

# Supplemental Materials for “Inverse design of phononic crystal with desired transmission via a gradient-descent approach”

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## THE TRANSMISSION IN TERMS OF NORMAL MODES

From the motion equation  $M\ddot{X} + KX = 0$ , we know that the amplitude  $X$  of the normal mode satisfies  $\omega^2 MX = KX$ . Let  $U = M^{\frac{1}{2}}X$ , then we can get  $\omega^2 U = M^{-\frac{1}{2}}KM^{-\frac{1}{2}}U$  which satisfies

$$F\Omega^2 F^\top = M^{-\frac{1}{2}}KM^{-\frac{1}{2}}, \quad (S1)$$

where eigenmatrix  $F_{ji} = e_j^i$  and eigenfrequencies  $\Omega_{ii} = \omega_i$ .

Define  $R = \Omega^2 - \omega^2 I$  and  $Z' = Z + \Sigma(\omega) = K - \omega^2 M$  where  $Z'_{1N}^* = Z_{1N}^*$  and  $I$  is identity matrix, then we obtain  $Z' = M^{\frac{1}{2}}FRF^\top M^{\frac{1}{2}}$ . Thus  $Z_{1N}^* = \text{Det}(MR)(M^{-\frac{1}{2}}FR^{-1}F^\top M^{-\frac{1}{2}})_{1N}$ . Then one can find

$$Z_{1N}^* = \frac{\text{Det}(MR)}{\sqrt{\gamma_L \gamma_R}} S_1 = 0, \quad (S2)$$

where  $S_1$  is given by

$$S_1 = \sum_{i=1}^N \frac{E_1^i E_N^i}{\omega_i^2 - \omega^2}. \quad (S3)$$

Next, we simplify  $\text{Det}(Z)$ . Due to the property of determinant, one has  $\text{Det}(Z) = \text{Det}(MF^\top M^{-\frac{1}{2}}ZM^{-\frac{1}{2}}F)$  and

$$F^\top M^{-\frac{1}{2}}ZM^{-\frac{1}{2}}F = R + A + B, \quad (S4)$$

where  $A = -i\frac{\gamma_L}{m_1}F_{(1,:)}^\top F_{(1,:)}$ ,  $B = -i\frac{\gamma_R}{m_N}F_{(N,:)}^\top F_{(N,:)}$ . The  $F_{(i,:)}$  means taking the  $i$ th row of matrix  $F$  as a vector.

Since  $R$  is a diagonal matrix and the rank of matrices  $A$  and  $B$  is 1, one can find

$$\text{Det}(R + A + B) = \text{Det}(R) \left[ 1 + \sum_{i=1}^N \frac{A_{ii} + B_{ii}}{R_{ii}} + \sum_{1=i<j}^N \frac{\text{Det} \begin{pmatrix} A_{ii} & B_{ij} \\ A_{ji} & B_{jj} \end{pmatrix} + \begin{pmatrix} B_{ii} & A_{ij} \\ B_{ji} & A_{jj} \end{pmatrix}}{R_{ii}R_{jj}} \right]. \quad (S5)$$

It results in

$$\text{Det}(Z) = \text{Det}(MR)(1 - i\omega S_3 - \omega^2 S_2), \quad (S6)$$

where  $S_2$  and  $S_3$  is given by

$$S_2 = \sum_{1=i<j}^N \frac{(E_1^i E_N^j - E_1^j E_N^i)^2}{(\omega_i^2 - \omega^2)(\omega_j^2 - \omega^2)}, \quad (S7)$$

$$S_3 = \sum_{i=1}^N \frac{(E_1^i)^2 + (E_N^i)^2}{\omega_i^2 - \omega^2}.$$

So far we have obtained  $Z_{1N}^*$  and  $\text{Det}(Z)$ . Finally, in terms of  $G_{1N} = Z_{1N}^*/\text{Det}(Z)$  and  $\mathcal{T}(\omega) = 4\gamma_L \gamma_R \omega^2 |G_{1N}|^2$ , one can get the transmission with respect to the normal mode as given by

$$\mathcal{T}(\omega) = \frac{4\omega^2 S_1^2}{(1 - \omega^2 S_2)^2 + \omega^2 S_3^2}. \quad (S8)$$

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