Theoretical limits for negative elastic moduli in subacoustic lattice materials

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An insightful mechanics-based bottom-up framework is developed for probing the frequency dependence of lattice material microstructures. Under a vibrating condition, effective elastic moduli of such microstructured materials can become negative for certain frequency values, leading to an unusual mechanical behavior with a multitude of potential applications. We have derived the fundamental theoretical limits for the minimum frequency, beyond which the negative effective moduli of the materials could be obtained. An efficient dynamic stiffness matrix based approach is developed to obtain the closed-form limits, which can exactly capture the subwavelength scale dynamics. The limits turn out to be a fundamental property of the lattice materials and depend on certain material and geometric parameters of the lattice in a unique manner. An explicit characterization of the theoretical limits of negative elastic moduli along with adequate physical insights would accelerate the process of its potential exploitation in various engineered materials and structural systems under dynamic regime across the length scales.

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I. INTRODUCTION

The global mechanical properties can be engineered in lattice materials by intelligently identifying the material microstructures as the properties in these materials are often defined by their structural configuration along with the intrinsic material properties of the constituent members. This novel class of materials with tailorable application-specific mechanical properties (like equivalent elastic moduli, buckling, vibration, and wave propagation characteristics with modulation features) have tremendous potential applications for future aerospace, civil, mechanical, electronics, and medical applications across the length scales. Naturally occurring materials cannot exhibit unprecedented and fascinating properties such as extremely lightweight, negative elastic moduli, negative mass density, pentamode material characteristics (metafluid), which can be achieved by an intelligent microstructural design [1,2]. For example, the conventional positive value of Poisson's ratio in a hexagonal lattice metamaterial can be converted to a negative value [3] by making the cell angle θ in Fig. 1(b) negative. Other unusual and exciting properties can be realized in metamaterials under dynamic condition, such as negative bulk modulus induced by monopolar resonance [4], negative mass density induced by dipolar resonance [5], and negative shear modulus induced by quadrupolar resonance [6]. Elastic cloaks [7] and various other unprecedented dynamic behavior of such materials have been widely reported in literature [8–14].

Lattice microstructures are often modeled as a continuous solid medium with a set of effective elastic moduli throughout the entire domain based on a unit cell approach [15–17]. The basic mechanics of deformation for the lattices being scale independent, the formulations developed in this context are generally applicable for a wide range of materials and structural forms. Two-dimensional hexagonal lattices of natural and artificial nature can be identified across different length scales (nano to macro) in auxetic and nonauxetic forms [18,19]. This has led to our focus on hexagonal lattices in this article while selecting a lattice configuration to demonstrate the concepts.

Honeycombs and other forms of lattice microstructures are often intended to be utilized in vibrating structures such as sandwich panels [20–22] used in aircraft structures [23]. Hexagonal latticelike structural form being a predominant material structure at nanoscale (such as graphene, hBN, etc. [24–27]), analysis of vibrating nanostructures are quite relevant to various applications at nanoscale. Besides that, recent developments in the field of metamaterials have prompted its use as advanced materials in aircraft and other machineries that experience vibration during operation. Dynamic homogenization of metamaterials have been reported in various recent papers [28,29]. For relatively low-frequency vibrations, the length of each unit cell will be significantly smaller than the wavelengths of the global vibration modes. As a result, each unit cell would effectively behave as a subwavelength scale resonator. Several exciting and unusual bulk properties of

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metamaterials have been reported exploiting subwavelength scale resonators [30]. These include negative stiffness [31], negative density (or mass) [32], or both [33], anisotropy in the effective mass or density [34,35], and nonreciprocal response [36,37].

Theoretically, lattice materials under the effect of dynamic forces can also show similar unusual behavior of negative elastic moduli due to the subwavelength scale resonator. However, this has not been widely reported primarily due to the difficulties in modeling complex lattice unit cells as subwavelength scale resonators. In principle, this is possible using very fine finite element discretizations of the individual beam elements in a unit cell. Such an approach will be purely numerical involving infeasible computationally intensive simulations. Besides that, a large-scale simulation based approach cannot provide an insightful physical framework for deriving the theoretical limits of the frequencies to obtain negative elastic moduli.

We aim to develop physically insightful theoretical limits of natural frequency to obtain negative axial and shear moduli in hexagonal lattice materials. We would exploit the tremendous implicit capabilities of the dynamic stiffness method [38] at high frequencies coupled with the concepts of structural mechanics to derive closed-form analytical limits, which are valid for steady-state dynamics under harmonic excitations. Though we concentrate on hexagonal lattices in this article, the basic concepts are general and it would be applicable to other two- and three-dimensional lattice geometries.

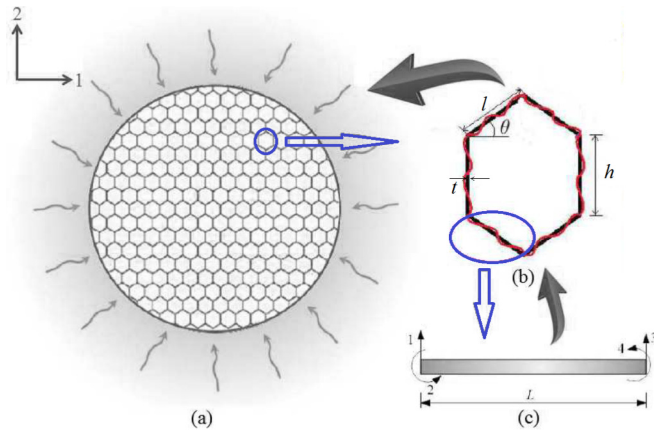


FIG. 1. Bottom-up approach (involving a hierarchy of analysis with beam element, unit cell, and lattice structure) for analyzing the frequency-dependent elastic moduli of lattice materials. (a) Typical representation of a hexagonal cellular structure in a dynamic environment (such as the honeycomb as part of a host structure experiencing wave propagation, vibrating structural component, etc.). The curved arrows are symbolically used to indicate propagation of wave. (b) One hexagonal unit cell under dynamic environment. (c) A dynamic beam element for the damped bending vibration with two nodes and four degrees of freedom.

II. NEGATIVE ELASTIC MODULI OF LATTICE MATERIALS AND THEIR THEORETICAL LIMITS

A bottom-up theoretical framework is developed here (refer to Fig. 1) to investigate the limits of natural frequency that would cause negative axial or shear moduli. A latticelike structure can be analyzed by considering a unit cell as shown in Fig. 1(b), while the unit cell consists of beam elements. In a vibrating condition, the dynamic motion of the overall lattice corresponds to vibration of individual beams, which would exhibit a different frequency-dependent deformation behavior compared to the conventional static analyses. Thus we first form the frequency-dependent elastic stiffness matrix for a beam element ($\mathbf{D}(\omega) = [D_{ij}]$, where $i, j \in [1, 2, \dots, 4]$ and ω is the frequency of vibration) and, thereby, the frequency-dependent deformation characteristics of a unit cell are developed. Here the dynamic stiffness matrix accounts for the compound effect of mass and stiffness matrices as $\mathbf{D}(\omega) = \mathbf{K}(\omega) - \omega^2\mathbf{M}(\omega)$, wherein the dynamic equilibrium $\mathbf{D}(\omega)\widehat{\mathbf{v}}(\omega) = \widehat{\mathbf{f}}(\omega)$ is satisfied (refer to Sec. 1.3 of the Supplemental Material [39] for further details). Eventually, frequency-dependent equivalent elastic moduli of the overall lattice structure are derived based on the deformation behavior of a unit cell. A multitude of critical analyses can be carried out based on the insightful closed-form expressions of frequency-dependent elastic moduli. The theoretical limits of frequencies to obtain negative elastic moduli are derived using their respective frequency-dependent expressions.

The frequency-dependent elastic stiffness matrix of a beam element is obtained based on an efficient dynamic stiffness method [40,41], which is a high fidelity approach at low to high frequencies compared to the conventional "static" finite element method. For characterizing the frequency-dependent elastic moduli, the conventional static finite element method could require very fine discretization for higher frequencies that may be practically impossible to achieve in a complex lattice metamaterial. The displacement field within the elements can be expressed by complex frequency dependent shape functions in dynamic stiffness method, leading to a radically significant computational efficiency at higher frequencies. The major advantages of this method and derivation of the frequency-dependent elastic moduli of the hexagonal lattices is provided as Supplemental Material [39]. Expressions of the frequency-dependent Young's moduli and shear modulus [42] can be obtained based on the concepts of structural mechanics using the elements of $[\mathbf{D}(\omega)]$ matrix as (refer to the Supplemental Material [39] for derivation)

$$E_1(\omega) = \frac{D_{33} l \cos\theta}{(h + l \sin\theta)\bar{b} \sin^2\theta}, \tag{1}$$

$$E_2(\omega) = \frac{D_{33}(h + l \sin\theta)}{l\bar{b} \cos^3\theta}, \tag{2}$$

$$G_{12}(\omega) = \frac{(h + l \sin\theta)}{2l\bar{b} \cos\theta} \frac{1}{\left(-\frac{h^2}{4lD^s_{43}} + \frac{2}{\left(D^v_{33} - \frac{(D^v_{34})^2}{D^v_{44}}\right)}\right)}. \tag{3}$$

For detailed description regarding the elements of dynamic stiffness matrix $[\mathbf{D}(\omega)]$ involved in the above expressions, refer to the Supplemental Material [39]. It can be noted in the above expressions that the elements of $[\mathbf{D}(\omega)]$ matrix are functions of the frequency-dependent parameter b, where

$b^4 = \frac{m\omega^2(1-i\zeta_m/\omega)}{EI(1+i\omega\zeta_k)}$. The quantities ζ_k and ζ_m are stiffness and mass proportional damping factors. Here E is the intrinsic Young's modulus of the lattice material, i.e., the Young's modulus of the material of the individual beam elements, while E_1 and E_2 are the equivalent Young's moduli of the entire lattice structure. The parameter m denotes mass per unit length and t is the thickness of the lattice wall. The quantities $h,\ l$, and θ are the length of cell walls and cell angle as shown in Fig. 1(b). Two in-plane Poisson's ratios are found to be independent of the frequency:

$$\nu_{12} = \frac{1}{\nu_{21}} = \frac{l\ \cos^2\theta}{(h + l\ \sin\theta)\sin\theta}. \tag{4}$$

The primary scope of this work is to extend the well-known Gibson and Ashby's formulas [15] for static elastic moduli of lattice structures to the dynamic domain. In most of the engineering applications, the elastic properties required in design are presented in terms of the two principle axes, such as $E_1,\ E_2,\ G_{12}$, etc. Thus we concentrated on these quantities in the current paper to find out the effect of vibration and deriving the expression for frequencies to cause the onset of negative elastic moduli.

It can be noted in this context that the expressions of E_1, E_2, and G_{12} for the undamped case converge to the closed-form solution provided in [15], when the frequency parameter (ω) tends to zero, while the expressions of the Poisson's ratios are exactly the same as that provided in [15]. The expressions of frequency dependent elastic moduli also conform the reciprocal theorem, i.e., $E_1(\omega)\nu_{21} = E_2(\omega)\nu_{12}$. Regular lattice material ($\theta = 30^\circ$) shows an isotropic behavior under dynamic condition

$$E_1 = E_2 = \frac{4}{\sqrt{3}}\frac{D_{33}}{\bar{b}}. \tag{5}$$

At the static limit ($\omega \to 0$), the isotropic behavior of a regular lattice material ($\theta = 30^\circ$) can be expressed as

$$E_1 = E_2 = \frac{4}{\sqrt{3}}E\left(\frac{t}{l}\right)^3. \tag{6}$$

The isotropic behavior of a regular lattice depends on two factors: the interaction between different elements of the $[D(\omega)]$ matrix (i.e., the dynamic stiffness matrix of a single beam element) and the geometry of a unit cell. It can be noted that the Young's moduli E_1 and E_2 of a hexagonal lattice depend on a single element D_{33} [refer to Eqs. (1) and (2)], except the geometric parameters. For a regular hexagonal lattice, the rest of the components in the expression of E_1 and E_2 (i.e., the geometric part) become the same for $h = l$ and $\theta = 30^\circ$. This causes the isotropy in a regular hexagonal system. For other kinds of regular lattices (e.g., triangular or square [43]), the isotropic behavior will depend on the above mentioned two factors, the crucial insights of which could be obtained following a similar framework as proposed in this paper.

The expressions of E_1 and E_2 are proportional to the complex frequency-dependent element D_{33} of the $[\mathbf{D}(\omega)]$ matrix. Therefore, we study its behavior in the undamped limit to understand if the real part of E_1 and E_2 can become negative. Assuming no damping in the system, the critical value of frequency beyond which the Young's moduli become negative can be obtained based on Taylor series expansion of D_{33} (refer to the Supplemental Material [39] for detailed derivation)

$$\omega^*_{E_1,E_2} \approx 5.598\frac{1}{l^2}\sqrt{\frac{EI}{m}}. \tag{7}$$

Here, $\omega^*_{E_1,E_2}$ represents the fundamental inflection frequency, where the Young's moduli change sign from positive to negative. For lightly damped systems, beyond this frequency value, the equivalent Young's moduli E_1 and E_2 will be negative for the first time when viewed on the frequency axis. As the frequency increases, the Young's moduli will become positive and negative again. The significance of the fundamental inflection frequency derived in Eq. (7) is that it is the *lowest* frequency value beyond which the effective Young's modulus can become negative. Physically, negative Young's modulus means that when a force is applied at the inflection frequency, the direction of the steady-state dynamic response will be in the opposite direction to the applied forcing at the same frequency.

Since the discovery of the Young's modulus over three centuries ago, it has been generally recognized as a positive quantity. This can be mathematically explained in the light of Eq. (7). Since $m \neq 0$, this implies that $\omega^*_{E_1,E_2} > 0$ for any lattice with finite-length beams. A static analysis normally used to obtain the classical Young's modulus can be viewed as a dynamic analysis with $\omega = 0$. Therefore, according to Eq. (7) it is not possible to observe a negative Young's modulus as $\omega^*_{E_1,E_2} > 0$. Only when a dynamic equilibrium is considered, our results show that for cellular metamaterials the Young's moduli can be negative, apparently contradicting notions established for centuries. It should be noted that a similar observation has been made in the context of acoustics metamaterials with subwavelength scale oscillators (see the review paper [30] for more discussions). The result derived through Eq. (7) is an explicit analysis towards establishing the existence of negative Young's modulus in the context of dynamics of elastic cellular metamaterials.

Unlike the case of Young's moduli, the frequency-dependent closed-form expression (3) for shear modulus shows a compound effect of multiple elements of the $[\mathbf{D}(\omega)]$ matrix. It is possible to obtain the expression of a tight bound for the frequency, beyond which the shear modulus becomes negative. Expanding the closed-form expression of G_{12} in a Taylor series, the following fundamental inequality regarding the frequency for negative value of G_{12} can be derived (refer to the Supplemental Material [39] for detailed derivation):

$$\frac{120}{\sqrt{160 + 75\,(h/l)^4}}\frac{1}{l^2}\sqrt{\frac{EI}{m}} \leqslant \omega^*_{G_{12}} \leqslant 30.2715\sqrt{\frac{1+2(h/l)}{8+9(h/l)^5}}\frac{1}{l^2}\sqrt{\frac{EI}{m}}. \tag{8}$$

Here, $\omega^*_{G_{12}}$ represents the fundamental inflection frequency for shear modulus, where the shear modulus changes sign.

Adequate physical insights can be drawn from the closed-form expressions for the elastic moduli in terms of explicit characterization of the parameters involved in the onset of negative Young's moduli or shear modulus. For example, if we notice Eq. (7), it is clear that $\omega^*_{E_1,E_2}$ is inversely proportional to the parameters l and m, while proportional to the flexural rigidity EI. Further, based on the power(/exponent) of the parameters, it can be realized that the sensitivity of l (with a power of 2) is much higher than the other two parameters m and EI (with a power of 0.5). Unlike the equivalent expression for the Young's moduli E_1 and E_2 in Eq. (7), the minimum frequency above which G_{12} becomes negative depends on the h/l ratio in addition to the other parameters (i.e., l, EI, and m). Similar conclusions as the Young's moduli can be readily derived in the case of the shear modulus on the dependence of the onset of negative shear modulus on different system parameters.

III. RESULTS AND DISCUSSION

Numerical results based on the derived expressions of analytical limits of negative elastic moduli are presented in the following paragraphs. However, before discussing the results concerning negative axial and shear moduli, the dynamic stiffness based framework needs to be validated first. We have presented representative results for validation of the analytical expression for frequency dependent Young's modulus in the Supplemental Material [39]. Unless otherwise mentioned, numerical results are presented for a structural configuration of $\theta = 30^\circ$ and $h/l = 1$, with $\zeta_k = 0.002$ and $\zeta_m = 0.05$. The geometric parameters of the honeycomb and intrinsic material properties are assumed as $l = 3.67$ mm, $h = l$, $E = 69.5 \times 10^3$ N/mm^2, $d = 0.8$ mm, $t = 0.0635$ mm, and $m = 0.137$ kg/mm.

The Young's moduli E_1 and E_2 are functions of only the frequency dependent coefficient D_{33} [refer to Eqs. (1) and (2)]. When E_1 and E_2 are normalized with respect to their equivalent static values, they both essentially become the same mathematical function

$$\frac{E_1}{E_{1_s}} = \frac{E_2}{E_{2_s}} = \frac{D_{33}}{12EI/l^3}. \tag{9}$$

For any positive values of the damping coefficients, D_{33} becomes complex. This in turn makes the Young's moduli E_1 and E_2 complex quantities. The real and imaginary parts and also the amplitude of the normalized value of E_1 and E_2 [see Eq. (9)] are shown in Fig. 2. It can be observed that the real part of E_1 and E_2 becomes negative and then changes to positive again with the change of frequency. This confirms that the value of the elastic moduli E_1 and E_2 (and subsequently the axial stiffness in the two directions) will be negative at certain frequencies. In Fig. 2, the frequency axis is zoomed to observe the first frequency point when D_{33} becomes negative. This frequency point is predicted by Eq. (7) as $\omega = 1.2231$. This matches exactly with what is observed (marked by "+") in Fig. 2 confirming the validity of Eq. (7). The frequency at which the Young's moduli E_1 and E_2 of a hexagonal lattice becomes negative is a fundamental property of the lattice and it depends only on the length of the inclined beams (l), the bending rigidity (EI), and mass density per unit length (m). The imaginary parts of E_1 and E_2 remain positive at all frequencies for any positive value of damping.

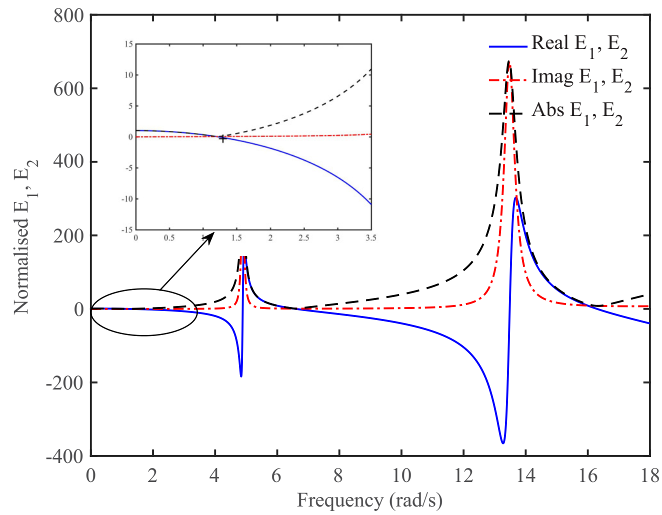
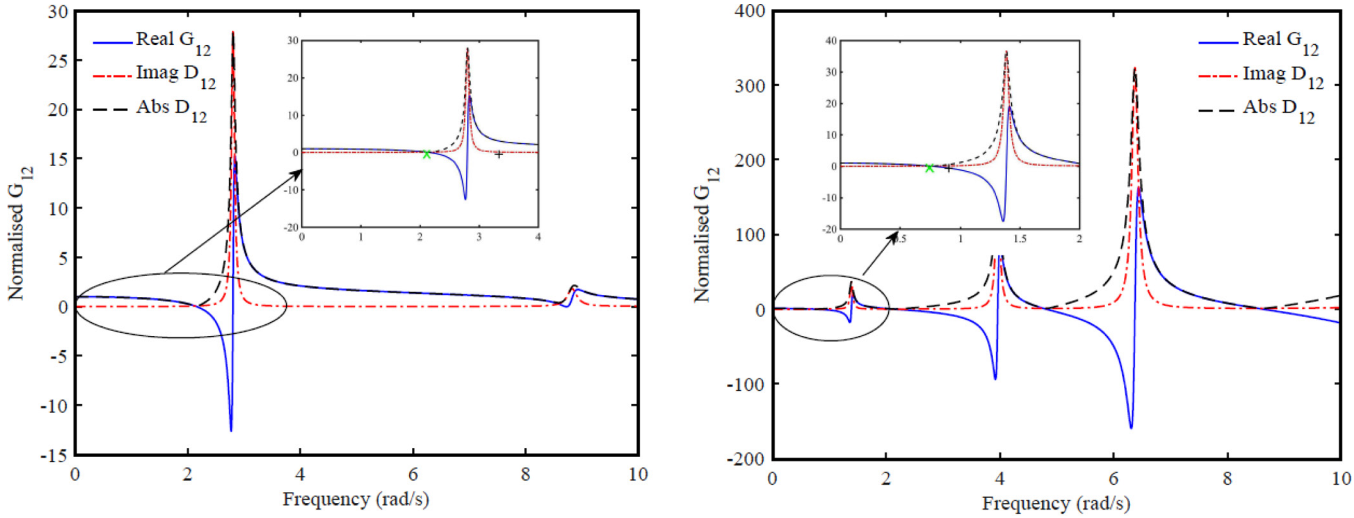


FIG. 2. Real and imaginary parts and the amplitude of the normalized value of E_1 and E_2 as a function of frequency. Here the first frequency value when the Young's moduli become negative is marked by "+".

The normalized shear modulus is presented in Fig. 3 for two different values of h/l ratios. The real and imaginary parts along with the absolute values are shown in the figure. The upper and lower bounds of the values of $\omega^*_{G_{12}}$, the frequency at which G_{12} becomes negative, are shown by "×" and "+" in the figure. It is found that the actual value of $\omega^*_{G_{12}}$ lies within the bounds given by Eq. (8). The value of $\omega^*_{G_{12}}$ reduces with the increase in h/l ratio, which is also evident from the derived inequality. It can be noted here that the real part becomes negative for all the three elastic moduli beyond the fundamental inflection frequency. Amplitude is always a positive quantity by definition. The imaginary part cannot be negative for a positive value of damping in a stable dynamic system.

IV. SUMMARY AND PERSPECTIVE

We have developed a robust analytical framework to explain the negative elastic moduli (the real parts of E_1, E_2, and G_{12}) of lattice materials under vibrating condition. In the steady-state dynamic environment, a metamaterial could subsequently be developed with both negative elastic moduli and negative Poisson's ratio when the cell angle becomes negative [refer to Fig. 1(b)]. Similar observation of negative stiffness was made for acoustic metamaterials [31] and through destabilizations of (meta)stable equilibria of the constituents [44,45]. Here we demonstrate such a possibility for lattice materials in the subacoustic range. Theoretical limits of frequencies are reported for the first time to achieve such negative axial and shear moduli. The main approach to establish the negative effective elastic moduli hinges upon exploitation of the dynamic stiffness matrix. In contrast to the conventional static analysis, the dynamic stiffness approach accurately models the subwavelength scale dynamics of the unit cells.



(a) G_{12} ($h/l = 0.5$, $2.0430 < \omega^*_{G_{12}} < 3.2502$) (b) G_{12} ($h/l = 2.0$, $0.71090 < \omega^*_{G_{12}} < 0.8596$)

FIG. 3. Real and imaginary parts and the amplitude of the normalized value of G_{12} as a function of frequency for two different values of h/l. Bounds of $\omega^*_{G_{12}}$, the frequency at which the G_{12} becomes negative, are calculated from Eq. (8). Here the upper and lower bounds of frequency where G_{12} becomes negative for the first time are shown by "×" and "+", respectively.

Assuming the undamped limit, an explicit closed-form expression of the minimum frequency value, referred to as fundamental inflection frequency [refer to Eq. (7)] beyond which the effective elastic moduli E_1 and E_2 become negative, has been obtained. This is achieved using a Taylor series expansion of a relevant dynamic stiffness coefficient. For the shear modulus, a closed-form solution for the frequency (fundamental inflection frequency) when it becomes negative was not found. However, a tight bound has been derived [refer to Eq. (8)]. The frequencies $\omega^*_{E_1,E_2}$ and $\omega^*_{G_{12}}$ are fundamental properties of a lattice metamaterial and they depend only on the length of the inclined and vertical beams, the bending rigidity, and the mass density per unit length. The imaginary part of the elastic moduli remain positive for all frequency values, indicating that the material would result in dynamically stable responses. The expressions of $\omega^*_{E_1,E_2}$ and $\omega^*_{G_{12}}$ clearly show the relative mass (m) and stiffness (EI) contributions on the critical frequencies. A higher value of the stiffness contribution increases the critical frequencies and vice versa, while the mass contribution has an opposite effect. The values of the fundamental inflection frequencies are proportional to the square root of the ratio ($\frac{EI}{m}$). In addition to this ratio, $\omega^*_{E_1,E_2}$ depends only on l, while $\omega^*_{G_{12}}$ depends on both l and h/l ratio. The expressions reveal another interesting fact in terms of static limits. In the static limit, the contribution of mass (effect of inertia) tends to zero. This leads to the value of $\omega^*_{E_1,E_2}$ and $\omega^*_{G_{12}}$ as infinity. In other words, there cannot be a negative value of the Young's modulus and the shear modulus in the static case. Thus, besides characterizing the negative elastic moduli, our analysis gives a new and alternative explanation of the classical positive elastic moduli of lattice metamaterials. Although we have focused here on hexagonal two-dimensional lattices to present numerical results, the disseminated concepts can be extended to other forms of lattices and metamaterials in two and three dimensions, the complexity of which will depend on the nature of microstructure.

Realization of negative elastic moduli in metamaterials is not new, as discussed in the Introduction section. However, the contribution of this paper is to develop the fundamental limits for the minimum frequency, beyond which the negative elastic moduli (Young's modulus and shear modulus) can be realized. These are derived in closed form for the first time. The limits turn out to be intrinsic properties of the lattice material and certain geometric parameters. Exact characterization of the influencing intrinsic mechanical properties at the onset of negative elastic properties is an important aspect for mechanical metamaterials. These closed-form limits will have tremendous impact in efficient development of future microstructured materials within a dynamic paradigm exploiting the accurate onset of negative elastic moduli.

In summary, this article sheds light on the negative axial and shear moduli of lattice materials under subacoustic conditions based on a physics-based insightful framework. Theoretical limits of the minimum frequency beyond which the elastic moduli change sign, referred to as the fundamental inflection frequencies, have been derived in closed form. These frequency values are intrinsic properties of the lattice and are unique to a given geometrical pattern and material properties. These expressions and the disseminated generic concepts can be used to pinpoint the onset of negative elastic moduli and help to design and develop the next generation of lattice materials in different length scales.

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