

Soft Modes and Elasticity of Nearly Isostatic Lattices: Randomness and Dissipation

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The square lattice with nearest neighbor central-force springs is isostatic and does not support shear. Using the coherent potential approximation (CPA), we study how the random addition, with probability $\mathcal{P} = (z - 4)/4$ ($z =$ average number of contacts), of next-nearest-neighbor (NNN) springs restores rigidity and affects phonon structure. The CPA effective NNN spring constant $\tilde{\kappa}_m(\omega)$, equivalent to the complex shear modulus $G(\omega)$, obeys the scaling relation, $\tilde{\kappa}_m(\omega) = \kappa_m h(\omega/\omega^*)$, at small \mathcal{P} , where $\kappa_m = \tilde{\kappa}'_m(0) \sim \mathcal{P}^2$ and $\omega^* \sim \mathcal{P}$, implying nonaffine elastic response at small \mathcal{P} and the breakdown of plane-wave states beyond the Ioffe-Regel limit at $\omega \approx \omega^*$. We identify a divergent length $l^* \sim \mathcal{P}^{-1}$, and we relate these results to jamming.

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Isostatic lattices [1–3] are systems at the onset of mechanical stability in which the average number of contacts z per particle in d dimensions is equal to $z_c = 2d$. A lattice with N particles and N_c two-particle contacts has $N_0 = dN - N_c$ zero modes. An infinite isostatic lattice is one in which $N_c = Nz_c/2$, and the fraction of zero modes vanishes. Because particles at the boundary have fewer contacts than those in the bulk, the number of zero modes in a finite isostatic lattice is subextensive ($N_0 \sim N^{(d-1)/d}$) and proportional to the area of the system boundary. As a result, the phonon spectrum of isostatic lattices is one-dimensional in nature. These properties underlie the elastic and vibrational properties of a variety of systems including network glasses [4,5], rigidity percolation [6,7], β -cristobalite [8], granular media [9,10], and networks of semiflexible polymers [11]. Isostatic lattices include d -dimensional hypercubic lattices and the $2d$ kagome, the $3d$ pyrochlore lattice, and their d -dimensional generalizations [12], all with central-force springs with spring constant k connecting nearest neighbor (NN) sites. They also include randomly packed spheres at the jamming transition [13–15].

As in critical phenomena at “standard” phase transitions, the approach to the critical isostatic state, which this Letter explores, is characterized by diverging length and time scales and by scaling behavior. Lattices can be moved off isostaticity in various ways, including (i) introducing springs with a tunable spring constant κ connecting next-nearest-neighbor (NNN) sites [16] and (ii) increasing the volume fraction ϕ of packed spheres above the critical value ϕ_c at jamming [13–15,17–19]. The isostatic lattices with their soft modes are then approached continuously as κ or $\Delta\phi = (\phi - \phi_c)$ approach zero, and divergent length scales l^* , vanishing frequencies ω^* , and possibly vanishing shear moduli G (isotropic for jamming and the anisotropic modulus $C_{44} \equiv C_{xyxy}$ for the square lattice as detailed

below) can be identified. In approach (ii), the number of contacts increases as $\Delta z = z - z_c \sim (\Delta\phi)^{1/2}$, $l^* \sim (\Delta z)^{-1}$, $\omega^* \sim \Delta z$, and $G \sim \Delta z$, whereas in approach (i) for the square lattice $l^* \sim \kappa^{-1/2}$, $\omega^* \sim \kappa^{1/2}$, and $G \sim \kappa$.

In this Letter, we investigate a third approach to isostaticity in the square lattice: we populate NNN bonds with springs of spring constant κ with probability \mathcal{P} as shown in Fig. 1. At nonzero \mathcal{P} , the addition of an extensive number of NNN bonds removes all zero modes with a probability that approaches unity [20] as the number of sites $N \rightarrow \infty$, and as a result, the infinite lattice has a nonzero shear modulus for all $\mathcal{P} > 0$. Thus, our model describes a rigidity percolation problem in which the percolation threshold is at $\mathcal{P} = 0$. It is the particular case [21,22] of the more general rigidity percolation problem on a square lattice [23] with NN and NNN bonds populated independently with respective probabilities \mathcal{P}_{NN} and \mathcal{P} in which $\mathcal{P}_{\text{NN}} = 1$. This model shares underlying periodicity with approach (i) but it includes randomness analogous to approach (ii). Adding a NNN spring increases the number of contacts by

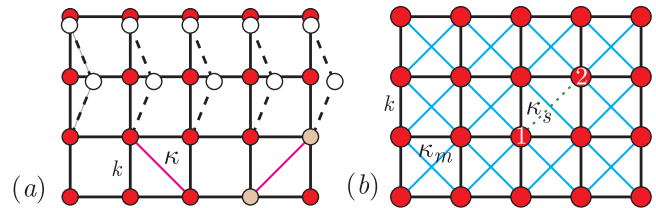


FIG. 1 (color online). (a) Square lattice with NN bonds with springs of spring constant k and NNN bonds with randomly placed springs with spring constant κ . The distortion depicted with dotted lines represents one of the zero modes of the lattice with no NNN springs. (b) Effective-medium lattice with springs of spring constant κ_m on all NNN bonds. In the CPA, the spring constant κ_s of a single NNN bond is changed to κ or to 0 with respective probabilities \mathcal{P} and $1 - \mathcal{P}$.

TABLE I. Dependence of l^* , ω^* , and G on \mathcal{P} and Δz .

$l^* \sim \mathcal{P}^{-1} \sim (\Delta z)^{-1}$	$\omega^* \sim \mathcal{P} \sim \Delta z$	$G \sim \mathcal{P}^2 \sim (\Delta z)^2$
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1 so that $\mathcal{P} = (z - z_c)/4$, where $z_c = 4$ in the NN square lattice. Unless otherwise stated in what follows, we use reduced units with $k = 1$ and lattice constant $a = 1$ and unitless spring constants, elastic moduli, and frequencies: $\kappa/k \rightarrow \kappa$, $Ga^2/k \rightarrow G$, and $\omega/\sqrt{k} \rightarrow \omega$.

We study this random NNN model using the coherent potential approximation (CPA) [23–25], which gives good results for the conductivity of random networks near percolation [26] and for rigidity percolation problems [23] except right in the vicinity of $\mathcal{P} = \mathcal{P}_c$, and we verify that it gives results that are in quantitative agreement with numerical simulations in our system. In the CPA, an effective medium of a uniform lattice with every NNN bond occupied by a spring with complex effective spring constant $\tilde{\kappa}_m(\omega) = \tilde{\kappa}'_m(\omega) - i\tilde{\kappa}''_m(\omega)$, determined by a proper self-consistency condition, is used to capture the disorder average of the random lattice. From $\tilde{\kappa}_m(\omega)$, which is also equal to the complex shear modulus $G(\omega)$, we can calculate (following the procedures of approach (i) [16]) the characteristic length l^* and frequency ω^* and the zero-frequency shear modulus $G = \tilde{\kappa}'(\omega = 0)$, as summarized in Table I. As in the case of jamming, $l^* \sim 1/\omega^* \sim (\Delta z)^{-1}$, in agreement with the general cutting arguments of Refs. [3,18]. The length l^* , being the average distance between NNN bonds in any row or column in the random lattice, marks the crossover from $1d$ to $2d$ behavior in the effective medium, because NNN bonds couple neighboring $1d$ rows or columns. The shear modulus, however, scales as $G \sim \mathcal{P}^2 \sim (\Delta z)^2$, rather than as $G \sim (\Delta z)$ at jamming, implying highly nonaffine response near $\mathcal{P} = 0$. If the response were affine, every equivalent NNN bond would distort the same way in response to shear, and G would be equal to $\mathcal{P}\kappa$. Response becomes more nearly affine with $G \approx \mathcal{P}\kappa$ when $\pi^2\mathcal{P} \gg \kappa$. Figure 2 shows $\kappa_m = G$ as a function of \mathcal{P} for different κ calculated from the CPA and via numerical simulations using the conjugate gradient method [27] to calculate the relaxed response of the system to an applied shear.

The frequency dependence of $\tilde{\kappa}_m(\omega)$ is plotted in Fig. 3. In the nonaffine regime, it obeys a scaling law, $\tilde{\kappa}(\omega) = \kappa_m h(\omega/\omega^*)$, where $h(w)$ approaches unity as $w \rightarrow 0$. $\tilde{\kappa}''(\omega)$ vanishes as ω^2 at small ω but becomes nearly linear in ω for $\omega \geq 0.5\omega^*$. This behavior corresponds to a shear viscosity that vanishes as ω at small ω but becomes a constant at large ω . A transverse phonon of frequency ω propagating along the y direction (i.e., with $q_x = 0$) has a wave number $q(\omega) = \omega/\sqrt{\tilde{\kappa}'_m(\omega)}$ and a mean-free path $l(\omega) = \sqrt{\tilde{\kappa}'_m(\omega)}\tau(\omega)$, where $\tau(\omega) = 2[\tilde{\kappa}''_m(\omega)q^2(\omega)/\omega]^{-1}$ is the decay time, implying that the Ioffe-Regel limit [28] $q(\omega)l(\omega) = 1$ occurs at $2\tilde{\kappa}'_m(\omega) = \tilde{\kappa}''_m(\omega)$, i.e., at $\omega \approx \omega^*$. Thus ω^* sets the frequency scale for the nearly isostatic

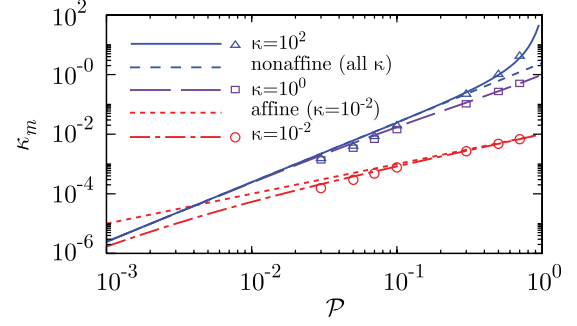


FIG. 2 (color online). Comparison of the CPA solution (lines) and numerical simulations on a 100×100 lattice (data points) for the effective-medium spring constant κ_m as a function of \mathcal{P} for $\kappa = 10^{-2}$, 10^0 , and 10^2 (in reduced units). Also shown are the nonaffine ($\kappa_m = (\pi\mathcal{P}/2)^2$) and affine limits ($\kappa_m = \mathcal{P}\kappa$). For the CPA at large \mathcal{P} , we used the full dynamical matrix [Eq. (1)] rather than the approximate forms of Eq. (2).

modes and the scale at which plane-wave states become ill defined in agreement with recent studies of thermal conductivity near jamming [19]. Because $q_y(\omega^*) \sim \pi/a$, plane-wave states with $q_x = 0$ are well defined up to the zone edge.

Because the zero modes on isostatic square lattice are uniform displacements of rows or columns, its phonon spectrum is identical to that of decoupled one-dimensional chains with frequencies $\omega_{x,y}(\mathbf{q}) = 2|\sin q_{x,y}/2|$ and density of states $\rho(\omega) = (2/\pi)/\sqrt{4 - \omega^2}$ with a nonzero value $1/\pi$ at $\omega = 0$ as shown in Fig. 4. When the effective-medium NNN coupling $\tilde{\kappa}_m(\omega)$ is added, the dynamical matrix becomes

$$\begin{aligned}
 D_{xx}(\mathbf{q}) &= D_{yy}(q_y, q_x) \\
 &= 4\sin^2(q_x/2) + 4\tilde{\kappa}_m(\omega)\sin^2(q_y/2) \\
 &\quad + 4\tilde{\kappa}_m(\omega)\sin^2(q_x/2) \\
 &\quad - 8\tilde{\kappa}_m(\omega)\sin^2(q_x/2)\sin^2(q_y/2), \\
 D_{xy}(\mathbf{q}) &= D_{yx}(\mathbf{q}) = 2\tilde{\kappa}_m(\omega)\sin(q_x)\sin(q_y).
 \end{aligned} \tag{1}$$

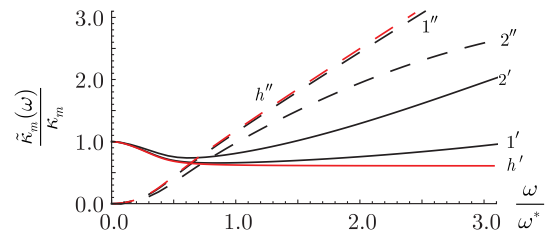


FIG. 3 (color online). Real and imaginary parts of $h(\omega/\omega^*) \equiv h' - ih''$ (labeled respectively h' and h'') and of $\kappa_m(\omega)/\kappa_m$ for $\mathcal{P} = 10^{-2}$ and 10^{-1} (labeled respectively $1'$, $1''$, $2'$, and $2''$) for $\kappa = 1$. Curves for $\mathcal{P} = 10^{-3}$ and 10^{-4} differ by less than 1% from the h curve and are not shown. The full dynamical matrix [Eq. (1)] was used in the $\mathcal{P} = 10^{-1}$ calculation.

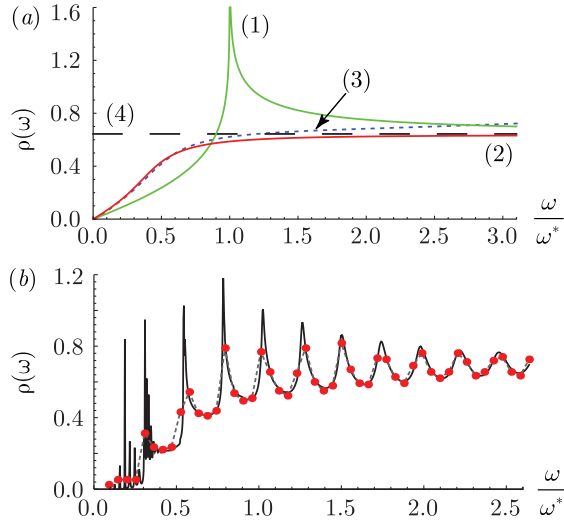


FIG. 4 (color online). (a) Density of states $\rho(\omega)$ for (1) (green) a uniform lattice with $\kappa = \kappa_m$ on all NNN bonds, (2) (red) in the scaling nonaffine limit where $\tilde{\kappa}_m(\omega) = \kappa_m h(\omega/\omega^*)$, and (3) (blue dotted line) for $\mathcal{P} = 10^{-1}$ (4) (black dashed line) Isostatic two-mode limit of $2/\pi \approx 0.64$. (b) Density of states for a 100×100 lattice with $\mathcal{P} = 10^{-1}$ obtained via direct numerical calculation (dots) and via the CPA (line) using the full rather than the approximate dynamical matrix of Eq. (2). Binning of the CPA result would wash out the spikes at low frequency at $\omega = q_x = 2\pi n/100$ (for integer n).

In the $\mathbf{q} \rightarrow 0$ limit, the dynamical matrix reduces to that of continuum elastic theory with $D_{xx} = C_{11}q_x^2 + C_{44}q_y^2$, where C_{11} is a compression modulus and C_{44} the shear modulus. $C_{44}(\omega)$ is the complex shear storage modulus $G(\omega)$. Comparison of the continuum form with the small \mathbf{q} limit of Eq. (1) yields $\tilde{\kappa}_m(\omega) = G(\omega)$.

When $|\tilde{\kappa}_m(\omega)| \ll 1$, the off-diagonal terms in D_{ij} can be ignored, and the low-frequency modes follow from

$$D_{xx}(\mathbf{q}) \approx q_x^2 + 4\tilde{\kappa}_m(\omega)\sin^2(q_y/2) \approx q_x^2 + \tilde{\kappa}_m(\omega)q_y^2 \quad (2)$$

and a similar approximation for $D_{yy}(\mathbf{q})$. Replacing $\tilde{\kappa}_m(\omega)$ by its $\omega \rightarrow 0$ limit κ_m yields a characteristic length $l^* = \sqrt{1/4\kappa_m}$ through the comparison of q_x^2 with $D_{xx}(0, \pi) = 4\kappa_m$ and a characteristic frequency at the zone edge of $\omega^* = \sqrt{D_{xx}(0, \pi)} = 2\sqrt{\kappa_m}$. For $q_x > 1/l^*$ (or $\omega > \omega^*$), the excitation spectrum is one dimensional in q_x . These observations along with $\kappa_m \sim \mathcal{P}^2$, which we derive below, lead to the results of Table I.

To proceed with the CPA, we use the 2×2 phonon matrix Green's function of this effective medium

$$\mathbf{G}(\mathbf{q}, \omega) = [\omega^2 \mathbf{I} - \mathbf{D}(\mathbf{q})]^{-1}. \quad (3)$$

In the CPA approximation [24,26], an arbitrary NNN bond, say, between particles 1 and 2 as shown in Fig. 1(b), is replaced by a new one with a random spring constant κ_s with values κ and 0 with respective probabilities \mathcal{P} and $1 - \mathcal{P}$. The dynamical matrix then changes to $\mathbf{D}^V = \mathbf{D} +$

\mathbf{V} , where \mathbf{V} is the potential given by [23]

$$\mathbf{V}_{l,l'} = (\kappa_s - \tilde{\kappa}_m)(\delta_{l,1} - \delta_{l,2})\hat{\mathbf{b}} \otimes (\delta_{l',1} - \delta_{l',2})\hat{\mathbf{b}}, \quad (4)$$

in real space, $\hat{\mathbf{b}} = (\mathbf{e}_x + \mathbf{e}_y)/\sqrt{2}$ is the unit vector along the chosen NNN bond, and l and l' specify sites on the lattice. The potential \mathbf{V} leads to a modification of the phonon Green's function, $G_{l,l'}^V(\omega)$, which can be calculated following standard procedures:

$$\mathbf{G}_{l,l'}^V(\omega) = \mathbf{G}_{l-l'}(\omega) + \sum_{l_1, l_2} \mathbf{G}_{l-l_1}(\omega) \cdot \mathbf{T}_{l_1, l_2} \cdot \mathbf{G}_{l_2-l'}(\omega), \quad (5)$$

where $\mathbf{G}_{l-l'}$ is the Fourier transform with respect to \mathbf{q} of $\mathbf{G}(\mathbf{q}, \omega)$ and where $\mathbf{T} = [\mathbf{I} - \mathbf{V} \cdot \mathbf{G}]^{-1} \cdot \mathbf{V}$ is the scattering T matrix. The effective spring constant $\tilde{\kappa}_m(\omega)$ is determined within the CPA through the requirement that the average \mathbf{T} vanish: $\mathcal{P}\mathbf{T}|_{\kappa_s=\kappa} + (1 - \mathcal{P})\mathbf{T}|_{\kappa_s=0} = 0$, so that

$$f(\tilde{\kappa}_m, \omega)\tilde{\kappa}_m^2(\omega) - [1 + \kappa f(\tilde{\kappa}_m, \omega)]\tilde{\kappa}_m(\omega) + \kappa\mathcal{P} = 0. \quad (6)$$

The function f can be expressed as $f(\tilde{\kappa}_m, \omega) = [2/(\pi\sqrt{\tilde{\kappa}_m})]\tilde{g}(\tilde{\kappa}_m, \omega/\sqrt{\tilde{\kappa}_m})$, where

$$\tilde{g}(r, s) = \frac{1}{2} \int_0^\pi dq \frac{1 - e^{-\sqrt{r}p(q,s)} \cos q}{p(q, s)}, \quad (7)$$

with $p(q, s) = \sqrt{4\sin^2(q/2) - s^2}$. In the limit $r, s \rightarrow 0$, $\tilde{g}(r, s) = 1$, and thus $f(\tilde{\kappa}_m, 0) \rightarrow [2/(\pi\sqrt{\tilde{\kappa}_m})]$ as $\tilde{\kappa}_m \rightarrow 0$. When $\sqrt{r}p(\pi, s) \ll 1$, the exponential in the numerator of $\tilde{g}(r, s)$ can be replaced by unity, and $\tilde{g}(0, s) \equiv g(s)$, $g(s) \rightarrow 1 + (s^2/8)\{\ln[8/(\sqrt{e}s)] + i(\pi/2)\}$. We expect $\tilde{\kappa}_m$ to tend to zero with \mathcal{P} so that in the small \mathcal{P} limit, we can generally ignore the first term in Eq. (6).

We consider first the static limit, $\omega = 0$, for which the self-consistency equation for small \mathcal{P} becomes

$$\kappa_m + \frac{2\kappa}{\pi}\sqrt{\kappa_m} - \mathcal{P}\kappa = 0. \quad (8)$$

The solution of this equation has two limits

$$\kappa_m \simeq \begin{cases} (\pi\mathcal{P}/2)^2 & \text{if } \pi^2\mathcal{P} \ll \kappa, \\ \mathcal{P}\kappa & \text{if } \pi^2\mathcal{P} \gg \kappa, \end{cases} \quad (9)$$

as shown in Fig. 2, together with solutions of the full CPA Eq. (6) and numerical simulations. In the first case, $\kappa\sqrt{\kappa_m} \gg \kappa_m$, and the solution for κ_m is obtained by ignoring the first term in Eq. (8); in the second case, the opposite is true, and κ_m is obtained by ignoring the second term in this equation. In the second case, every NNN bond distorts in the same way under stress, and response is affine. In the first case $\kappa_m = (\pi\mathcal{P}/2)^2 \ll \mathcal{P}\kappa$, and response is nonaffine with local rearrangements in response to stress that lower the shear modulus to below its affine limit. Within the CPA, this result emerges because of the divergent elastic response encoded in \mathbf{G} (and $f(\kappa_m, 0)$) as $\kappa_m \rightarrow 0$. As κ

approaches zero at fixed \mathcal{P} , distortions produced by the extra bond decrease and the nonaffine regime becomes vanishingly small.

For finite frequency ω , the effective-medium spring constant is complex, $\tilde{\kappa}(\omega) = \tilde{\kappa}'(\omega) - i\tilde{\kappa}''(\omega)$, where the imaginary part $\tilde{\kappa}''(\omega)$, which is odd in ω and positive for $\omega > 0$, describes damping of phonons in this random network. As in the static case, the nonaffine limit of the CPA result for $\tilde{\kappa}(\omega)$ at small \mathcal{P} is the solution to $\tilde{\kappa}_m f(\tilde{\kappa}_m, \omega) = \mathcal{P}$ obtained from Eq. (6) by ignoring all but its last two terms. Following Eq. (7), at small $\tilde{\kappa}_m$ and ω , $f(\tilde{\kappa}_m, \omega) = [2/(\pi\sqrt{\tilde{\kappa}_m})]g(2\sqrt{\kappa_m/\tilde{\kappa}_m}\omega/\omega^*)$. Thus in this limit, $\tilde{\kappa}_m(\omega)$ satisfies a scaling equation $\tilde{\kappa}_m(\omega) = \kappa_m h(\omega/\omega^*)$. As $\omega \rightarrow 0$, $h(\omega) \rightarrow 1 - \omega^2\{\ln[4/(\sqrt{e}\omega)] + i(\pi/2)\}$, and $\tilde{\kappa}''(\omega) \sim \omega^2$ at small ω . We calculated $\tilde{\kappa}_m(\omega)/\kappa_m$ for $\mathcal{P} = 10^{-4}$, 10^{-3} , 10^{-2} and 10^{-1} with the full CPA Eq. (6) and the nonaffine scaling function $h(\omega/\omega^*)$ for $\kappa = 1$. The crossover from nonaffine to affine behavior in the static limit is at $\mathcal{P} = 1/\pi^2 \approx 10^{-1}$, so all cases but $\mathcal{P} = 10^{-1}$ are at or near the nonaffine limit. $\kappa_m''(\omega)$ becomes greater than $\kappa_m'(\omega)$, and thus according to the Ioffe-Regel criterion [28], plane-wave phonon modes become heavily damped and ill defined at $\omega \approx \omega^*$ for all four values of \mathcal{P} .

The phonon density of states (DOS) $\rho(\omega)$, calculated from $\text{ImTr}\mathbf{G}^m(\mathbf{q}, \omega)$ in the usual way, is plotted in Fig. 4(a) as a function of ω/ω^* . Curves for the three lowest \mathcal{P} in Fig. 4(a) collapse on to a common curve for $\omega \leq 3\omega^*$. The curve for $\mathcal{P} = 10^{-1}$ departs from the common curve at $\omega \approx 0.5\omega^*$ and is plotted in the figure. The large value of $\kappa_m''(\omega^*)$ in the random system removes the strong van Hove singularity at ω^* of the uniform system. Figure 4(b) compares the DOS for a finite lattice calculated from CPA and by direct numerical diagonalization of the Hessian matrix using ARPACK [29]. The peaks in Fig. 4(b) at $\omega = q_x = (2\pi n/L)$ are due to finite size effects of the lattice with size L .

We have used the CPA to analyze the static and dynamic properties of a simple system on the threshold of isostaticity, namely, a square lattice with NN springs and randomly distributed NNN springs. This system provides clean analytic results about a random system near isostaticity, including nonaffine response near $\mathcal{P} = 0$, and the scaling form for $\tilde{\kappa}_m(\omega)$ (which to our knowledge has not been observed in jamming systems), that can serve as a comparison point for more complicated systems. Our results strongly suggest that the divergent length $l^* \sim 1/\omega^* \sim (\Delta z)^{-1}$ is a common feature of all nearly isostatic systems in agreement with the arguments of Ref. [3]. They also unambiguously demonstrate that elastic moduli are not universal but depend on the geometry of the isostatic lattice. Further study is needed to determine exactly what properties of the isostatic lattice lead, for example, to a finite bulk modulus and a shear modulus vanishing as Δz

(as in jamming) or $(\Delta z)^2$ (current system) or as $(\Delta z)^0$ (kagome lattice [30]) or to one in which both B and G vanish as Δz as in Ref. [31].

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