correlated with the mean stiffness, where higher gaps occur at lower mean stiffness (Fig. 4(a); Pearson’s \( r = -0.995 \)). Surprisingly, systems with two, three or four gaps do not follow this trend as strongly and their stiffness distribution is less correlated with the position of the gap (Pearson’s \( r = -0.79 \) for two, \( r = -0.73 \) for three, \( r = -0.64 \) for four gaps). To gain further understand about the stiffness distributions of gapped networks, we computed the radial stiffness autocorrelation

![Figure 4](image-url)
functions for networks with a single gap at various positions, where we define distance between springs (edges) in the sense of the shortest path between nodes of the associated line graph. In agreement with our earlier observation that optimized networks often contain high-stiffness clusters embedded in a lower stiffness matrix, we find a weak anticorrelation between any particular spring stiffness and its immediate neighbors. Correlations are strongest for a gap in the middle of the spectrum and weaker for low or high lying gaps (the full autocorrelation functions along lattice symmetry directions are provided in the Supplementary Information, Fig. S1).

However, this local structure is insufficient to explain the global behavior. A shift of the upper half of a periodic network destroys the global stiffness structure while mostly retaining local correlations. As a result, the gap closes, although there remains a region with low density of states in the spectrum. Further destroying all correlations but retaining the stiffness distribution by randomly shuffling the stiffnesses completely eradicates any trace of a spectral gap. This suggest that a generic gap result from the interplay between local and global structures in the network.

Robustness. With regard to applications, it is important to investigate robustness of the gap to perturbations. For the same networks as before, we add random Gaussian noise with varying standard deviation to the stiffnesses, clipping any values under- or overshooting the stiffness bounds. Averaging over the networks, the relative gap becomes significantly disturbed once the random noise is on the scale of the smallest stiffnesses $k_{\text{min}} = 0.1$, suggesting that the smallest springs play a crucial role in supporting the gap. Similarly, when fabricating networks, springs or rods with continuous stiffnesses are usually difficult to produce. To this end, we quantize the stiffnesses by introducing $n$ uniformly distributed thresholds, effectively constructing an approximation of the continuous network using $n+1$ different spring constants. As shown in Fig. 4(f), three or four different stiffnesses are often sufficient to retain a relatively large spectral gap.

Sensitivity to optimization schemes. Generally, we find that the finer details of designed networks can vary depending on the choice of the numerical optimization scheme. In our simulations, the L-BFGS-B algorithm (Methods) generally produced robust results, but comparison with other methods showed that other algorithms can give slightly different network structures. The outcome of individual simulation runs can also depend on the choice of initial conditions due to non-convexity and non-differentiability of Eq. 2 when degenerate states exist near the gap. In general, many local maxima exist that we only approximate. If one were interested in the largest possible gap, which would correspond to the global maximum of the objective function, more sophisticated global optimization methods such as simulated annealing would be appropriate. However, for most practical design purposes fast gradient-based methods seem sufficient (Supplementary Information, Fig. S2).

Thresholding and fabrication. Due to the discrete nature of mechanical networks other types of optimization algorithms relying on a discrete set of stiffnesses become feasible as well. One can thus envision relatively straightforward fabrication of phononic networks by using improved scalable additive manufacturing techniques for mass production (such as 3D printing) or by employing elastic rods and pin joints. Even when only a discrete set of spring stiffnesses is available for manufacturing, our results for thresholded networks demonstrate that it is possible to preserve a spectral gap in many cases. Conversely, this means that our continuous method is a good replacement for more involved integer optimization or Monte Carlo schemes that could be used to tune networks with fundamentally discrete stiffnesses.

Transmission of sound. Many important applications of phononic metamaterials involve the transmission of sound. To verify the transmission properties of our tuned networks, we simulated gapped systems that were harmonically driven at a fixed frequency at one boundary of the unit cell. Then, the transmission coefficient was computed as the average amplitude at the opposite boundary. Networks tuned using gradient methods generically show a highly pronounced drop in the transmission spectrum at the position of the spectral gap when compared to networks with randomized stiffnesses, and have comparable transmission properties to those obtained with subspace methods (Supplementary Information, Fig. S3).

CONCLUSIONS

Our study shows that direct numerical optimization of spring networks can robustly predict 2D and 3D material structures with both simple and complex gaps in the phononic spectrum of the unit cell and these spectral properties can be carried over to the corresponding periodic crystal. We also demonstrated how extensions involving a summed objective function are able to produce gaps in periodic crystals if the simplest method fails. The proposed spectral design approach is robust with respect to the underlying topology of the network which may be ordered or disordered, and produces generally amorphous, disordered stiffnesses in the unit cell. Refining our results with sophisticated subspace optimization methods, we found relatively little improvement for generic gaps, suggesting that for most practical design purposes fast gradient-based methods can be sufficient.

The engineered networks appear in general to consist of two material phases with maximally different stiffnesses, presumably because impedance mismatch is responsible for gap formation. This allows gaps to largely
survive when only a small number of discrete stiffnesses is accessible, suggesting that the above ideas can be efficiently implemented in practice to fabricate new classes of phononic metamaterials. We conclude by noting that the proposed design framework can be straightforwardly extended to tune gaps at specified frequencies instead of mode indices, different gaps at different positions in the Brillouin zone, or even more complex spectral features, paving the way towards a comprehensive spectral design of mechanical networks.

METHODS

Gradient-based optimization. Numerical maximizations were performed using the L-BFGS-B bound constrained algorithm as implemented in SciPy 1.0 [27].

Subspace-based optimization. The subspace semidefinite programming algorithm was implemented using the packages CVXOPT 1.1.9 [28] and CVXPY 1.0 [29]. In contrast to the original implementation from Ref. [24] (Table 1), for phononic networks, the stiffness matrix $K$ is relevant instead of a finite element discretization of Maxwell’s equations in a medium. The objective function $\text{Eq. (2)}$ is a fractional linear program, which was converted into a linear program using the Charnes-Cooper transformation [30]. The subspaces (eigenspaces corresponding to eigenfrequencies above and below the gap) were approximated using up to 30% of all available eigenvectors directly adjacent to the gap. The iteration was said to have converged when the Euclidean norm of relative changes in the stiffnesses was less than a tolerance of $10^{-4}$ after consecutive iterations.

Randomized topology. Networks with randomized topology were constructed by first distributing points $x_i$ in the unit cell uniformly at random, and then performing 20 gradient descent steps for the potential function $V = 10^{-5} \sum_{\sigma \neq i} |x_i - x_j|^{-1}$ in order to make the points appear more ordered. At each step, gradient components larger than 0.01 in absolute value were clipped. In addition, points were constrained to remain inside the unit cell. In order to generate periodic connectivity, the basic unit cell points were copied into the directly adjacent unit cells and a Delaunay triangulation was calculated to obtain the network topology and unit vectors along the bonds. Finally, equivalent points were identified in the basic unit cell and the adjacent unit cells deleted to obtain a periodic network.
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