# Appendix A. Auxiliary proofs

**Proof of Lemma 2**: Let us add (3.2) and (3.3) to their respective complex conjugates. Since $G,\rho$ and $\tilde{\lambda}_n^\circ$ are real-valued, we find that

$$\left.\begin{array}{rcl} -\nabla\cdot\big(G\nabla(\tilde{\phi}_n^\circ+\overline{\tilde{\phi}_n^\circ})\big) &=& \tilde{\lambda}_n^\circ\rho(\tilde{\phi}_n^\circ+\overline{\tilde{\phi}_n^\circ}) \quad \text{in } Y, \\ \boldsymbol{\nu}\cdot G\nabla(\tilde{\phi}_n^\circ+\overline{\tilde{\phi}_n^\circ})|_{x_j=0} &=& -\boldsymbol{\nu}\cdot G\nabla(\tilde{\phi}_n^\circ+\overline{\tilde{\phi}_n^\circ})|_{x_j=\ell_j} \end{array}\right\} \implies \tilde{\phi}_n^\circ+\overline{\tilde{\phi}_n^\circ}=c\,\tilde{\phi}_n^\circ, \quad c=\text{const.}$$

i.e. that $\arg(c\tilde{\phi}_n^\circ(\boldsymbol{x}))=0$. On taking $c\in\mathbb{R}$, we obtain $\operatorname{Im}(\tilde{\phi}_n^\circ)=0$ which completes the proof. □

**Proof of Lemma 3**: On recalling (3.2) and the fact that $\tilde{\phi}_n^\circ$ is taken as real-valued by Lemma 2, we compute the difference between (3.14) and its complex conjugate to show that

$$\left.\begin{array}{rcl} \tilde{\lambda}_n^\circ\rho(\boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}})+\nabla\cdot\big(G\nabla(\boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}})\big) &=& 0 \quad \text{in } Y \\ \boldsymbol{\nu}\cdot G\nabla(\boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}})|_{x_j=0} &=& -\boldsymbol{\nu}\cdot G\nabla(\boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}})|_{x_j=\ell_j} \end{array}\right\} \implies \boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}} = \boldsymbol{c}\tilde{\phi}_n^\circ,$$

for some vector constant $\boldsymbol{c}$. However, one also has $\boldsymbol{c}=\langle\boldsymbol{c}\tilde{\phi}_n^\circ\rangle=\langle\boldsymbol{\chi}^{(1)}-\overline{\boldsymbol{\chi}^{(1)}}\rangle=\langle\boldsymbol{\chi}^{(1)}\rangle-\langle\overline{\boldsymbol{\chi}^{(1)}}\rangle\equiv\boldsymbol{0}$, which establishes the claim. □

**Proof of Lemma 4**: On multiplying (3.22) by $\boldsymbol{\chi}^{(1)}$ and integrating by parts, we obtain

$$\tilde{\lambda}_n^{\boldsymbol{a}}\int_Y\rho\eta^{(0)}\boldsymbol{\chi}^{(1)}\,\mathrm{d}\boldsymbol{x}-\int_Y G\nabla\eta^{(0)}\cdot\nabla\boldsymbol{\chi}^{(1)}\,\mathrm{d}\boldsymbol{x} = \int_Y\Big(\frac{\langle 1\rangle}{\rho^{(0)}}\rho\tilde{\varphi}_n^{\boldsymbol{a}}-1\Big)\boldsymbol{\chi}^{(1)}\mathrm{d}\boldsymbol{x}. \tag{A.1}$$

Integrating by parts one more time, the second term on the left-hand side becomes

$$\begin{aligned} -\int_Y G\nabla\eta^{(0)}\cdot\nabla\boldsymbol{\chi}^{(1)}\,\mathrm{d}\boldsymbol{x} &= -\int_Y\nabla\eta^{(0)}\cdot G\big(\nabla\boldsymbol{\chi}^{(1)}+\boldsymbol{I}\tilde{\varphi}_n^{\boldsymbol{a}}\big)\,\mathrm{d}\boldsymbol{x}+\int_Y\nabla\eta^{(0)}G\tilde{\varphi}_n^{\boldsymbol{a}}\,\mathrm{d}\boldsymbol{x} \\ &= \int_Y\eta^{(0)}\nabla\cdot\big(G\big(\nabla\boldsymbol{\chi}^{(1)}+\boldsymbol{I}\tilde{\varphi}_n^{\boldsymbol{a}}\big)\big)\,\mathrm{d}\boldsymbol{x}+\int_Y\nabla\eta^{(0)}G\tilde{\varphi}_n^{\boldsymbol{a}}\,\mathrm{d}\boldsymbol{x} \\ &= -\tilde{\lambda}_n^{\boldsymbol{a}}\int_Y\eta^{(0)}\rho\boldsymbol{\chi}^{(1)}\,\mathrm{d}\boldsymbol{x}-\int_Y\eta^{(0)}G\nabla\tilde{\varphi}_n^{\boldsymbol{a}}\,\mathrm{d}\boldsymbol{x}+\int_Y\nabla\eta^{(0)}G\tilde{\varphi}_n^{\boldsymbol{a}}\,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

By virtue of this result and the fact that $\tilde{\varphi}_n^{\boldsymbol{a}}$ and $\boldsymbol{\chi}^{(1)}$ are real-valued, (A.1) reduces to

$$\langle G\nabla\eta^{(0)}\rangle-(G\eta^{(0)},\nabla\tilde{\varphi}_n^{\boldsymbol{a}}) = \frac{1}{\rho^{(0)}}((\langle 1\rangle\rho\tilde{\varphi}_n^{\boldsymbol{a}}-\rho^{(0)})\boldsymbol{\chi}^{(1)},1) = \frac{\langle 1\rangle}{\rho^{(0)}}\boldsymbol{\rho}^{(1)}-(\boldsymbol{\chi}^{(1)},1).$$

□

**Proof of Lemma 5**: By way of (3.18), field equation (3.26) can be recast as

$$-\big(\boldsymbol{\mu}^{(0)}\!:(i\hat{\boldsymbol{k}})^2+\sigma\rho^{(0)}\hat{\omega}^2\big)w_1-\Big(\boldsymbol{\mu}^{(1)}-\frac{1}{\rho^{(0)}}\{\boldsymbol{\rho}^{(1)}\otimes\boldsymbol{\mu}^{(0)}\}\Big)\!:(i\hat{\boldsymbol{k}})^3w_0 = -(\boldsymbol{\chi}^{(1)},1)\cdot i\hat{\boldsymbol{k}}. \tag{A.2}$$

On recalling (3.14) and (3.21), however, one can conveniently symmetrize and integrate by parts their weighted difference $\big(\{(3.21)\otimes\boldsymbol{\chi}^{(1)}-(3.14)\otimes\boldsymbol{\chi}^{(2)}\},1\big)$. Noting in particular that

$$\begin{aligned} \big(\{\nabla\cdot\big(G(\nabla\boldsymbol{\chi}^{(2)}+\{\boldsymbol{I}\otimes\boldsymbol{\chi}^{(1)}\}')\big)\otimes\boldsymbol{\chi}^{(1)}\},1\big) &= -\big(\{G(\nabla\boldsymbol{\chi}^{(1)})^{\mathrm{T}}\cdot\nabla\boldsymbol{\chi}^{(2)}\},1\big)-\big(\{G(\nabla\boldsymbol{\chi}^{(1)})^{\mathrm{T}}\otimes\boldsymbol{\chi}^{(1)}\},1\big), \\ \big(\{\nabla\cdot\big(G(\nabla\boldsymbol{\chi}^{(1)}+\boldsymbol{I}\tilde{\phi}_n^\circ)\big)\otimes\boldsymbol{\chi}^{(2)}\},1\big) &= -\big(\{G(\nabla\boldsymbol{\chi}^{(1)})^{\mathrm{T}}\cdot\nabla\boldsymbol{\chi}^{(2)}\},1\big)-\big(\{G\nabla\boldsymbol{\chi}^{(2)}\tilde{\phi}_n^\circ\},1\big), \end{aligned}$$

where "$(\cdot)^{\mathrm{T}}$" denotes tensor transpose, we obtain $\rho^{(0)}\boldsymbol{\mu}^{(1)}=\{\boldsymbol{\rho}^{(1)}\otimes\boldsymbol{\mu}^{(0)}\}$ thanks to the fact that $\tilde{\varphi}_n^{\boldsymbol{a}}$ is real-valued. A substitution of the last result into (A.2) immediately recovers (3.29). □

**Proof of Lemma 6**: The first claim is a direct result of Lemma 3 since (5.19) is a replica of (3.14) with $Y$ and $\tilde{\phi}_n^\circ$ replaced by $Y_{\boldsymbol{a}}$ and $\tilde{\varphi}_n^{\boldsymbol{a}}$, respectively. On the other hand, the inner product of (4.22) with $\tilde{\varphi}_n^{\boldsymbol{a}}$ reads

$$-\big(\tilde{\lambda}_n^{\circ}\rho\tilde{w}_1,\tilde{\varphi}_n^{\boldsymbol{a}}\big) - \big(\nabla\cdot(G(\nabla\tilde{w}_1+i\hat{\boldsymbol{k}}\tilde{w}_0)),\tilde{\varphi}_n^{\boldsymbol{a}}\big) \;=\; w_0\big(i\hat{\boldsymbol{k}}\cdot(G\nabla\tilde{\varphi}_n^{\boldsymbol{a}}),\tilde{\varphi}_n^{\boldsymbol{a}}\big) + w_0\big(\rho\tilde{\varphi}_n^{\boldsymbol{a}},\tilde{\varphi}_n^{\boldsymbol{a}}\big)\sigma\breve{\omega}^2, \quad (A.3)$$

thanks to (4.21). On exercising repeated integration by parts and recalling (4.21) anew, the second term on the left-hand side of (A.3) is computed as

$$\begin{aligned} -\big(\nabla\cdot(G(\nabla\tilde{w}_1+i\hat{\boldsymbol{k}}\tilde{w}_0)),\tilde{\varphi}_n^{\boldsymbol{a}}\big) \;&=\; -\big(\nabla\cdot(G(\nabla\tilde{w}_1+i\hat{\boldsymbol{k}}\tilde{w}_0)\tilde{\varphi}_n^{\boldsymbol{a}}),1\big) \\ &+\big(\nabla\cdot(G\nabla\tilde{\varphi}_n^{\boldsymbol{a}}\tilde{w}_1),1\big) - \big(\tilde{w}_1,\nabla\cdot(G\nabla\tilde{\varphi}_n^{\boldsymbol{a}})\big) + w_0(i\hat{\boldsymbol{k}}G\tilde{\varphi}_n^{\boldsymbol{a}},\nabla\tilde{\varphi}_n^{\boldsymbol{a}}), \end{aligned} \quad (A.4)$$

since $\tilde{\varphi}_n^{\boldsymbol{a}}=\overline{\tilde{\varphi}_n^{\boldsymbol{a}}}$, see Remark 7. The first (resp. second) term on the right-hand side of (A.4) vanishes thanks to (i) the divergence theorem, (ii) boundary condition (4.17) with $m=1$ (resp. the flux boundary condition in (4.8)), and (iii) the fact that $\tilde{\varphi}_n^{\boldsymbol{a}}$ (resp. $\tilde{w}_1$) is an element of $H_p^1(Y_{\boldsymbol{a}})$. On rewriting the third term on the right-hand side of (A.4) as $-\big(\tilde{w}_1,\nabla\cdot(G\nabla\tilde{\varphi}_n^{\boldsymbol{a}})\big)=\big(\tilde{\lambda}_n^{\boldsymbol{a}}\rho\tilde{w}_1,\tilde{\varphi}_n^{\boldsymbol{a}}\big)$ by way of (4.7) and substituting the result back into (A.3), we find that

$$\sigma\breve{\omega}^2\big(\rho\tilde{\varphi}_n^{\boldsymbol{a}},\tilde{\varphi}_n^{\boldsymbol{a}}\big)\,w_0 \;=\; \big[(i\hat{\boldsymbol{k}}G\tilde{\varphi}_n^{\boldsymbol{a}},\nabla\tilde{\varphi}_n^{\boldsymbol{a}})-(i\hat{\boldsymbol{k}}\cdot(G\nabla\tilde{\varphi}_n^{\boldsymbol{a}}),\tilde{\varphi}_n^{\boldsymbol{a}})\big]\,w_0 \;\equiv\; 0 \quad\Longrightarrow\quad \breve{\omega}w_0=0 \quad (A.5)$$

since $\tilde{\varphi}_n^{\boldsymbol{a}}$ is real-valued and $\big(\rho\tilde{\varphi}_n^{\boldsymbol{a}},\tilde{\varphi}_n^{\boldsymbol{a}}\big)>0$. To preserve the leading-order solution, one must have $\breve{\omega}=0$ which completes the proof. □

**Proof of Lemma 7**: We premultiply the conjugate transpose of (5.11) by $\sum_p w_{0p}$, and we subtract the result from (5.11) premultiplied by $\sum_p \overline{w_{0p}}$. On relabeling dummy indexes, we obtain

$$\sum_p\sum_q \overline{w_{0p}}\,\big(A_{pq}-\overline{A_{pq}}^{\mathrm{T}}\big)\,w_{0q} \;-\; (\tau-\overline{\tau})\sum_q \overline{w_{0p}}\,D_{pq}\,w_{0q} \;=\; 0.$$

Since $A_{pq}$ is Hessian and $D_{pq}$ is positive definite, we find that $\tau=\overline{\tau}$ which establishes the first claim. By virtue of this result and the fact that $\overline{A_{pq}}=-A_{pq}$, we next take the complex conjugate of (5.11) to show that the latter also holds with $w_{0q}$ and $\tau$ superseded by $\overline{w_{0q}}$ and $-\tau$, respectively. Finally, we note that for $Q$ odd, there is at least one eigenvalue such that $\tau=-\tau$, whereby the maximum rank of $A_{pq}$ in this case is $Q-1$. □

**Proof of Lemma 8**: We integrate (4.25)$\otimes\boldsymbol{\chi}_p^{(1)}$ by parts over $Y_a$ to obtain

$$\big(G\tilde{\varphi}_{nq}^{\boldsymbol{a}}\nabla\boldsymbol{\chi}_p^{(1)},1\big)_{\overline{Y}_{\boldsymbol{a}}} - \big(G\nabla\tilde{\varphi}_{nq}^{\boldsymbol{a}}\otimes\boldsymbol{\chi}_p^{(1)},1\big)_{\overline{Y}_{\boldsymbol{a}}} \;=\; \tilde{\lambda}_n\,\big(\rho\boldsymbol{\chi}_q^{(1)}\otimes\boldsymbol{\chi}_p^{(1)},1\big)_{\overline{Y}_{\boldsymbol{a}}} - \big(G\nabla\boldsymbol{\chi}_q^{(1)}\cdot\nabla\boldsymbol{\chi}_p^{(1)},1\big)_{\overline{Y}_{\boldsymbol{a}}}.$$

The proof then immediately follows from (5.21) upon rewriting $\boldsymbol{\mu}_{pq}^{(0)}$ as

$$\boldsymbol{\mu}_{pq}^{(0)} \;=\; \big(G\{\tilde{\varphi}_{np}^{\boldsymbol{a}}\nabla\boldsymbol{\chi}_q^{(1)}\},1\big)_{\overline{Y}_{\boldsymbol{a}}} - \big(G\{\nabla\tilde{\varphi}_{np}^{\boldsymbol{a}}\otimes\boldsymbol{\chi}_q^{(1)}\},1\big)_{\overline{Y}_{\boldsymbol{a}}} + \boldsymbol{I}\,\big(G\tilde{\varphi}_{np}^{\boldsymbol{a}}\tilde{\varphi}_{nq}^{\boldsymbol{a}},1\big)_{\overline{Y}_{\boldsymbol{a}}}.$$

□

**Proof of Lemma 10**: We first recall that $A_{pq}$ is real-valued symmetric and that $B_{pq}$ is imaginary skew-symmetric, whereby there exists a real-valued orthogonal matrix $R_{pq}$ with the sought properties in each case. Next, we demonstrate the invariance of $\rho^{(0)}$ under transformation (5.33) by observing from (5.30) that

$$\sum_p \widetilde{\rho_p^{(0)}} \;=\; \sum_{p,r} T_{pr}\,\rho_r^{(0)}\,T_{rp}^{\mathrm{T}} \;=\; \rho^{(0)}\sum_r \rho_r^{(0)}\sum_{p,q,s} R_{pq}D_{qr}^{-1/2}R_{ps}D_{sr}^{-1/2} \;=\; \rho^{(0)}Q \;=\; \sum_r \rho_r^{(0)}.$$

To show the uniqueness of $\widetilde{\tilde{\varphi}_{nq}^{\boldsymbol{a}}}$ when $M_{pq}$ $(M=A,B)$ has no repeated eigenvalues, we let

$$\tilde{\pi}_{nq}^{\boldsymbol{a}} \;=\; (\rho^{(0)}/\rho_q^{(0)})^{1/2}\,\tilde{\varphi}_{nq}^{\boldsymbol{a}}, \qquad q=\overline{1,Q} \qquad \text{(no summation)}$$

be the rescaled eigenfunction basis satisfying $(\rho\tilde{\pi}_{nq}^{\boldsymbol{a}},\tilde{\pi}_{nr}^{\boldsymbol{a}})_{\overline{Y}_{\boldsymbol{a}}}=\delta_{qr}\,\rho^{(0)}$, and we note that all such orthonormal bases can be "rotated" into one another by some orthogonal transformation $W_{pq}$. Next, we restart the analysis from $\rho$-orthogonal basis $\tilde{\varphi}_{nq}^{\boldsymbol{a}\prime}$ that is distinct from $\tilde{\varphi}_{nq}^{\boldsymbol{a}}$, but normalized so that $(\tilde{\varphi}_{nq}^{\boldsymbol{a}\prime},\tilde{\varphi}_{nq}^{\boldsymbol{a}\prime})_{\overline{Y}_{\boldsymbol{a}}}=1$ as before. In this case, we find that $\rho^{(0)\prime}=\rho^{(0)}$ by the earlier argument and that

$$\tilde{\varphi}^{\boldsymbol{a}\prime}_{nq} \;=\; \sum_{r} V_{qr}\,\tilde{\varphi}^{\boldsymbol{a}}_{nr}, \qquad V_{qr} \;=\; \sum_{t,s} D'^{1/2}_{qt}\,W_{ts}\,D^{-1/2}_{sr}, \qquad q,r=\overline{1,Q},$$

where $W_{ts}$ is orthogonal and $D'_{qt}$ is the "mass matrix" $D_{qt}$ computed for basis $\tilde{\varphi}^{\boldsymbol{a}\prime}_{nq}$. As a result, the counterpart of $R_{pq}$ in (5.33) computed for $\tilde{\varphi}^{\boldsymbol{a}\prime}_{nq}$ reads $R'_{pq}=\sum_s R_{ps}W^{\mathrm{T}}_{sq}$ and consequently $\widetilde{\tilde{\varphi}^{\boldsymbol{a}\prime}_{nq}} = \sqrt{\rho^{(0)}}\sum_{r,s} R'_{qr}\,D'^{-1/2}_{rs}\tilde{\varphi}^{\boldsymbol{a}\prime}_{ns} = \widetilde{\tilde{\varphi}^{\boldsymbol{a}}_{nq}}$, as long as $M_{pq}$ has no repeated eigenvalues which guarantees the uniqueness of $R_{ps}$.

On substituting (5.33) into the transformation rule for dyads $M_{pq}$ in (5.31), we immediately recover both (5.34) and the claimed orthonormality of $\widetilde{\tilde{\varphi}^{\boldsymbol{a}}_{nq}}$. Finally, the invariance of $\widetilde{A_{pq}}$ and $\widetilde{B_{pq}}$ in (5.34) is demonstrated by an argument similar to that used to establish the uniqueness of $\widetilde{\tilde{\varphi}^{\boldsymbol{a}}_{nq}}$, noting in particular that $\rho^{(0)}\sum_{r,s} D^{-1/2}_{pr}M_{rs}D^{-1/2}_{sq}$ due to $\tilde{\varphi}^{\boldsymbol{a}}_{nq}$ and $\rho^{(0)}\sum_{r,s} D'^{-1/2}_{pr}M'_{rs}D'^{-1/2}_{sq}$ due to $\tilde{\varphi}^{\boldsymbol{a}\prime}_{nq}$ share the same eigenvalues $\lambda^{M}_{p}$ $(M=A,B)$ irrespective of their multiplicity. $\square$

## Appendix B. Application to polyatomic chains

Consider a periodic chain of alternating masses and springs whose unit cell contains $N$ masses $m_j$ $(j=\overline{1,N})$ that are spatially separated by $\Delta x=\ell/N$. We denote by $c_j$ the stiffness of spring connecting $m_j$ and $m_{j+1}$. The chain is excited by a "plane-wave" body force with frequency $\omega$ and wavenumber $k$ such that mass $m_j$, with spatial coordinate $x_l$ $(l\in\mathbb{Z})$, is subjected to external force $\tilde{f}e^{i(kx_l-\omega t)}$. Without loss of generality, we write $l=j$ for the reference unit cell and omit the time factor $e^{-i\omega t}$, which gives the balance of linear momentum as

$$-\omega^2 m_j u_j + (c_j+c_{j-1})u_j - c_{j-1}u_{j-1} - c_j u_{j+1} \;=\; \tilde{f}e^{ikx_j}, \quad j=\overline{1,N} \tag{B.1}$$

where $u_j$ is the displacement of the $j$th mass. By analogy to (2.3), we seek the Bloch-wave solution $u_j=\tilde{u}_j e^{ikx_j}$ where $\tilde{u}_j$ is $N$-periodic. This reduces (B.1) to

$$\sum_j \Big(C_{lj}(ik)-\omega^2 M_{lj}\Big)\tilde{u}_j \;=\; \tilde{f}, \qquad l=\overline{1,N}, \tag{B.2}$$

where $M_{lj}$ is a diagonal mass matrix; $i=\sqrt{-1}$; $k$ is the wave number, and $C_{lj}(ik)$ is a Hermitian stiffness matrix that depends on wavenumber $k$. On setting $\tilde{f}=0$, (B.2) yields the eigenvalues $\lambda_n(k)=\omega_n^2(k)$ and affiliated eigenvectors $\phi_j^n(k)\in\mathbb{R}$ $(j,n=\overline{1,N})$ for the chain. In this setting, the definition of effective motion (2.15) near point $(\omega_n,0)$ in the frequency-wavenumber domain degenerates to

$$\langle u\rangle \;=\; \sum_j \tilde{u}_j\overline{\phi_j^n}, \qquad \phi_j^n=\phi_j^n(0);$$

a formula that is readily generalized to include both "apex" points $(\omega_n,\pi/\ell)$, repeated eigenvalues, and nearby eigenvalues by applying the developments from Section 4, Section 5, and Section 6, respectively. Then, by way of scalings

$$k \;=\; k^a+\epsilon\hat{k}, \qquad \omega^2 \;=\; \tilde{\lambda}_n^a+\epsilon\sigma\breve{\omega}^2+\epsilon^2\sigma\hat{\omega}^2, \qquad k^a\in\{0,\pi/\ell\}, \qquad \epsilon\;=\;o(1), \quad \sigma=\pm1,$$

and the asymptotic expansion $\tilde{u}_j=\epsilon^{-2}\tilde{u}_{j0}+\epsilon^{-1}\tilde{u}_{j1}+\tilde{u}_{j2}+\epsilon\tilde{u}_{j3}+\cdots$, (B.2) can be expanded in powers of $\epsilon$ to produce a cascade of matrix equations that form the basis for establishing both leading- and second-order descriptions of the effective motion.

**Remark 1.** *The exact dispersion relationship due to (B.2) reads* $cos(k\ell)=1-\mathscr{P}(\omega)$, *where* $\mathscr{P}$ *is a real-valued polynomial of degree* $2N$. *Inside (the positive half of) the first Brillouin zone, this relationship can be inverted as* $k\ell=g(\omega)$, *where* $g(\omega)=\cos^{-1}(1-\mathscr{P}(\omega))$ *is a single-valued function mapping* $\{\omega\in\mathbb{R}^+ : 0<\mathscr{P}(\omega)<2\}$ *to* $(0,\pi/\ell)$. *In light of Theorem 3, repeated eigenvalues at* $k^a$ *with multiplicity* $Q>2$ *are thus not possible in a polyatomic chain for each such situation would violate the single-valuedness of* $g(\omega)$.

**Remark 2.** *When* $Q=2$ *at* $k^a\in\{0,\pi/\ell\}$, *we find that* $dk/d\omega=\ell^{-1}[P(\omega)(2-P(\omega))]^{-1/2}P'(\omega)$ *is bounded at* $k^a$, *i.e. that* $|d\omega/dk|>0$ *there. By Theorem 3, this further precludes the situations with* $Q=2$ *and* $rank(A_{pq})=0$ *in a polyatomic chain.*

## Appendix C. Comparison with the results in [11]

To evaluate the effective parameters $\rho^{(0)}$, $\boldsymbol{\mu}^{(0)}$, $\boldsymbol{\rho}^{(2)}$, $\boldsymbol{\mu}^{(2)}$ and $\boldsymbol{\mu}^{(0)}_{pq}$ for a chessboard-like medium according to (4.28), (4.33), (5.21) and (5.32), eigenfunctions $\tilde{\varphi}^{\boldsymbol{a}}_n(\boldsymbol{x})$ and cell functions $\boldsymbol{\chi}^{(m)}(\boldsymbol{x})$ ($m$=1, 2, 3) are computed using the finite element platform NGSolve [28]. The unit cell (either $Y$ or $Y_{\boldsymbol{a}}$, depending on the apex) is discretized using fourth-order finite elements, with the maximum element size bounded from above by $0.05|Y|^{1/2}$. Before examining the general case with variable shear modulus and mass density, we first evaluate the effective tensor $\boldsymbol{T}=\boldsymbol{\mu}^{(0)}/\rho^{(0)}$ for a medium with *constant shear modulus* as in [11] by taking $\ell_1$=$\ell_2$=2, $\boldsymbol{G}=(1,1,1,1)$, and $\boldsymbol{r}=(1,101,201,101)$. This particular configuration, while bearing little relevance from the viewpoint of elastic solids, is nonetheless useful as a vehicle to verify the numerical implementation.

**Remark 3.** *At this point, we recall our premise that $|Y|=1$. This limitation can, however, be handled with little difficulty; for instance, at every apex $\boldsymbol{k}^{\boldsymbol{a}}$ with $\boldsymbol{a}\neq\boldsymbol{0}$, the foregoing results remain valid for any $|Y|>0$ by taking $|Y_{\boldsymbol{a}}|=|Y|\prod_{j=1}^{d}(1+a_j)$ in lieu of the measure given in (4.6). When $\boldsymbol{a}=\boldsymbol{0}$, a similar modification (omitted herein for brevity) can be implemented.*

For all apex points and solution branches under consideration, we find by simulations that: (i) $\boldsymbol{T}$ is diagonal when the eigenvalue is simple; (ii) so are tensors $\boldsymbol{T}_{pq}=\boldsymbol{\mu}^{(0)}_{pq}/\rho^{(0)}$ (using the eigenfunction basis as in Lemma 10) when the eigenvalue is repeated, and (iii) $\boldsymbol{T}_{pq}=\boldsymbol{0}$ for $p\neq q$. In this setting, Table C.1 compares the present results with those in [11] at apexes $A$, $B$, and $C$ for the first four solution branches. For brevity of notation, we refer to the effective tensors $\boldsymbol{T}_{11}$ and $\boldsymbol{T}_{22}$ simply as "$\boldsymbol{T}$" when listing the results for repeated eigenvalues. As can be seen from the display, there is a good overall agreement between the two sets of results.

**Table C.1.** Non-trivial components of the effective tensor $\boldsymbol{T}=\boldsymbol{\mu}^{(0)}/\rho^{(0)}$ at apexes $A$, $B$, and $C$ for the first four branches versus the values obtained in [11], assuming a chessboard-like medium as in Fig. 3 with $\ell_1$=$\ell_2$=2, $\boldsymbol{G}=(1,1,1,1)$ and $\boldsymbol{r}=(1,101,201,101)$. For clarity, all instances of repeated eigenvalues ($Q=2$) are indicated by an asterisk.

| Apex | $\boldsymbol{a}$ | $\omega_n$ | $\boldsymbol{T}[1,1]$ | $\boldsymbol{T}[2,2]$ | $\boldsymbol{T}[2,2]$ [11] | $\boldsymbol{T}[2,2]$ [11] |
|---|---|---|---|---|---|---|
| A | (0,0) | 0.2853* | −0.1605 | 0.0046 | −0.1605 | 0.0046 |
| A | – | 0.2853* | 0.0046 | -0.1605 | 0.0046 | −0.1605 |
| A | – | 0.3098* | 0.1723 | 0.0052 | 0.1723 | 0.0052 |
| A | – | 0.3098* | 0.0052 | 0.1723 | 0.0052 | 0.1723 |
| B | (1,0) | 0.1339 | −0.0541 | 0.0069 | −0.0542 | 0.0068 |
| B | – | 0.1784 | 0.0692 | 0.0107 | 0.0692 | 0.0107 |
| B | – | 0.2946 | −0.0066 | -0.1289 | −0.0066 | −0.1289 |
| B | – | 0.3192 | −0.0067 | 0.1430 | −0.0067 | 0.1430 |
| C | (1,1) | 0.1716 | −0.0254 | -0.0254 | −0.0254 | −0.0254 |
| C | – | 0.2156* | 0.0397 | -0.0220 | 0.0400 | −0.0220 |
| C | – | 0.2156* | −0.0220 | 0.0397 | −0.0220 | 0.0400 |
| C | – | 0.3118 | 0.0401 | 0.0401 | 0.0401 | 0.0401 |

## References

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# Appendix D. Effective description of nearby dispersion branches

## (a) Tetratomic chain

Consider first the tetratomic chain behavior featuring $Q=2$ nearby eigenvalues at $k\ell=\pi$, see the circled region in Fig 2(b). We pursue asymptotic expansion about the first (i.e. *bottom*) eigenvalue at $k\ell=1$, which yields $\gamma_1=0$, $\gamma_2=0.073487$, and

$$[A_{pq}] = \begin{bmatrix} 0 & 0.008724 \\ -0.008724 & 0 \end{bmatrix} \hat{k}, \qquad [\gamma_q D_{pq}] = \begin{bmatrix} 0 & 0 \\ 0 & 0.073487 \end{bmatrix}. \tag{D.1}$$

Accordingly we find that $rank(A^{\gamma}_{pq})=2$, whereby the "*twin cones*" model (6.13) applies. For completeness, we note that alternative expansion about the second (i.e. *top*) eigenvalue at $k\ell=1$ only reverses the sign of $A_{pq}$ and $D_{pq}$, and consequently does not affect the result shown in Fig. 6(a).

## (b) Chessboard-like solid

For the cluster of $Q=3$ nearby eigenvalues at apex $A$ of the chessboard medium (branches 3–5 in Fig. 4), we expand about the (repeated) fourth eigenvalue at $\boldsymbol{k}^{\boldsymbol{a}}=\boldsymbol{0}$, which yields $\gamma_1=\gamma_2=0$, $\gamma_3=-1.508519$, and

$$[A_{pq}] = \begin{bmatrix} 0 & 0 & 8.730555 \\ 0 & 0 & -8.349118 \\ -8.730555 & 8.349118 & 0 \end{bmatrix} \|\hat{\boldsymbol{k}}\| \quad \text{for} \quad \frac{\hat{\boldsymbol{k}}}{\|\hat{\boldsymbol{k}}\|}=(1,0), \tag{D.2}$$

$$[A_{pq}] = \begin{bmatrix} 0 & 0 & -0.269717 \\ 0 & 0 & -12.077152 \\ 0.269717 & 12.077152 & 0 \end{bmatrix} \|\hat{\boldsymbol{k}}\| \quad \text{for} \quad \frac{\hat{\boldsymbol{k}}}{\|\hat{\boldsymbol{k}}\|}=\tfrac{1}{\sqrt{2}}(1,1), \tag{D.3}$$

$$[\gamma_q D_{pq}] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1.536198 \end{bmatrix}, \tag{D.4}$$

which demonstrate that $rank(A^{\gamma}_{pq})=2$. In this case, we also find that $\boldsymbol{\theta}_{12}=\boldsymbol{\theta}_{21}=\boldsymbol{0}$, $\boldsymbol{\theta}_{13}\perp\boldsymbol{\theta}_{23}$, and $\|\boldsymbol{\theta}_{13}\|=\|\boldsymbol{\theta}_{23}\|=12.08016$. This allows us to identify "rotation" (5.29) of the eigenfunction basis, affecting only the first two eigenfunctions (representing the fourth and the fifth branch), so that (5.22) holds in each direction $\hat{\boldsymbol{k}}/\|\hat{\boldsymbol{k}}\|$. After such "rotations", we obtain $\widetilde{D_{pq}}=D_{pq}$ and

$$[\widetilde{A_{pq}}] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 12.08016 \\ 0 & -12.08016 & 0 \end{bmatrix} \|\hat{\boldsymbol{k}}\| \quad \text{for} \quad \frac{\hat{\boldsymbol{k}}}{\|\hat{\boldsymbol{k}}\|}=(1,0), \tag{D.5}$$

$$[\widetilde{A_{pq}}] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 12.08016 \\ 0 & -12.08016 & 0 \end{bmatrix} \|\hat{\boldsymbol{k}}\| \quad \text{for} \quad \frac{\hat{\boldsymbol{k}}}{\|\hat{\boldsymbol{k}}\|}=\tfrac{1}{\sqrt{2}}(1,1), \tag{D.6}$$

according to (5.30). We note that the transformed matrix $\widetilde{A_{pq}}$ is *the same* in both directions; however the applied "rotation" (5.29) is *different* in each case. This suggests a mixing of phonons that is dependent on $\hat{\boldsymbol{k}}/\|\hat{\boldsymbol{k}}\|$. By virtue of (D.5) and (D.6), we find that the "*parabola with cones*" model (6.19)–(6.20) applies uniformly in all perturbation directions.