Soft Modes in a Square Lattice with Random Next-Nearest-Neighbor Bonds

Martin J. Falk
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In this project, we compute dispersion relations for a particular distortion of the 2D square lattice with NN bonds. We find that the lattice supports lines of "soft modes" within the BZ for which $w \propto q^2$, and relate these modes to the zero-energy Guest strain, arguing that this suggests a "mildly topological" characterization of the property. We then consider the effect of randomly populating the lattice with NNN bonds, and review the use of a coherent potential approximation to justify replacing our heterogeneous lattice with a homogeneous effective lattice. We then find that the lines of soft modes do not survive within the BZ after adding NNN bonds.

I. PRELIMINARIES

As of late, there has been interest in understanding the mechanical properties of isostatic lattices - lattices where the number of bonds connecting at each site is twice the dimensionality of the space it is embedded in. This interest comes from a number of areas; isostatic lattices are normally on the verge of mechanical instability, and occur frequently in natural systems of interest, for example in glasses and as biopolymer networks in cells[1]. However, they have also recently drawn attention for being natural mechanical analogues of electronic topological insulators[2]. In this final project, we will review properties of a "distorted" two-dimensional square lattice. In particular, it supports two directions in its Brillouin Zone for which the dispersion is weaker that $\propto q^1$, and that a small perturbation of the basis sites is not sufficient to remove these two soft modes.

A natural extension of this work is to consider the effects of disorder on these results. While in the course we have considered the effect of disorder on coarse-grained models of two-dimensional elastic media by allowing for topological defects, we adopt a different approach here. We instead add next-nearest-neighbor (NNN) bonds randomly with probability p and of strength equal to the strength of the bonds in the original nearest-neighbor-only lattice. The mean-field-esque Coherent Potential Approximation is then subsequently employed to justify replacing the heterogeneous network with an effective, regular lattice with NNN bonds of strength $\kappa(p)$. In doing so, we take cues from Refs. 3, 4 which successfully employed the CPA to analytically investigate the approach to isostaticity for a regular 2D lattices. We will then analyze the spectrum of this effective regular lattice.

II. RESULTS FROM THE NEAREST-NEIGHBOR LATTICE

The system we consider is a regular, square array of unit cells, each of length 1. Each cell possesses four basis sites, and the rest configuration of this lattice is shown in Fig. I, with bonds drawn as solid lines. We parameterize movement away from the rest configuration by defining the collection of distortions $\mathbf{u}_{\mathbf{R},i}$ with $i = 0, 1, 2, 3$ and

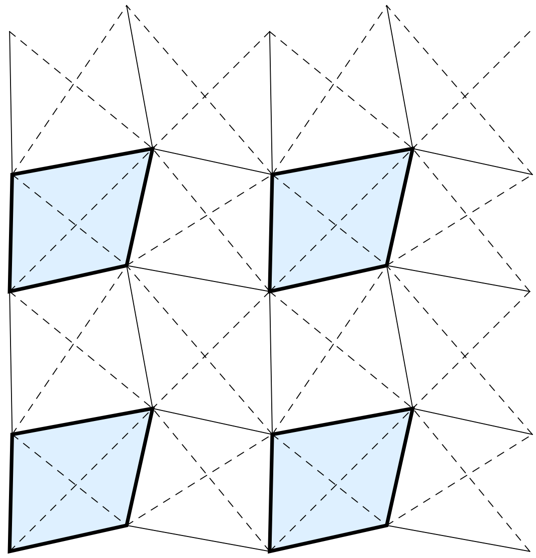

FIG. 1: Four unit cells of the lattice under consideration. Relative to the origin of each unit cell, the basis sites are located at (.45,.1), (.55,.55), (.01,.45), going counter-clockwise.

$\mathbf{R} \equiv n_1\ell_1 + n_2\ell_2$. Here ℓ_1, ℓ_2 are the Bravais lattice vectors for the system, $(1, 0)$ and $(0, 1)$.

Attaching linear central-force springs with force constant k set to unity between all NN sites, we can define $\mathbf{D}$, the dynamical matrix, the linear map between vectors of distortions $\mathbf{u}$ to vectors of the forces at correspondingly enumerated sites $\mathbf{f}$. In other words, $\mathbf{Du} = \mathbf{f}$. Employing a Fourier transform, we write $\mathbf{u}$ in a basis of the form

$$\mathbf{u} = \exp(i\mathbf{q}\cdot\mathbf{R})\exp(-iw(\mathbf{q})t) \tag{1}$$

In this new basis, $\mathbf{D}$ is block-diagonal, and $\mathbf{Du} = \mathbf{f}$ becomes

$$mw^2(\mathbf{q})\mathbf{u}(\mathbf{q}) = \mathbf{D}(\mathbf{q})\mathbf{u}(\mathbf{q}). \tag{2}$$

where $\mathbf{q}$ is a vector in $\mathbb{C}^2$ with $Re[\mathbf{q}]$ confined to the Brillouin Zone (BZ).

To complete the characterization of the NN lattice, we diagonalize $\mathbf{D}(\mathbf{q})$ to find dispersion relations. However,

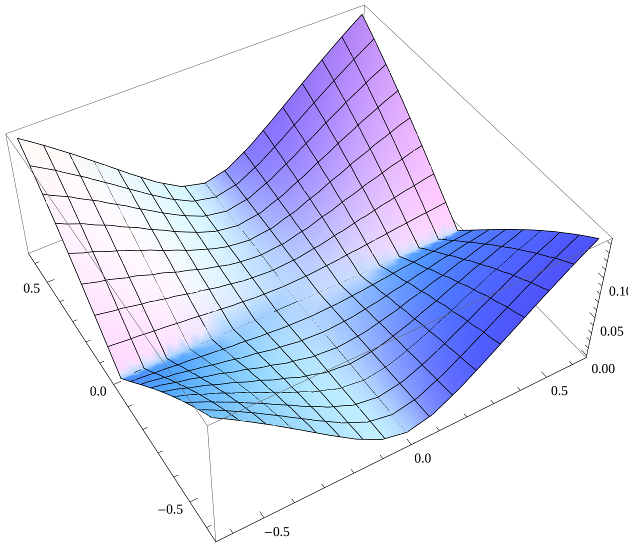

FIG. 2: One of the dispersion relations $w(\mathbf{q})$ for the distorted lattice under consideration which displays a soft mode near the origin of the BZ, seen as the sharp flat line.

of note is the fact that some of the acoustic dispersion relations, such as the one in Fig. II, have directions in the BZ for which the w grows very slowly.

Indeed, if we expand $\det(\mathbf{D})$ to lowest non-zero order near the origin of the BZ, we find that there are lines in the BZ along which $\det(\mathbf{D})$ vanishes. These lines represent "soft modes," which have dispersions $w \propto q^2$ as opposed to the usual $w \propto q$ for acoustic modes. In the end, this should come as no surprise, since most isostatic lattices guarantee the existence of a "Guest mode,"[1] which is defined as a uniform strain which costs the lattice zero energy. And, as expected, Guest modes are intimately related to the dispersion of the lattice at long wavelengths.

For any strain μ, consider an acoustic mode (ignoring intracellular displacements) $(t_x, t_y)\exp(i\mathbf{q}\cdot\mathbf{R})\exp(-iw(\mathbf{q})t)$ of the following form:

$$\mathbf{t} = (\mu_{xx}/(iq_x), \mu_{yy}/(iq_x\alpha_\pm(\mu))); \tag{3a}$$

$$q_y = \alpha_\pm(\mu)q_x; \tag{3b}$$

$$\alpha_\pm(\mu) \equiv \left(\mu_{xy} \pm \sqrt{\mu_{xy}^2 - \mu_{xx}\mu_{yy}}\right)/\mu_{xx}. \tag{3c}$$

As we take q_x to zero, this mode converges to our strain μ. But, just as the mode converges continuously to the strain, so must the energy of the mode converge to the elastic energy of the strain. Since the mode will have energy proportional to $w^2 q_x^{-2}$, this has consequences for lattices with zero energy Guest modes; along the lines $q_y = \alpha_\pm(\mu)q_x$, the dispersion relation must soften from $w \propto k^2$ to $w \propto k^2$.

Focusing again on our particular distorted square lattice, the fact that we have soft modes implies it has a Guest strain with negative determinant. If we wanted to remove these soft modes, we would have to change the basis sites of the lattice to a configuration where the Guest strain had positive determinant. Thus, in order for us to remove soft modes from the BZ and make α complex, we need to pass through a critical Guest strain which is singular. In this sense the soft modes are "mildly topological". Their presence can only be changed at very specific configurations of the lattice - configurations with singular Guest strains, and this is certainly not the generic case. We are therefore interested in whether or not the presence of disorder in the form of randomly added NNN bonds still respects this "mildly topological" property of the NN lattice.

III. RESULTS FROM THE NEXT-NEAREST-NEIGHBOR LATTICE

One way to deal with the form of disorder included by randomly populating an isostatic lattice with NNN bonds is the CPA, which adopts a mean-field approach to the problem. We assume that we can self-consistently choose a $\kappa(p, w)$ such that a homogeneous lattice with NNN bonds of strength κ reproduces the behavior of the heterogeneous lattice. This κ is determined by the requirement that the Green's function of the effective medium be unchanged after averaging over all configurations with one NNN bond missing with probability p. The Green's function for the effective medium is

$$\mathbf{G}(\mathbf{q}, w) = [w^2\mathbf{I} - \mathbf{D}(\mathbf{q})] \tag{4}$$

However, when we remove a bond from the lattice, the dynamical matrix is no longer translation invariant, and hence its computation becomes more involved. Nevertheless, the calculation has been carried out for the regular square lattice and the 2D Kagome lattice, and its validity has been confirmed via numerical simulation[3, 4]. The important information from those calculations are that, for $w = 0$, $\kappa(p) \propto p^2$ for p small, and $\kappa(p) \propto p$ elsewhere.

While we can calculate $\kappa(p, w)$ via the CPA, ultimately we are less interested in the specific form of its dependence on p and w. More important is the behavior of the soft mode as a function of κ. While the κ obtained via the CPA is generically complex, since we are interested in the behavior of the soft mode we only look in a small neighborhood of the BZ. There $w = 0$, and $\kappa(p, 0)$ is real for all p.

Adding in a homogeneous NNN interaction to our lattice, we can compute $\mathbf{D}$ as we did for the lattice with only NN interactions, and expand to lowest non-zero order near the origin of the BZ. We then solve for the slopes m such that $\det(\mathbf{D}(q_x, qy = mq_x))$ vanishes. However, we

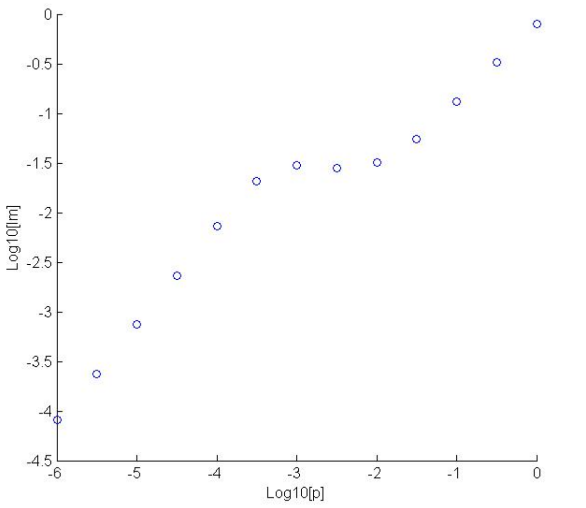

FIG. 3: Log-log plot of the imaginary component of one of the possible m's as a function of the probability p of populating a NNN bond.

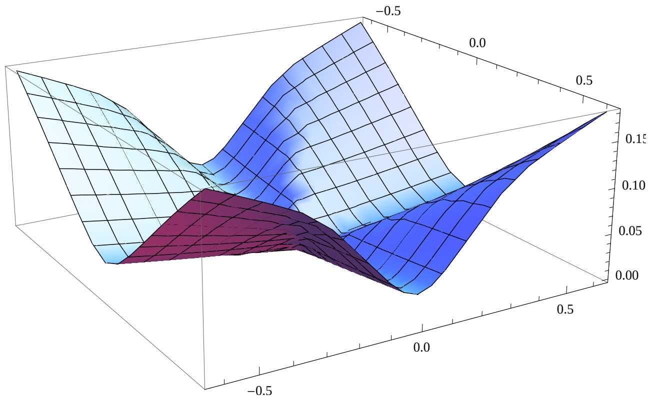

FIG. 4: One of the dispersion relations $w(\mathbf{q})$ for the distorted lattice with NNN bonds of strength $\kappa = .1$, no longer displaying a soft mode near the origin of the BZ.

find that in this case, unlike in the lattice with only NN interactions, all m's acquires an imaginary component which appears to grow continuously from 0, as illustrated in Fig. III. Thus the soft modes of the NN lattice disappear from the BZ upon addition of NNN interactions. This is born out by looking at the dispersion relation in Fig. III, where the soft mode in Fig. IV has been lifted.

IV. CONCLUSIONS AND FUTURE WORK

To summarize: in this project, we have computed dispersion relations for a particular distortion of the 2D square lattice with NN bonds. We found that the lattice supported lines of "soft modes" within the BZ for which $w \propto q^2$, and related these modes to the zero-energy Guest strain. We then considered the effect of randomly populating the lattice with NNN bonds, and reviewed the use of a coherent potential approximation to justify replacing our heterogeneous lattice with a homogeneous effective lattice. It was then found that the lines of soft modes do not survive within the BZ after adding NNN bonds, implying that soft modes are not necessarily protected by virtue of their connection to the Guest strain.

In terms of verification, while the CPA is a good starting point, it is of course important to also compare these results to simulation. Future directions to pursue are looking at the behavior of soft modes, sweeping over all possible distorted square lattices. Finally, there are more robustly topological features of the system, such as topologically protected surface and bulk modes. However, these topological characterizations are understood only in the context of isostatic lattices[2], and hence there is no intuition as to whether they too are inured to NNN bond disorder. This will require computing the CPA at finite w.

[1] T. C. Lubensky, C. L. Kane, Xiaoming Mao, A. Souslov, Kai Sun, arXiv:1503.01324 (2015)
[2] C. L. Kane, T. C. Lubensky Nature Physics 10 (1), 39-45
[3] Xiaoming Mao and T. C. Lubensky, Phys. Rev. E 83, 011111 (2011).
[4] Xiaoming Mao, Ning Xu, and T. C. Lubensky, PRL 104, 085504 (2010).