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1 Phonon transmission through a nonlocal metamaterial slab

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12

13 Abstract:

14 Previous theory and experiment has shown that introducing strong (nonlocal) beyond-nearest-neighbor interactions in addition to (local) nearest-neighbor interactions into rationally designed periodic lattices 15 called metamaterials can lead to unusual wave dispersion relations of the lowest band. For roton-like 16 17 dispersions, this especially includes the possibility of multiple solutions for the wavenumber at a given frequency. Here, we study the one-dimensional frequency-dependent acoustical phonon transmission of 18 19 a slab of such nonlocal metamaterial in a local surrounding. In addition to the usual Fabry-Perot 20 resonances, we find a series of bound states in the continuum. In their vicinity, sharp Fano-type 21 transmission resonances occur, with sharp zero-transmission minima next to sharp transmission maxima. 22 Our theoretical discussion starts with a discrete mass-and-spring model. We compare these results with 23 solutions of a generalized wave equation for heterogeneous nonlocal effective media. We validate our 24 findings by numerical calculations on three-dimensional metamaterial microstructures for one-25 dimensional acoustical wave propagation.

27 Introduction

28 The wave properties of ordinary crystals are determined by the atoms forming the crystal as well as by their interactions. Likewise, the wave properties of rationally designed artificial periodic lattices called 29 30 metamaterials¹⁻³ are determined by the interior of the metamaterial unit cells as well as by the interactions among the unit cells⁴⁻⁶. A bulk of literature has used the approximation of considering 31 interactions among only the nearest neighbors⁷⁻⁹. Interactions beyond the nearest neighbors have been 32 considered to test the validity of this approximation¹⁰. However, in metamaterials, the interactions 33 beyond the nearest neighbors can be designed rationally and can be made strong¹⁰⁻¹⁴. This additional 34 design freedom has lately been used to realize unusual dispersion relations of the lowest acoustic or 35 elastic metamaterial band¹⁵⁻¹⁸. For example, the latter can resemble the unusual dispersion relation, 36 $\omega(k)$, of sound waves in superfluid helium^{19, 20} that starts with an angular frequency of the wave, ω , 37 38 proportional to its wavenumber, k, followed by a maximum (the "maxon") and a minimum (the "roton") versus $k^{21, 22}$. Such unusual phonon dispersion relations have been observed experimentally using three-39 dimensional macroscopic metamaterials for airborne sound at audible frequencies^{17, 18} and using three-40 dimensional microstructured metamaterials for elastic waves at ultrasound frequencies¹⁷. 41

42 However, structures and devices in applications usually exploit multiple dissimilar materials and the 43 interplay between them and their interfaces. A paradigmatic textbook heterostructure geometry is a slab 44 with thickness L of material A clad between two semi-infinite half spaces of material B. For usual local 45 materials A and B, it is well-known that this setting leads to Fabry-Perot resonances connected to unity wave transmission, $|T(\omega)| = 1$, through the slab at particular angular frequencies $\omega = \omega_i$ of the incident 46 47 wave²³. At these particular frequencies, the phase that the wave accumulates in one round trip through the slab is an integer multiple of 2π . For a slab with a sufficiently large number of unit cells within, this 48 49 condition translates into $2kL = n_i 2\pi$, where $k = k(\omega_i)$ is the single wavenumber in material A at the 50 angular frequency ω_i and n_i is an integer. Fabry-Perot resonances with high quality factors have numerous applications, e.g., as optical filters or interferometry²⁴. 51

Here, we discuss the case that material A in the slab is replaced by a nonlocal metamaterial. At a given angular frequency ω , such medium generally supports more than a single wave mode with single wavenumber k. For different wavenumbers $k_j(\omega)$, with j = 1, 2, ... N, at a given angular frequency ω , the behavior is richer than for local material slabs. We start by discussing the problem using a previously introduced simple discrete one-dimensional (1D) mass-and-spring model¹⁵. Apart from the nearestneighbor interactions via Hooke's springs, it contains N-th nearest-neighbor interactions with integer $N \ge$ 58 2. Here, we emphasize the example of N = 3, which is the smallest N for which the roton-like minimum fully lies inside of the first Brillouin zone (for N = 2 it lies right at the Brillouin zone border). We find a 59 60 series of sharp Fano-type resonances in the frequency-dependent transmission $|T(\omega)|$ in the frequency region for which multiple solutions $k_i(\omega)$ for the wavenumber exist. We show that the linewidth of the 61 Fano-type resonances tends to zero towards special points in material-parameter space corresponding to 62 bound states in the continuum (BIC)²⁵. BIC physics in general, not related to beyond-nearest-neighbor 63 interactions in periodic lattices, has a long history in acoustics²⁶, elasticity^{27, 28}, as well as optics^{29, 30}, and 64 has recently attracted renewed attention in the metamaterials community³¹. We refer the reader to the 65 review articles^{25, 29} for an introduction to and comprehensive reviews of the BIC field. Next, we discuss the 66 67 nonlocal slab transmission on the level of a 1D effective-medium approximation for the displacement field 68 of the heterogeneous 1D mass-and-spring model, which leads to a phenomenological generalized wave 69 equation containing spatial derivatives up to order 2N. Finally, we present numerical calculations for three-dimensional nonlocal metamaterial microstructures for wave propagation along one direction, 70 71 again showing BIC behavior.

72

73 Results and Discussion

74 Mass-and-spring model. Figure 1(a) illustrates the infinite one-dimensional mass-and-spring toy model that we have discussed previously¹⁵. Herein, identical masses m, periodically arranged with period or 75 lattice constant a, are connected to their immediate neighbors along the x-axis on the left and on the 76 77 right by linear elastic Hooke' springs with spring constant K_1 . In this form (i.e., for $K_N = 0$), Fig. 1(a) 78 corresponds to the paradigmatic one-dimensional model for acoustical phonons in usual local media as 79 described in any solid-state-physics textbook³². For the nonlocal case, the masses in Fig. 1(a) are 80 additionally connected to their *N*-th nearest neighbor on the left and on the right by Hooke's springs with spring constant K_N . Shown is the example of N = 3. This is the lowest integer for which roton-like 81 dispersion relations¹⁵ can occur within the first Brillouin zone of the model. For N = 2, the roton-like 82 minimum is right at the boundary of the first Brillouin zone. Clearly, the model can be extended to contain 83 84 multiple orders of beyond-nearest-neighbor interactions³³. Here, for simplicity, we only consider nearest 85 neighbors plus neighbors with N = 3. We will see that the resulting behavior of slabs is extremely rich 86 and complex already. The beyond-nearest-neighbor springs in Fig. 1 are meant symbolically, an actual 87 feasible realization is discussed in Section V.

88 As an example for N = 3, Fig. 1(b) shows a slab of relative thickness L/a = 6 of such nonlocal material 89 clad between a local mass-and-spring model. The thinnest possible slab corresponds to L/a = N, for 90 which only a single *N*-th nearest-neighbor spring is left. For simplicity and clarity, we depict and study in what follows the case that the lattice constant a, the masses m, and the spring constants K_1 are constant 91 throughout the entire structure considered. We notice that, for a given well-defined integer ratio L/a, 92 93 the left and right boundaries of the nonlocal slab in Fig. 1(b) cannot be defined unambiguously anymore. 94 Six of the seven masses in the slab have only third-nearest-neighbor springs to one side. Further inside of 95 the nonlocal slab (in Fig. 1(b) only the middle mass), the masses have long-range interactions to their left 96 and to their right-hand side. For the phenomenological effective-medium description to be discussed 97 below, this obvious fact means that the boundaries between the local and the nonlocal medium cannot 98 be considered as being sharp or discontinuous anymore. The boundaries are rather smeared out, which 99 is a direct consequence of the nonlocality of the slab. This simple observation will become important for 100 an intuitive interpretation of our results and for the effective-medium description described below.

Before discussing the nonlocal slab, let us briefly recapitulate the expected transmission, $T(\omega)$, of a slab of a local material embedded in a different local material, at the real-valued angular frequency ω . We define the complex-valued transmission as the ratio of the transmitted displacement amplitude or output, u_{out} , and the displacement amplitude incident onto the slab, u_{in} , i.e.,

105 $T(\omega) = \frac{u_{\text{out}}}{u_{\text{in}}}.$ (1)

106 The phase of $T(\omega)$ clearly depends on at which lattice site exactly we take the incident and the 107 transmitted displacement, respectively. This dependence drops out when considering the modulus, 108 i.e., $|T(\omega)|$. Therefore, we consider $|T(\omega)|$ in what follows. As pointed out in the introduction, for a local 109 slab in a local surrounding, $|T(\omega)|$ generally exhibits Fabry-Perot resonances with $|T(\omega_i)| = 1$ at 110 particular angular frequencies ω_i which fulfill the standing-wave condition²³

111 $k(\omega_i)L = n_i \pi,$ (2)

with integer n_i . Clearly, this reasoning implies that the slab contains sufficiently many unit cells, such that the wavenumber k can assume nearly any value. For these particular angular frequencies, the wave accumulates a phase in one round trip within the slab that is an integer multiple of 2π . For the special case that the impedances between the two materials are matched, we have $|T(\omega)| = 1$ for all angular frequencies. 117 Let us apply this intuitive reasoning to a nonlocal slab with sufficiently many unit cells inside. As we have shown previously¹⁵ and as can be seen from roton-like dispersion relation shown in Fig. 2(a), one generally 118 has three solutions (for N = 3) for each direction (left/right or +k/-k) for the (real part of the) 119 wavenumber at a given angular frequency, i.e., $k(\omega_i) \rightarrow k_i(\omega_i)$ and $n_i \rightarrow n_{ij}$ with j = 1,2,3. Intuitively, 120 a standing-wave condition Eq. (2) has to be fulfilled for each one of them simultaneously to obtain a 121 "special" behavior of $|T(\omega)|$ at certain angular frequencies ω_i . Below, we will connect this "special" 122 behavior to bound states in the continuum (BIC). For arbitrary parameter choices of m, K_1 , K_3 , and a, and 123 hence arbitrary dispersion relations $\omega(k)$, it is unlikely that the condition Eq. (2) can be fulfilled three 124 125 times simultaneously for any one angular frequency ω_i . However, as pointed out above (see Fig. 1(b)), 126 the boundaries of the nonlocal slab are not sharp (see above discussion on Fig. 1(a)), and, hence, the effective slab thickness, L_i^{eff} , may be different from L in Eq. (2), i.e., we have to replace $L \to L_i^{\text{eff}}$ in Eq. (2). 127 Together, we obtain 128

$$k_i(\omega_i)L_i^{\rm eff} = n_{ij}\pi \,. \tag{3}$$

130 Unfortunately, there is no obvious and unambiguous way to calculate the effective slab thicknesses L_j^{eff} 131 and thereby the special frequencies ω_i from Eq. (3) and the given dispersion relation $k(\omega)$. Nevertheless, 132 this simple reasoning connects the textbook treatment of Fabry-Perot resonances for ordinary local slabs 133 to the more unusual resonances in nonlocal slabs discussed in this paper.

Before we discuss the problem more rigorously, especially including the possibility of only a small number of unit cells within the slab, let us address a subtlety of the dispersion relation connected to the finitethickness slab that turns out to be important for an intuitive interpretation of our results. For the infinitely extended periodic nonlocal mass-and-spring model (see Fig. 1(a)), Newton's law for the displacement u_l of the mass m at site l along the x-axis reads

139
$$m\frac{\partial^2 u_l}{\partial t^2} = K_1(u_{l+1} - 2u_l + u_{l-1}) + K_N(u_{l+N} - 2u_l + u_{l-N}), l = -\infty, ..., 0, ... + \infty.$$
(4)

140 Without further assumptions or approximations, the plane-wave ansatz $u_l = \tilde{u} \exp(i(kx - \omega t))$, with 141 x = la and constant prefactor \tilde{u} , leads to the phonon dispersion relation $\omega(k)$ given by¹⁵

142
$$\omega^2(k) = \frac{4}{m} \left(K_1 \sin^2 \left(\frac{ka}{2} \right) + K_N \sin^2 \left(\frac{Nka}{2} \right) \right).$$
(5)

143 Clearly, when taking the square root on both sides of Eq. (5), we obtain two signs for ω . As usual, we 144 follow the convention to consider positive (real parts of the) angular frequencies. For an infinite non-145 dissipative nonlocal medium, according to Bloch's theorem³², the wavenumber must be real. However, 146 for a finite-thickness nonlocal slab, the wavenumber is not necessarily real because evanescent modes 147 may appear. For the considered transmission *Gedankenexperiment*, the angular frequency is purely real (by definition) and positive by convention. Nevertheless, we plot in Fig. 2 all mathematical solutions of Eq. 148 (5) for the most general case of complex-valued k and complex-valued ω . Panel (a) is for a parameter set 149 (see caption) for which $Re(\omega)$ versus Re(k) shows a roton-like dispersion relation with a pronounced 150 151 maximum and a pronounced minimum. Panel (b) is for a parameter set (see caption) for which $\text{Re}(\omega)$ versus $\operatorname{Re}(k)$ shows no roton minimum in the phonon dispersion relation. Nevertheless, in Fig. 2(b), we 152 153 still obtain three solutions (three modes) for the complex-valued wavenumber k for real and positive ω 154 in the range of Re(k) > 0. We repeat that $\text{Im}(k) \neq 0$ indicates evanescent modes that drop out for an 155 infinite medium, but that we have to consider for a finite-thickness nonlocal slab. For a local medium with $K_N = 0$, be it finite or infinite in thickness, this subtlety does not apply because Im(k) = 0 holds 156 true for any real-valued $\omega > 0$. 157

158 We note in passing that the behavior shown in Fig. 2 can be understood in terms of the roton minimum being an exceptional point³⁴⁻³⁶. In fact, any k-position of a minimum or maximum of $\omega(k)$ in the first 159 160 Brillouin zone of any type of wave in any kind of lossless system is an exceptional point in the sense that two eigenmodes coalesce in both eigenvalues and eigenvectors for the angular eigenfrequency ω at the 161 k-position of the maximum or minimum. At the position of a saddle point (see Fig. 2(b)), even three 162 eigenmodes coalesce. This exceptional degeneracy is lifted as soon as one introduces a perturbation. It is 163 164 also lifted as soon as one considers finite imaginary parts of k (i.e., evanescent waves). As a result, one 165 black line emerges from the roton minimum for increasing imaginary part of the wavenumber in Fig. 2(a). In Fig. 2(b), two black lines emerge from the saddle point for Im(k) > 0. 166

167 Next, we discuss solutions for $|T(\omega)|$ of the nonlocal slab. As our model contains no losses, the sum of 168 kinetic and potential energy is conserved, and the reflectivity spectrum, $|R(\omega)|$, is directly connected to 169 the transmission spectrum by the relation

170

$$|R(\omega)|^2 + |T(\omega)|^2 = 1.$$
 (6)

This expression is only meaningful and valid for a local surrounding that supports only a single relevant mode (in either direction). This condition is automatically fulfilled for the discrete mass-and-spring model (cf. Fig. 1), but has to be taken with caution for the below approximate effective-medium description in which a very small but finite nonlocality needs to be added to the surrounding of the slab. We will come back to this point below. To mathematically compute the transmission spectrum for the discrete model (see Fig. 1(b)), we proceed as follows. An incident wave with angular frequency ω impinges onto the slab from the left-hand side. We aim at computing the frequency-dependent reflection and transmission coefficients. We write the displacements corresponding to masses with label $l \leq 0$ (see Fig. 1(b)) as

180
$$u_l = u_{\rm in} \exp(ikla) + u_{\rm ref} \exp(-ikla), \tag{7}$$

181 where u_{in} indicates the complex-valued amplitude of the incident wave, k is the wavenumber, and u_{ref} 182 represents the unknown amplitude of the reflected wave, respectively. To ease readability, the time 183 harmonic factor exp $(-i\omega t)$ is omitted here and throughout the following. It can be shown that the 184 displacements of the masses with label $l \leq -1$ satisfy their balance equations automatically. Likewise, 185 we represent the displacements of the masses with label $l \geq L/a$ by,

186
$$u_l = u_{\text{out}} \exp(ik(l - L/a)a), l \ge L/a$$
(8)

Here, u_{out} indicates the unknown amplitude of the transmitted wave. In total, we have L/a + 1unknowns, including u_{ref} , u_{out} , and the displacements, u_l , with $l = 1, 2 \dots (L/a - 1)$. These unknowns are obtained from L/a + 1 equilibrium equations for the masses with labels $l = 0, 2 \dots L/a$. As defined above, the transmission coefficient is obtained via $T(\omega) = u_{out}/u_{in}$.

191 For example, for
$$L/a = 4$$
, we obtain the transmission spectrum

192
$$T(\omega) = \frac{2i\sin(ka)K_1^2(K_1(K_1+K_3)(K_1+5K_3)-2K_3(4K_1+K_3)m\omega^2+2K_3m^2\omega^4)}{F_1(\omega)F_2(\omega)}.$$
 (9)

193 Herein,

194
$$F_1(\omega) = \exp(ika) K_1(2K_1 + K_3 - m\omega^2) - (3K_1 - m\omega^2)(K_1 + 2K_3 - m\omega^2), \tag{10}$$

195 and

196
$$F_{2}(\omega) = 2(\exp(ika) - 1)K_{1}^{3} + m^{2}\omega^{4}(M\omega^{2} - 2K_{3}) + (\exp(ika) - 6)K_{1}m\omega^{2}(M\omega^{2} - K_{3}) + K_{1}^{2}(9m\omega^{2} - 2K_{3} + 2\exp(ika)(K_{3} - 2m\omega^{2})).$$
(11)

198 The corresponding explicit expressions become very lengthy for slab length $L/a \ge 5$, and are hence not 199 provided here.

Fig. 3(a) depicts an example of the calculated transmission $|T(\omega)|$ (gray scale) of the nonlocal slab (see Fig. 1(b)) versus ω and versus the spring-constant ratio K_3/K_1 . For simplicity, all other model parameters are fixed (see caption). For reference, panel (b) shows the phonon dispersion relation for the slab for selected values of K_3/K_1 (see dashed lines). We find a complex behavior. In Fig. 3(a), for low frequencies, transmission peaks occur that follow the expectation for ordinary Fabry-Perot resonances (labelled "FP" in Fig. 3). At higher frequencies, near specific special frequencies (see arrows in Fig. 3(a)), the resonances in transmission become more and more narrow. Exactly at these special frequencies and spring constant ratio K_3/K_1 , the resonances disappear. We interpret these special frequencies as being due to bound states in the continuum (BIC).

209 To test this interpretation, we have performed additional numerical calculations of the eigenfrequencies 210 and eigenmodes of the slab alone, i.e., without the surrounding (not shown). We find eigenfrequencies, 211 $\omega_{\rm BIC}$, for which the corresponding eigenmodes exhibit strictly zero displacement amplitude at the left and right end of the slab for all times t. Obviously, an incident plane wave with non-zero amplitude impinging 212 213 from the surrounding cannot couple to such an eigenmode. Correspondingly, the lifetime of this mode is 214 infinitely long – provided that friction plays no role, as implied in our model, see Fig. 1 or Eq. (4). This 215 means that the special frequencies of BIC resonances only depend on the slab properties, but not on the 216 properties of the surrounding. The same holds true for usual Fabry-Perot resonances.

To connect to our above intuitive discussion for sufficiently many unit cells within the slab, we can decompose the BIC modes of the slab corresponding to the BIC angular frequencies ω_i into the three (j =1, 2, 3) eigenmodes with wavenumbers $k_j(\omega_i)$ of the nonlocal dispersion relation according to Eq. (5) to fulfill the three standing-wave conditions Eq. (3) simultaneously. However, the reverse is not true. Just any arbitrary linear combination of the three standing-wave solutions fulfilling Eq. (3) will generally not lead to a BIC mode as the displacement of the masses at the two ends of the slab is not necessarily strictly zero.

224 For special (small) integer values of the relative slab thickness L/a, the BIC resonance frequencies ω_{BIC} 225 can be obtained analytically. We consider those (1 + L/a) eigenfrequencies of the (1 + L/a) coupled 226 masses in the slab in Fig. 1(b) for which the corresponding eigenmode is such that the mass on the left-227 hand side and the right-hand side of the slab have strictly zero displacement amplitude at all times t (but 228 the masses in between have nonzero amplitude). Such solutions occur only for special combinations of the three slab parameters m, K_1 , and K_N . For any N and $K_N = 0$, BIC solutions do not occur for any value 229 of L/a. For $K_N \neq 0$, N = 3 and L/a = 3 (i.e., only a single third-nearest-neighbor spring), a BIC does not 230 231 occur either. The simplest non-trivial case is N = 3 and L/a = 4, for which we have only two third-232 nearest-neighbor springs in the slab. It is straightforward to obtain the eigenstates for this system 233 composed of five coupled masses. By demanding that the displacements of the two masses on the left 234 end and on the right end of this chain are zero for all times (see Supplementary Note 1), we obtain

$$(K_3/K_1)_{\rm BIC} = 1; \ \omega_{\rm BIC} = \sqrt{\frac{3K_3}{m}}.$$
 (12)

For large relative slab thicknesses L/a we find BIC modes numerically as it seems hard to obtain closed analytical solutions.

238 For frequencies and parameters near but not identical to these BIC conditions, an incident propagating 239 plane wave can couple to the resonance mode localized within the slab. The interference of a continuum 240 of propagating modes and a spectrally-sharp localized mode is well known to give rise to Fano-type line shapes³⁷, the detailed form of which depends on the Fano coupling parameter. In Fig. 4(a), we show a 241 242 zoomed-in view of one BIC point highlighted by the yellow box in Fig. 3(a). For K_3/K_1 values below the 243 BIC points and with increasing angular frequency ω , we find a transmission dip (zero transmission) followed by a transmission peak (complete transmission), whereas for K_3/K_1 ratios above the BIC 244 245 frequency, the sequence flips and we find a transmission peak followed by a transmission dip with increasing frequency. This behavior is more clearly seen from the selected cuts shown in Fig. 4(b) 246 corresponding to three different K_3/K_1 values. 247

Further examples for other L/a, represented likewise in Fig. 3(a), are shown in Supplementary Figure 1. We find BIC modes even if only two third-nearest neighbor Hooke's springs are kept (L/a = 4 and N = 3, see Eq. (6)). In the opposite limit of a thick slab, $L/a \gg 1$ (see Fig. 1(b)), in which we expect that we can consider the slab as an effective medium, the BIC resonances survive as well. This brings us to a possible effective-medium description.

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235

Effective-medium description. For an infinitely periodic nonlocal mass-and spring model and for N = 3, we have previously argued¹⁷ that one gets the following general form for the displacement field u = u(x, t) within the long-wavelength limit ($ka \rightarrow 0$)

257
$$m\frac{\partial^2 u}{\partial t^2} = A_2\frac{\partial^2 u}{\partial x^2} + A_4\frac{\partial^4 u}{\partial x^4} + A_6\frac{\partial^6 u}{\partial x^6}.$$
 (13)

In a previous study¹⁷, we have derived explicit expressions for the parameters A_2 , A_4 , and A_6 . However, it should be noted that one gets different explicit expressions for A_2 , A_4 , and A_6 depending on which terms of the expansion one keeps. For example, even for the nearest-neighbor interactions alone (i.e., for $K_1 \neq 0$ and $K_3 = 0$) one can obtain finite terms for all three coefficients A_2 , A_4 , and A_6 in Eq. (13). Unless $K_1 \ll K_3$ (which does not hold true for the parameters considered in this paper), these terms are not negligible compared to the ones originating from the third-nearest-neighbor interactions. Therefore, we have assumed a phenomenological spirit and have considered the parameters A_2 , A_4 , and A_6 in the general form Eq. (13) as fit parameters when plotting the phonon dispersion relations as gray curves in Fig. 4B and 4D in Martínez et al.¹⁷. Further examples are given in Wang et al.¹⁶.

If one wants to go beyond this phenomenological treatment, one would have to expand the finite differences on the right-hand side of Eq. (4) to yet much-higher orders of spatial derivatives than in Eq. (13) in order to quantitatively reproduce the results of the discrete mass-and-spring model. However, in this case, nothing is gained because the point of a meaningful effective-medium description is that it should be simpler than the underlying discrete model (or microstructure or atomic structure). Otherwise, one could rather continue working with the more complete discrete model.

We assume the same phenomenological spirit here. However, importantly, for the slab geometry of interest in this paper, the coefficients A_2 , A_4 , and A_6 are no longer constant versus the *x*-coordinate (see Fig. 1(b)). For this case of a heterogeneous nonlocal medium, it is straightforward to derive, starting from Eq. (4), the more general form

277
$$m\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(A_2(x)\frac{\partial u}{\partial x} \right) + \frac{\partial^2}{\partial x^2} \left(A_4(x)\frac{\partial^2 u}{\partial x^2} \right) + \frac{\partial^3}{\partial x^3} \left(A_6(x)\frac{\partial^3 u}{\partial x^3} \right), \tag{14}$$

in the limit of $a \to 0$. The coefficients $A_2(x)$, $A_4(x)$, and $A_6(x)$ can be expressed by the model 278 parameters $K_1(x)$, $K_N(x)$ and spatial derivatives up to third order thereof (see Supplementary Materials 279 of Martínez et al.¹⁷ for the case of constant coefficients). However, again, the expressions for $A_2(x)$, 280 $A_4(x)$, and $A_6(x)$ depend on which terms of the expansion one keeps. If one considers the 281 282 mathematically strict limit of $a \rightarrow 0$, one gets discontinuous steps of the coefficients $A_2(x)$, $A_4(x)$, and $A_6(x)$ at the interfaces of the slab, leading to diverging derivatives on the right-hand side of Eq. (14). One 283 possible strategy to solve Eq. (14) with such discontinuous jumps of parameters is to introduce additional 284 continuity conditions (as described for low-order differential equations in many textbooks³⁸) or to treat 285 the derivatives in a distributional sense³⁹. However, in the current paper, we rather assume continuous 286 coefficients as detailed below. 287

We rather make a second phenomenological assumption: We search for reasonable coefficients $A_2(x)$, $A_4(x)$, and $A_6(x)$ that lead to a behavior of the transmission $|T(\omega)|$ of the nonlocal slab that at least roughly qualitatively resembles the behavior we have found for the discrete mass-and-spring model shown in Fig. 3 or Fig. 4. By "reasonable", we mean that the dependencies $A_2(x)$, $A_4(x)$, and $A_6(x)$ must assume constant values far away from the interfaces. However, we must assume phenomenological shapes of the transition in the smeared-out interface regions (see above discussion on Fig. 1(b)). Intuitively, the smearing out extends over a length scale Na given by the nonlocal interaction of order N. Furthermore, the coefficients $A_4(x)$ and $A_6(x)$ must be extremely small in the local surrounding. Conceptually, they should be zero in a local medium. However, mathematically, they cannot be strictly zero there, because this would again lead to discontinuous jumps and hence divergences of spatial derivatives when attempting to solve Eq. (14).

We do *not* expect a quantitative agreement with our results for the discrete heterogeneous mass-andspring model (see, e.g., Fig. 3) because this form of a phenomenological effective-medium description does not even capture the dispersion relation of the nonlocal model quantitatively (see Figs. 4B and 4D in a previous study¹⁷). The asymptotics for $|k| \rightarrow \pi/a$ is incorrect, too⁴⁰. Our effective-medium description can only capture roughly and qualitatively the fact that there is a roton minimum at a finite wavenumber within the first Brillouin zone. Nevertheless, we feel that it is interesting and relevant to identify a simple effective-medium description that can at least capture the existence of BIC behavior for nonlocal slabs.

306 To compute the transmission spectrum of a nonlocal slab according to Eq. (14) within the effective-307 medium description numerically, we proceed as follows. Figure 6(a) and (b) illustrate the discrete model 308 and the corresponding continuum model. Here, L = 9a serves as an example. In the discrete model (see 309 Fig. 5(a)), all springs connecting two neighboring masses are the same. Therefore, we can naturally set 310 $K_1(x) = 1$ in the continuum model. The spatial dependence of the non-local spring constant $K_3(x)$ needs 311 to be manually constructed. We assume a smooth function for $K_3(x)$ in the region of 0 < x < 3a, roughly 312 corresponding to the boundary length scale of the discrete slab (compare Fig. 5(a) and (b)). Due to mirror 313 symmetry of the discrete system, $K_3(x)$ for L - 3a < x < L is obtained by symmetry. For the central part 314 of the slab, i.e., 3a < x < L - 3a, and the two surroundings to the left and right of the slab, i.e., x < 0and x > L, $K_3(x)$ becomes constant. This constant is determined by the value of the graded profiles at 315 x = 0 and x = L. The effective coefficients, $A_2(x)$, $A_4(x)$, and $A_6(x)$ of the continuum model are 316 chosen phenomenologically as described above. 317

Now, we consider a plane wave with angular frequency ω incident onto the left interface of the slab. Since the surrounding has small but non-zero coefficients A_4 and A_6 , three reflected modes exist, one with a real wavenumber, corresponding to a propagating mode, and two with complex wavenumbers, denoting evanescent modes that exponentially decay away from the interface. The total displacement field can be written as

323
$$u(x) = u_{in} \exp(ikx) + R_1 \exp(-ik_1x) + R_2 \exp(-ik_2x) + R_3 \exp(-ik_3x), x \le 0.$$
(15)

The wavenumber k_1 is purely real, while k_2 and k_3 should have positive imaginary parts to ensure exponential decay for x < 0. The three wavenumbers all satisfy the dispersion relation

326
$$\omega^2 = A_2 k_i^2 - A_4 k_i^4 + A_6 k_i^6 \tag{16}$$

for i = 1, 2, 3. In the transmission region, we start from the displacement field

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328
$$u(x) = T_1 \exp(ik_1 x) + T_2 \exp(ik_2 x) + T_3 \exp(ik_3 x), x \ge La.$$
(17)

Here, the three wavenumbers k_i , i = 1, 2, 3 are the same as in Eq. (15). In the above two expressions, R_i and T_i , i = 1, 2, 3, are the corresponding unknown reflection and transmission coefficients for the three modes.

To solve the six unknown coefficients, R_i and T_i , i = 1, 2, 3, wave propagation inside the non-local slab must be considered. However, due to inhomogeneous material parameters, the displacement fields cannot be constructed analytically. Here, we implement a state-space approach for solving the high-order ordinary differential equation⁴¹.

336 We first re-write the above sixth-order ordinary differential equation (14) into the following matrix form,

337
$$\frac{\mathrm{d}\mathbf{S}(x)}{\mathrm{d}x} = \mathbf{P}(x) \cdot \mathbf{S}(x), \tag{18}$$

 $\mathbf{S}(x) = \begin{pmatrix} u(x) \\ A_2(x)u'(x) \\ A_4(x)u''(x) \\ A_6(x)u'''(x) \\ (A_6(x)u'''(x))' + A_4(x)u''(x) \\ (A_6(x)u'''(x))'' + (A_4(x)u''(x))' + A_2(x)u'(x) \end{pmatrix},$ (19)

339
$$\mathbf{P}(x) = \begin{pmatrix} 0 & \frac{1}{A_2(x)} & 0 & 0 & 0 & 0\\ 0 & \frac{A'_2(x)}{A_2(x)} & \frac{A_2(x)}{A_4(x)} & 0 & 0 & 0\\ 0 & 0 & \frac{A'_4(x)}{A_4(x)} & \frac{A_4(x)}{A_6(x)} & 0 & 0\\ 0 & 0 & -1 & 0 & 1 & 0\\ 0 & -1 & 0 & 0 & 0 & 1\\ -m\omega^2 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$
(20)

Here, the prime symbol ' represents the spatial derivative with respect to the coordinate x and $\mathbf{S}(x)$ is called the state-space vector.

Next, the slab is discretized into many thin layers. The left location and right location of the j^{th} layer are denoted as x_{j-1} and x_j , respectively. Each layer is assumed to be homogeneous with its material parameters being evaluated at its middle, i.e., $A_2((x_{j-1} + x_j)/2)$, $A_4((x_{j-1} + x_j)/2)$, and $A_6((x_{j-1} + x_j)/2)$, respectively. The discretized problem will converge to the original problem with graded material parameter distribution if the discretized layers are sufficiently thin.

Within the j^{th} layer, the matrix $\mathbf{P}(x)$ becomes a constant matrix and the Eq. (19) has an exponential solution⁴¹. Furthermore, the two state-space vectors at both ends of the thin layer have the following transfer relation,

350
$$\mathbf{S}(x_j) = \mathbf{t}(x_j) \cdot \mathbf{S}(x_{j-1}), j = 1, 2 ...,$$
 (21)

351 with

352

$$\mathbf{t}(x_j) = \exp\left(\left(x_j - x_{j-1}\right)\mathbf{P}\left(\frac{x_{j-1} + x_j}{2}\right)\right).$$
(22)

Note that the state-space vector is continuous across the interface between two adjacent thin layers. Therefore, we can apply the transfer relation Eq. (21) sequentially to obtain the transfer relation between the two state space vectors at both ends, i.e., x = 0 and x = La, of the slab region,

356
$$\mathbf{S}(La) = \mathbf{T} \cdot \mathbf{S}(0), \mathbf{T} = \prod_j \mathbf{t}(x_j).$$
(23)

The two state-space vectors $\mathbf{S}(La)$ and $\mathbf{S}(0)$ are also obtained from the derived displacement fields Eqs. (21) - (22) for the incidence region and transmission region. Together with the transfer relation Eq. (23), the six unknown coefficients, R_i and T_i , i = 1, 2, 3 can be obtained.

In Fig. 6(a), we show the numerically calculated transmission results by using the above effective-medium 360 model for a slab with relative length L/a = 9. The other chosen parameters are given in the figure caption. 361 362 By comparing Fig. 3(a) and Fig. 6(a), we see that the effective model can capture the BIC behavior as well 363 as the usual Fabry-Perot resonance qualitatively well. The BIC behavior also occurs in the frequency range 364 where multiple eigenstates coexist (the roton part of the dispersion relation). The agreement with respect to the discrete model cannot be quantitative because the dispersion relations for the discrete model and 365 the effective-medium model do not match exactly (Fig. 6(b)). As for previous discrete model (see Fig. 4), 366 Figure 7 shows an enlarged view of the BIC point enclosed by the yellow box in Fig. 6(a). While the BIC 367 point appears in both, Fig. 4(b) and Fig. 7(b), the transmission line shapes are qualitatively different. 368 369 Results for different relative slab thicknesses in the effective-medium model are shown in Supplementary 370 Figure 2. There, one can again see the trend that, as the slab thickness increases, more and more BIC 371 points appear.

373 **Metamaterial microstructures.** So far, we have only considered a conceptual discrete mass-and-spring 374 toy model and an effective-medium simplification thereof. This model itself can hardly be called a 375 metamaterial. We have previously discussed that acoustic metamaterials for airborne sound can be 376 described approximately by the mass-and-spring toy model¹⁶. Therefore, in this section, we perform 377 numerical calculations for a slab of a specific acoustic metamaterial.

378 Figure 8(a) illustrates the considered metamaterial for airborne sound. The metamaterial is composed of 379 acoustical cavities (blue cylinders) and acoustical tubes (green and red pipes). Based on our previous theoretical and numerical studies¹⁶, the acoustical cavities can be treated as masses in the discrete model 380 381 in Fig. 1(a), and the green (red) acoustical tubes correspond to nearest-neighbor (third-nearest-neighbor) 382 springs. The ratio between the strength of the third-nearest-neighbor interactions and that of the nearest-383 neighbor interactions can be tuned through the geometry parameter R_3/R_1 . The metamaterial structure 384 shown in Fig. 10(a) forms the basis for the following calculations. Figure 8(b) exhibits a specific realization 385 of the discrete model in Fig. 1(b) by using the illustrated nonlocal metamaterial in Fig. 8(a). The length of 386 the metamaterial structure in Fig. 8(b) is about L = 5a. The surrounding tubes have no cut-off frequency, 387 which is similar to the continuum model in the preceding section. Viscosity of air usually leads to losses in acoustic systems⁴² and can influence the high-quality-factor resonances near the expected BIC points. 388 Therefore, in what follows, we will show and discuss numerical results with and without losses. 389

We simulate the sound wave propagation in the metamaterial shown in Fig. 8(b) by using the commercial software COMSOL Multiphysics. A plane-wave radiation condition is applied at the bottom of the model to mimic an incident plane wave. A perfectly matched layer is employed at the top to mimic a semi-infinite transmission region with no reflections⁴³. All other boundaries are treated as acoustic rigid boundaries²³. The linear acoustic equation in frequency,

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$$\nabla \cdot (\nabla p_{\omega}(\mathbf{r})) = -\frac{\omega^2}{c_{\mathrm{air}}^2} p_{\omega}(\mathbf{r})$$
(24)

is solved with the above specified boundary conditions. ω again represents the excitation angular frequency, $p_{\omega}(\mathbf{r})$ is the corresponding pressure field, and c_{air} is the speed of sound wave in air. The transmission coefficient *T* is extracted from the pressure field in the transmission region.

Results for the transmission behavior of the lossless microstructured slab are given in Fig. 9. Panel (a) depicts the transmission amplitude |T| versus the wave frequency ω and the geometry parameters R_3/R_1 . Panel (b) exhibits the calculated lowest phonon band for the periodic metamaterial in Fig. 9(a) for 402 different ratios R_3/R_1 . In the numerical simulations, we fix the radius $R_1 = 0.1a$ and vary the parameter 403 R_3 . In analogy to the above mass-and-spring model and continuum model, Fabry-Perot resonances are 404 observed in Fig. 9(a). Furthermore, a BIC behavior is clearly identified within that frequency range, for 405 which multiple Bloch wave modes coexist. Near by the BIC point, very sharp Fano resonances appear – as 406 for the discrete model as well as for the effective-medium model (see above).

In Fig. 10, we show the calculated transmission amplitude |T| as in Fig. 9(a), but with losses accounted for. Here, viscous damping in the acoustic pipes is treated *via* the "narrow region acoustics" in COMSOL Multiphysics. A quasi-BIC behavior is still observed from the plot. Here, the resonances near the BIC points have much smaller quality factors compared to the lossless case in Fig. 10(a). Nevertheless, the behavior is qualitatively similar to that of the discrete model and that of the effective-medium model, respectively.

We expect that our findings for nonlocal elastic slabs can be translated to other systems. For example, a thin film of superfluid helium, for which rotons were originally discovered, in a local surrounding should show a similar overall transmission behavior according to our intuitive interpretation. The detailed mathematical description might be quite different though. Furthermore, the nonlocal discrete mass-andspring model discussed here can be exactly mapped onto an electrical circuit composed of lumped capacitors and inductors, where the capacitors correspond to the masses and two types of inductors to the nearest-neighbor and beyond-nearest-neighbor Hooke's springs, respectively.

Finally, we note again that the minimum in the roton-like dispersion relation corresponds to an exceptional point. Furthermore, we have shown that the roton-like dispersion relation leads to BIC for a nonlocal metamaterial slab. This BIC behavior has already occurred at frequencies near to those of the roton minimum of the slab. We speculate that further interesting behavior might occur if one tunes the system parameters such that the BIC frequency coincides with that of the roton exceptional point.

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425 Data availability

The data that support the plots within this paper and other findings of this study are published on the open access data repository of the Karlsruhe Institute of Technology (<u>https://doi.org/10.35097/860</u>).

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431 Code availability

The numerical simulations in this work for the mass-and-spring model have been performed by using the
 commercial software MATLAB. Numerical simulations for the elastic metamaterials are performed using

the commercial software COMSOL Multiphysics. The code and models are published on the open access

- data repository of the Karlsruhe Institute of Technology (<u>https://doi.org/10.35097/860</u>).
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444 Author contributions

445 Y.C. and K.W. performed the numerical simulations. K.W. and M.K. designed the metamaterials. Y.C. and

- 446 S.G. developed the theory. M.W. wrote the first draft. C.W. and M.W. supervised the effort. All authors
- discussed the results and contributed to the writing and reviewing of the manuscript.
- 448

449 **Competing interests**

- 450 All authors declare no competing interests.
- 451
- 452

453 Figures and Captions



455 Figure 1. Illustration of mass-and-spring model. (a) An infinite periodic one-dimensional mass-and-spring model composed of masses (light yellow), m, connected to their nearest neighbors by Hooke's springs 456 (blue) with spring constant K_1 and additionally connected to their N-th nearest neighbors by Hooke's 457 458 springs (red) with spring constant K_N . Shown is the example of N = 3, which we emphasize in this paper 459 because it is the smallest integer for which one obtains a roton-like minimum inside of the first Brillouin 460 zone. The lattice constant is a. (b) A slab of such nonlocal material clad between half spaces of an ordinary 461 local mass-and-spring model with only nearest-neighbor interactions. The slab thickness is defined by the integer ratio L/a. Shown is the example of L/a = 6 and N = 3. Note that the boundaries of the slab are 462 smeared out in the sense that only the center mass out of the (1 + L/a) masses in the slab has two third-463 nearest-neighbor connections. The remaining six masses have only one such connection. This smearing-464 out is an immediate consequence of the nonlocality. 465

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Figure 2. Dispersion relations of the mass-and-spring model. (a) Surface plot of real component of 468 469 frequency ω versus the real and the imaginary components of the wavenumber k following Eq. (5). For 470 the conditions discussed in this paper, the angular frequency ω is purely real. The wavenumber k is also 471 purely real for a Bloch-periodic solution of an infinite periodic model. For a finite-thickness slab (see Fig. 1(b), evanescent modes can play a role and the imaginary part of k is generally not zero. The imaginary 472 473 part of the complex-valued angular frequency ω is shown by the false-color scale. Only the positive parts 474 of the real and imaginary components of the wavenumber are shown here as the corresponding negative 475 parts can be obtained by mirror symmetry. The four highlighted black lines on the surface lead to purely 476 real angular frequency ω . Among them, one corresponds to purely real wavenumber and the other three correspond to complex wavenumbers in the range of $\operatorname{Re}(k) > 0$. For a normalized frequency of $\omega/\omega_0 =$ 477 478 1.0, in between the local maximum and roton minimum, three real wavenumbers (see the three gray dots) can be obtained from the dispersion relation. For $\omega/\omega_0 = 0.2$ below the roton minimum, a real 479 480 wavenumber and a pair of complex conjugate wavenumber are obtained (see two yellow dots). Parameters are $K_3/K_1 = 1.0$ and the normalization frequency is $\omega_0 = \sqrt{4K_1/m}$. (b) Parameters 481 482 corresponding to the critical case without roton minimum in the dispersion relation, i.e., m = 1 and $K_3/K_1 = 1/3$. Note that still three solutions for the complex-valued k in the range of Re(k) > 0 occur at 483 484 a given angular frequency ω .

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Figure 3. Phonon transmission results of the mass-and-spring model. (a) Calculated transmission 488 amplitude $|T(\omega)|$ of the discrete nonlocal mass-and-spring-model slab (see Fig. 1(b)) shown on a gray 489 scale versus ω and K_3/K_1 . In the hatched region above the cut-off frequency $\omega/\omega_0 = 1.0$, waves cannot 490 propagate in the surrounding medium. "FP" denotes Fabry-Perot resonances, "BIC" bound-states-in-the-491 continuum points. Note the Fano-type line shapes of $|T(\omega)|$ near the BIC points. Two "BIC" points are 492 indicated. A zoom into one of them (see yellow box) is shown in Fig. 4(a). The normalization frequency is 493 $\omega_0 = \sqrt{4K_1/m}$. Parameters are: m = 1, L/a = 9. (b) Illustration of the corresponding dispersion 494 relations of the slab region for purely real ω and purely real k for different ratios of K_3/K_1 . 495

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Figure 4. Zoomed-in view of the BIC and sharp resonances. (a) Zoomed-in view of the bound-states-inthe-continuum (BIC point) highlighted by the yellow box in Fig. 3(a). (b) Cuts through the data in panel (a) at three selected ratios K_3/K_1 (see dashed vertical lines in (a)). Extremely sharp resonance versus frequency ω occur for parameters close to the BIC point (yellow and purple curves). At the BIC point (red curve), the sharp resonance disappears as incident waves strictly do not couple to the BIC.



507 Figure 5. Illustration of the effective-medium model. (a) Discrete system with slab thickness L. L = 9ais used as an example. (b) Scheme of the continuum model composed of the slab region and the two semi-508 infinite surroundings. The slab is further decomposed into a central uniform region, i.e., 3a < x < L - C509 3a, and two graded regions, i.e., 0 < x < 3a, and L - 3a < x < L. The graded regions represent smooth 510 transitions of the effective parameters to those in the two surroundings. In the region of 0 < x < 3a, a 511 function that increases smoothly from an extremely small value to a finite value is assumed for $K_3(x)$, 512 indicating the third-nearest-neighbor constants. $K_3(x)$ for L - 3a < x < L is obtained from mirror 513 514 symmetry of the system. For the central uniform part of the slab, i.e., 3a < x < L - 3a, and the two surroundings, i.e., x < 0 and x > L, $K_3(x)$ becomes constant and is obtained from continuity. The 515 parameter $K_1(x)$ is assumed to be constant throughout the 1D system, $K_1(x) = 1$. The effective 516 parameters of the continuum model are constructed from the two spring constants $K_1(x)$ and $K_3(x)$, i.e., 517 from $A_2(x) = K_1(x) + 9K_3(x)$, $A_4(x) = 6K_3(x)$, and $A_6(x) = K_3(x)$, respectively. 518

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Figure 6. Phonon transmission results for the phenomenological effective-medium model rather than the discrete mass-and-spring model. (a) Phonon transmission results. Parameters are L = 9a and $K_3(x)/K_1 = 1 - 1/(1 + \exp(2(x - 3a/2)))$ for 0 < x < 3a. The assumed $K_3(x)$ ensures that the two surrounding regions exhibit extremely small non-local stiffness parameters (about two orders of magnitude smaller than for the slab). (b) Dispersion relations for the effective-medium model (solid curves). The dashed curves correspond to the data in Fig. 3(b) for the discrete mass-and-spring model and can be compared directly to the effective-medium model.

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Figure 7. Zoomed-in view of the BIC and sharp resonances. (a) Zoomed-in view of the bound-states-inthe-continuum (BIC) point highlighted by the yellow box in Fig. 6(a). (b) Cuts through the data in panel (a) at three selected ratios K_3/K_1 (see dashed vertical lines in (a)).



537 Figure 8. Illustration of the considered 3D acoustical metamaterial for airborne sound. (a) Infinite 538 periodic metamaterial with non-local interactions. The metamaterial is composed of acoustical cavities (yellow cylinders) and acoustical channels (blue and red pipes). Colors are for illustration only, all parts 539 540 represent voids for air. The yellow cylinders, with height h and diameter d, correspond to masses in the discrete mass-and-spring model, and the blue (red) pipes, with diameter $2R_1$ ($2R_3$), represent the 541 nearest-neighbor interactions (third-nearest-neighbor interactions). The helix part of the red pipes has a 542 543 major radius, D/2. (b) A specific realization of the discrete model in Fig. 1(b) by using the metamaterial 544 structure in (a). The two semi-infinite pipes at both ends represent the surrounding. Therefore, the surrounding medium has no cut-off frequency, analogous to the effective-medium model shown in Fig. 6. 545 Geometry parameters are: h = 0.5a, d = 0.6a, D = 1.5a, $R_1 = 0.1a$, and a = 0.1 m, respectively. For 546 air, we choose the sound velocity $c_{\rm air} = 343~{\rm m~s^{-1}}$ and the mass density $\rho_{\rm air} = 1.29~{\rm kg~m^{-3}}$. 547



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Figure 9. Phonon transmission results of the designed metamaterial. (a) Numerically obtained transmission spectrum |T| for the metamaterial structure shown in Fig. 8(b) versus exciting frequency $\omega/(2\pi)$ and versus the ratio R_3/R_1 . Damping is neglected. The bound-states-in-the-continuum (BIC) point is marked by the red arrow. (b) Calculated phonon dispersion relation for three selected ratios R_3/R_1 (see legend). The lowest acoustic band exhibits a pronounced roton-like behavior. For comparison, the dispersion relation of the surrounding (a straight line) is depicted by the black solid curve.



Figure 10. Numerically obtained transmission spectrum |T| with viscous damping in the acoustic pipes is accounted for. As a result, the resonances around the BIC point are smeared out, but the overall qualitative behavior remains unchanged.

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