Appendix D

Detailed Errata for Geremia 2002

In this appendix, I will give a detailed account of the various flaws and errors in the original photonic inverse problem paper [67] published in Physical Review E in 2002. I feel strongly that these errors should be documented somewhere, and of course to the extent possible, I have corrected these in the work I have done subsequent to this paper. Unfortunately, as I was not an author in the original paper, I did not feel it was my place to publish an errata, nor did Dr. Geremia seem motivated to do so when I approached him with some of the initial errors. Nevertheless, if and when the decision is made to do so, this appendix provides a sufficiently detailed account that should be more than adequate for that purpose. Unless otherwise specified in this appendix, reference to equation and figure numbers are meant to be for those in Geremia 2002, while equation numbers beginning with the letter D refer to equations in this appendix.

D.1 Introduction

D.1.1 Relevant abstract of Geremia 2002

In Geremia 2002, optimal photonic crystal cavity design results were presented using an analytical 2D model, as well as a numerical 3D model. To date, there has not been further investigation on the 3D work, but the 2D results have been examined extensively. To summarize the work in Geremia 2002, the 2D analytical approach can

be separated into two distinct and separate steps. The first step is an optimization of the desired mode without consideration as to the dielectric that can generate the mode. The particular optimization that it claims to do is a maximization of pseudo-Q factor (Q) and electric field at the origin($E(0)$), and a minimization of mode volume (V). Quantitatively, this means a maximization of $\beta_Q Q+\beta_E E(0)-\beta_V V$, where the β's balance the importance of the various terms. Without loss of generality, β_Q is taken to be 1. The second step extracts the dielectric required to produce the optimized mode from step 1 by solving the inverse Helmholtz equation. The inverse Helmholtz equation is derived in the bulk mode basis into a set of linear equations. A 'radially symmetric' defect and an asymmetric defect design were provided as illustrations to the technique.

There are various errors or omissions in the description of the first step, the optimization of the desired mode. We will examine these in section D.2. The more critical error in the paper is in the derivation of the inverse Helmholtz equation which we will address in section D.3, and of course the most notable omission is the discussion of regularization. Before we can even address these errors though, it turns out there are some typographical errors in the equations. In order to make a comparison between the corrected version of the inverse Helmholtz equation and the ones in Geremia 2002, we first need to correct the typos. We will first assume that the derivation is correct and fix the typos in section D.1.2.

D.1.2 Typographical errors

The typos appear in equation 25 in the main text, and then A2, A3 and A4 in the appendix. Again, actual flaws in the reasoning will be addressed later. Following the reasoning outlined in the paper, we write out explicitly all the steps in full. We include it all here because the derivation is extremely cumbersome, particularly keeping track of all the indices. Of course, since the inverse problem is unstable, if you don't know about regularization, then even the correct equations will give bad answers, so at a practical level when trying to code up the equations, it was rather difficult trying to

catch these errors. Also keep in mind that these equations will ultimately be proven incorrect. The reader not interested in the grunge here can safely skip to section D.1.3 for the summary of the typos on page 144.

Detailed Steps of PRE Derivation

Recall the defect mode is expanded in the TE bulk mode basis

$$\mathbf{H}_m(\mathbf{r}) = \frac{1}{N}\sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}}\mathbf{H}_{n,\mathbf{k}}(\mathbf{r}) \tag{D.1}$$

where the bulk modes are computed in the plane wave expansion method:

$$\mathbf{H}_{n,\mathbf{k}}(\mathbf{r}) = \mathbf{z}\sum_{\mathbf{G}} h_{n,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \tag{D.2}$$

$$\int_{V_N} \mathbf{H}^*_{n',\mathbf{k}'}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r} = N\delta_{n,n'}\sum_{\mathbf{G}}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{G}} \tag{D.3}$$

The $\mathbf{z}$ vector will be omitted in the following notation for compactness unless required for completeness under curl operations. We start with Maxwell's equation, but separate out the defect dielectric from the unperturbed lattice:

$$\nabla\times\eta_0(\mathbf{r})\nabla\times\mathbf{H}_m(\mathbf{r}) + \nabla\times\delta\eta(\mathbf{r})\nabla\times\mathbf{H}_m(\mathbf{r}) = \frac{\omega_m^2}{c^2}\mathbf{H}_m(\mathbf{r}) \tag{D.4}$$

$$\nabla\times\eta_0(\mathbf{r})\nabla\times\mathbf{H}_m(\mathbf{r}) - \frac{\omega_m^2}{c^2}\mathbf{H}_m(\mathbf{r}) = -\nabla\times\delta\eta(\mathbf{r})\nabla\times\mathbf{H}_m(\mathbf{r}) \tag{D.5}$$

Next, substitute into equation (D.5) the defect and bulk mode expansion of equations (D.1) and (D.2), left multiply by $\mathbf{H}_{n'',\mathbf{k}''}$ and integrate over the size of the supercell. The left hand side (LHS) of equation (D.5) becomes

$$\frac{1}{N}\sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}}\frac{\omega^2_{n,\mathbf{k}}-\omega^2_m}{c^2}\int \mathbf{H}^*_{n'',\mathbf{k}''}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r}$$

Evaluating the right hand side (RHS) of equation (D.5) requires a (truncated) Fourier

expansion of the defect dielectric.

$$\delta\eta(\mathbf{r}) \equiv \sum_{\mathbf{k}} \delta\eta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

The $\mathbf{k}$ points used in the summation are the ones consistent with the specified Born-von Karman boundary conditions (i.e. geometry of the supercell), and the series is truncated with a finite number of reciprocal lattice vectors used to tile the reciprocal superlattice, identical to the truncation in calculating the band structure of the bulk lattice.

The RHS now becomes:

$$\begin{aligned}
& -\nabla \times \left(\sum_{\mathbf{k}'} \delta\eta_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r}} \right) \nabla \times \frac{1}{N} \sum_{n,\mathbf{k}} a_{n,\mathbf{k}}^{(m)} \mathbf{H}_{n,\mathbf{k}}(\mathbf{r}) \\
= & -\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} \nabla \times e^{i\mathbf{k}'\cdot\mathbf{r}} \left(\nabla \times \mathbf{z} \sum_{\mathbf{G}} h_{n,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \right) \\
= & -\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} \sum_{\mathbf{G}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} h_{n,\mathbf{k}+\mathbf{G}} \nabla \times e^{i\mathbf{k}'\cdot\mathbf{r}} \left(i(\mathbf{k}+\mathbf{G}) \times \mathbf{z} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \right) \\
= & -\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} \sum_{\mathbf{G}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} h_{n,\mathbf{k}+\mathbf{G}} \nabla \times e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \left(i(\mathbf{k}+\mathbf{G}) \times \mathbf{z} \right) \\
= & -\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} \sum_{\mathbf{G}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} h_{n,\mathbf{k}+\mathbf{G}} [i(\mathbf{k}'+\mathbf{k}+\mathbf{G})] \times [i(\mathbf{k}+\mathbf{G}) \times \mathbf{z}] e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \\
= & -\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} \sum_{\mathbf{G}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} h_{n,\mathbf{k}+\mathbf{G}} (\mathbf{k}'+\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}) e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \mathbf{z}
\end{aligned}$$

Next we left multiply by plane wave expansion of $\mathbf{H}_{n'',\mathbf{k}''}$ and integrate over the size

of the supercell again. (Omitting again the $\mathbf{z}$ vector for compactness)

$$
\begin{aligned}
& -\int \sum_{\mathbf{G}''} h^*_{n'',\mathbf{k}''+\mathbf{G}''} e^{-i(\mathbf{k}''+\mathbf{G}'')\cdot\mathbf{r}} \times \cdots \\
& \quad \left(\frac{1}{N} \sum_{\mathbf{k}'} \sum_{n,\mathbf{k}} \sum_{\mathbf{G}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} (\mathbf{k}'+\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}) h_{n,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \right) d\mathbf{r} \\
= & -\int \sum_{\mathbf{G}''} \frac{1}{N} \sum_{\mathbf{G},\mathbf{k}',n,\mathbf{k}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} (\mathbf{k}'+\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}) \times \cdots \\
& \qquad\qquad h^*_{n'',\mathbf{k}''+\mathbf{G}''} e^{-i(\mathbf{k}''+\mathbf{G}'')\cdot\mathbf{r}} h_{n,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} d\mathbf{r} \\
= & -\frac{1}{N} \sum_{\mathbf{G}'',\mathbf{G},\mathbf{k}',n,\mathbf{k}} a_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} (\mathbf{k}'+\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}) \times \cdots \\
& \qquad\qquad h^*_{n'',\mathbf{k}''+\mathbf{G}''} h_{n,\mathbf{k}+\mathbf{G}} \int e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}} d\mathbf{r} \\
= & -\frac{1}{N} \sum_{\mathbf{G}'',\mathbf{G},\mathbf{k}',n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}} \delta\eta_{\mathbf{k}'} (\mathbf{k}'+\mathbf{k}+\mathbf{G}) \cdot (\mathbf{k}+\mathbf{G}) \times \cdots \\
& \qquad\qquad h^*_{n'',\mathbf{k}''+\mathbf{G}''} h_{n,\mathbf{k}+\mathbf{G}} \int e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}} d\mathbf{r}
\end{aligned}
$$

We have now arranged Maxwell's equation with defect dielectric into equation (A3) of [67]. To get to equation (A4), we simply 'evaluate' the integrals and collapse the appropriate delta functions. The LHS of equation (A3) is :

$$
\begin{aligned}
& \frac{1}{N} \sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}} \frac{\omega^2_{n,\mathbf{k}} - \omega^2_m}{c^2} \int \mathbf{H}^*_{n'',\mathbf{k}''}(\mathbf{r}) \mathbf{H}_{n,\mathbf{k}}(\mathbf{r}) d\mathbf{r} \\
= & \sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}} \frac{\omega^2_{n,\mathbf{k}} - \omega^2_m}{c^2} \delta_{n'',n} \sum_{\mathbf{G}} \delta_{\mathbf{k}'',\mathbf{k}+\mathbf{G}} \text{ , using equation (D.3)} \\
= & \sum_{\mathbf{k}} a^{(m)}_{n'',\mathbf{k}} \frac{\omega^2_{n'',\mathbf{k}} - \omega^2_m}{c^2} \sum_{\mathbf{G}} \delta_{\mathbf{k}'',\mathbf{k}+\mathbf{G}}
\end{aligned}
$$

We note that by Bloch's theorem, $\omega_{n,\mathbf{k}} = \omega_{n,\mathbf{k}+\mathbf{G}}$, so we can in this instance substitute $\sum_{\mathbf{G}} \delta_{\mathbf{k}'',\mathbf{k}+\mathbf{G}}$ with $N\delta_{k'',k}$. Finally, we obtain the expression

$$
N a^{(m)}_{n'',\mathbf{k}''} \frac{\omega^2_{n'',\mathbf{k}''} - \omega^2_m}{c^2}
$$

The RHS of equation (A4) simply involves collapsing the integral into a delta function. Only note here is that since we are integrating over the supercell, we pick up a factor of N.

$$\int_V e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}} d\mathbf{r} = N\delta_{\mathbf{G},\mathbf{k}''+\mathbf{G}''-\mathbf{k}-\mathbf{k}'}$$

The RHS of equation (A3) after collapsing this delta function on $\mathbf{G} = \mathbf{k}'' + \mathbf{G}'' - \mathbf{k} - \mathbf{k}'$ is

$$\begin{aligned}
& -\frac{1}{N}\sum_{\mathbf{G},\mathbf{G}''}\sum_{\mathbf{k}'}\sum_{n,\mathbf{k}} a_{n,\mathbf{k}}^{(m)}\delta\eta_{\mathbf{k}'}(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G})\times\ldots \\
& \qquad\qquad h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}+\mathbf{G}}\int e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}}d\mathbf{r} \\
= & -\sum_{\mathbf{G}''}\sum_{\mathbf{k}'}\sum_{n,\mathbf{k}} a_{n,\mathbf{k}}^{(m)}\delta\eta_{\mathbf{k}'}(\mathbf{k}''+\mathbf{G}''-\mathbf{k}')\cdot(\mathbf{k}''+\mathbf{G}'')\times h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}''+\mathbf{G}''-\mathbf{k}'} \\
= & -\sum_{\mathbf{G}''}\sum_{\mathbf{k}'}\sum_{n,\mathbf{k}} a_{n,\mathbf{k}}^{(m)}h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}''+\mathbf{G}''-\mathbf{k}'}(\mathbf{k}''+\mathbf{G}''-\mathbf{k}')\cdot(\mathbf{k}''+\mathbf{G}'')\delta\eta_{\mathbf{k}'}
\end{aligned}$$

Multiply the collapsed versions of equation (A3) by $-\frac{1}{N}$ to recover equation (A4). Next we note as in equation (A5) that we can fold summations over $\mathbf{k}$ back into the First Brillouin zone using the identity:

$$\sum_{n,\mathbf{k}} a_{n,\mathbf{k}}^{(m)} = N\sum_{n,\mathbf{q}} a_{n,\mathbf{q}}^{(m)}$$

Next we make the following index transformations: $n \to n'$, $\mathbf{G}'' \to \mathbf{G}$, $n'' \to n$. We also collapse $\mathbf{k}$ to $\mathbf{q}'$ using the above identity, and rename $\mathbf{k}'$ to $\mathbf{k}$. Finally we restrict the indices $\mathbf{k}''$ to within the first Brillouin zone, and rename it $\mathbf{q}$, since they are not summed.

The LHS of equation (A4) is:

$$\begin{aligned}
& \frac{1}{N}\sum_{\mathbf{G}''}\sum_{\mathbf{k}'}\sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}} h^{*}_{n'',\mathbf{k}''+\mathbf{G}''} h_{n,\mathbf{k}''+\mathbf{G}''-\mathbf{k}'}(\mathbf{k}''+\mathbf{G}''-\mathbf{k}')\cdot(\mathbf{k}''+\mathbf{G}'')\delta\eta_{\mathbf{k}'} \\
= & \sum_{\mathbf{G}}\sum_{\mathbf{k}}\sum_{n',\mathbf{q}'} a^{(m)}_{n',\mathbf{q}'} h^{*}_{n,\mathbf{q}+\mathbf{G}} h_{n',\mathbf{q}+\mathbf{G}-\mathbf{k}}(\mathbf{q}+\mathbf{G}-\mathbf{k})\cdot(\mathbf{q}+\mathbf{G})\delta\eta_{\mathbf{k}} \\
= & \sum_{\mathbf{k}}\left\{\sum_{\mathbf{G}}\sum_{n',\mathbf{q}'} a^{(m)}_{n',\mathbf{q}'} h^{*}_{n,\mathbf{q}+\mathbf{G}} h_{n',\mathbf{q}+\mathbf{G}-\mathbf{k}}(\mathbf{q}+\mathbf{G}-\mathbf{k})\cdot(\mathbf{q}+\mathbf{G})\right\}\delta\eta_{\mathbf{k}} \\
\equiv & \sum_{\mathbf{k}} D^{(m)}_{n,\mathbf{q};\mathbf{k}}\delta\eta_{\mathbf{k}}
\end{aligned}$$

Finally the RHS of equation (A4) is:

$$\begin{aligned}
& -a^{(m)}_{n'',\mathbf{k}''}\frac{\omega^2_{n'',\mathbf{k}''}-\omega^2_m}{c^2} \\
= & \; a^{(m)}_{n,\mathbf{q}}\frac{\omega^2_m-\omega^2_{n,\mathbf{q}}}{c^2}
\end{aligned}$$

This gives us equation (24) as desired, with the inversion matrix D given by equation (25).

D.1.3 Proposed typographical errata

Equation 25 should read:

$$D^{(m)}_{n,\mathbf{q};\mathbf{k}} = \sum_{n'}\sum_{\mathbf{G},\mathbf{q}'} a^{(m)}_{n'\mathbf{q}'} h^{*}_{n,\mathbf{q}+\mathbf{G}} h_{n',\mathbf{q}+\mathbf{G}-\mathbf{k}} \times (\mathbf{q}+\mathbf{G})\cdot(\mathbf{q}+\mathbf{G}-\mathbf{k})$$

rather than

$$D^{(m)}_{n,\mathbf{q};\mathbf{k}} = \sum_{n'}\sum_{\mathbf{G},\mathbf{q}'} a^{*}_{n'\mathbf{q}'} h^{*}_{n,\mathbf{q}+\mathbf{G}} h_{n',\mathbf{q}'+\mathbf{G}-\mathbf{k}'} \times (\mathbf{q}+\mathbf{G})\cdot(\mathbf{q}+\mathbf{G}-\mathbf{k}')$$

Equation A2 should read:

$$\int_{V_N} \mathbf{H}^*_{n',\mathbf{k}'}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r} = N\delta_{n',n}\sum_{\mathbf{G}}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{G}}$$

rather than

$$\int_{V_N} \mathbf{H}^*_{n',\mathbf{k}'}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r} = \delta_{n',n}\sum_{\mathbf{G}}\delta_{\mathbf{k}',\mathbf{k}+\mathbf{G}}$$

Equation A3 should read:

$$\begin{aligned}
&\frac{1}{N}\sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}}\frac{\omega^2_{n,\mathbf{k}}-\omega^2_m}{c^2}\int \mathbf{H}^*_{n'',\mathbf{k}''}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r}\\
= \;& -\frac{1}{N}\sum_{\mathbf{k}'}\sum_{n,\mathbf{k}}\sum_{\mathbf{G},\mathbf{G}''} a^{(m)}_{n,\mathbf{k}}\delta\eta_{\mathbf{k}'}h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}+\mathbf{G}}\cdots\\
&\qquad\times(\mathbf{k}'+\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G})\int e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}}d\mathbf{r}
\end{aligned}$$

rather than

$$\begin{aligned}
&\frac{1}{N}\sum_{n,\mathbf{k}} a^{(m)}_{n,\mathbf{k}}\frac{\omega^2_{n,\mathbf{k}}-\omega^2_m}{c^2}\int \mathbf{H}^*_{n'',\mathbf{k}''}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r}\\
= \;& \frac{1}{N}\sum_{\mathbf{k}}\sum_{n,\mathbf{k}}\sum_{\mathbf{G},\mathbf{G}''} a^{(m)}_{n,\mathbf{k}}\delta\eta_{\mathbf{k}}h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}+\mathbf{G}}\cdots\\
&\qquad\times(\mathbf{k}''+\mathbf{G}'')\cdot(\mathbf{k}''+\mathbf{G}''-\mathbf{k}')\int e^{i(\mathbf{k}'+\mathbf{k}+\mathbf{G}-\mathbf{k}''-\mathbf{G}'')\cdot\mathbf{r}}d\mathbf{r}
\end{aligned}$$

Equation A4 should read:

$$\begin{aligned}
&\frac{1}{N}\sum_{n,\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{G}''} a^{(m)}_{n,\mathbf{k}}\delta\eta_{\mathbf{k}'}h^*_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{k}''+\mathbf{G}''-\mathbf{k}'}(\mathbf{k}''+\mathbf{G}'')\cdot(\mathbf{k}''+\mathbf{G}''-\mathbf{k}')\\
= \;& -a^{(m)}_{n'',\mathbf{k}''}\frac{\omega^2_{n'',\mathbf{k}''}-\omega^2_m}{c^2}
\end{aligned}$$

rather than

$$\begin{aligned} & \frac{1}{N}\sum_{n,\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{G}''} a^{(m)}_{n,\mathbf{k}}\delta\eta_{\mathbf{k}'}h^{*}_{n'',\mathbf{k}''+\mathbf{G}''}h_{n,\mathbf{G}''-\mathbf{k}'}(\mathbf{k}''+\mathbf{G}'')\cdot(\mathbf{k}''+\mathbf{G}''-\mathbf{k}') \\ = \quad & -\frac{1}{N}a^{(m)}_{n'',\mathbf{k}''}\frac{\omega^2_{n'',\mathbf{k}''}-\omega^2_m}{c^2} \end{aligned}$$

D.2 Mode Optimization Errors

The three physical quantities that were optimized were maximizing **E** field intensity at the central defect location, minimizing the mode volume, and maximizing the Q factor. In the paper, the optimization is performed using Lagrange multipliers. Equation (23) from the paper states:

$$\sum_{n',\mathbf{q}'}\left[\frac{\omega_{n',\mathbf{q}'}\omega_{n,\mathbf{q}}}{qq'}+\beta_I H^{*}_{n',\mathbf{q}'}(0)H_{n,\mathbf{q}}(0)-\beta_V\langle\psi_{n',\mathbf{q}'}|\psi_{n,\mathbf{q}}\rangle\right]a^{(m)}_{n',\mathbf{q}'}=\Lambda a_{n,\mathbf{q}}$$

The first term maximizes Q by removing bulk mode contribution above the light-line, the second term maximizes the intensity at the origin, and the final term minimizes the mode volume. As it appears in the paper, it is unclear how it actually optimizes any of the three quantities. We will address each expression in the next sections.

D.2.1 *Q* factor

The Q factor optimization incorrectly applies the lightline model to mimic the behavior of the cavity Q. The light cone rule of thumb originates from the idea of lossy modes coupling into free space. The relevant traits that describe modes lying above the light line (lossy modes) is that they have high frequencies and small in-plane fourier components. For a defect mode of a given frequency, correct application of this rule of thumb is to restrict fourier components lying within a small circle (sphere in 3D) in k-space determined by the mode frequency. This is the approach consistent with Oskar Painter's group [9]. So there are two errors in using the frequency of the

associated bulk mode and its quasi k-vector in determining where it lies in relation to the light line. The first point is that the actual frequency of the defect free bulk mode is irrelevant, since we are trying to determine the lossiness of the *defect mode*. Hence only the *defect mode frequency* will give the relevant coupling condition. Secondly, it is the fourier components that compose the mode that is relevant, and not the quasi k-vector. A bulk mode in fact is composed of the fourier components of the k-vector in the first Brillouin zone as well as all others by addition of reciprocal lattice vectors. In fact, many of the upper band bulk modes actually have large fourier components, and are minimally lossy (i.e. minimal, though finite contribution from small fourier components). A reduced zone scheme picture is actually rather deceptive in trying to visualize the light line. On the other hand, the bulk modes originating from the low lying bands (of which most of the 'optimized' modes are composed) actually have a significant amount of small fourier components. Therefore, if one were to use these low lying bulk modes to form a defect mode, since the defect frequency is in the band gap, these contributions are in fact highly lossy due to the expanded region of unfavorable k-space. In misapplying the light line constraint, the optimization should make things worse by incorporating more of these low lying modes. Finally, this analysis ignores the fact that coherent superposition of lossy bulk modes can lead to cancellation of small (i.e. leaky) fourier components. Going back to our linear algebra language, the bulk modes are a non-diagonalized basis for the purpose of Q factor considerations. The point is moot when only using 5 layers of photonic crystal as in [67], because there are so few small fourier components for such a small supercell (although note the observation in section D.4 about figures 3 and 5).

D.2.2 E field intensity

In the paper, it is unclear whether it is the **H** field or the **E** field that actually gets optimized. The equations in the paper throughout only show expressions for the **H** field (cf. eqns. (5,21,23)), whereas the plots in the results section show the **E** field. One can obtain the **E** field by taking the curl of **H**, but because TE polarization

is assumed, the **E** field lies in the xy-plane (as opposed to the H field which only has z components), it must be treated as a vector quantity. The expression for the **E** optimization is not discussed in the paper. One way to treat this is to allow for vectored expansion coefficients for the optimized **E**, but then it is not immediately obvious that the Lagrange multipliers method is applicable. Convex optimization cannot be applied here either because the norm of **E(0)** is convex, and we cannot maximize a convex function using convex optimization. In fact, the local extremum of a norm must be a local minimum, so the global maximum must be some end point. In any case, equations (23) in the paper is an incorrect expression for a cavity mode optimization, since maximizing the **H** field intensity will yield a zero **E** field at the origin.

D.2.3 Mode volume

There are also problems with the expression for the mode volume optimization in the paper. Again, there is the ambiguity over whether it is the **H** field or **E** field that is optimized (cf. eqns. (4,19,20,23)). Even if we were to assume that it is sufficient to minimize the mode volume of **H** to get the desired result, the expressions are still incorrect. In the paper, ψ refers to a max 1 normalized mode function that satisfies

$$\mathbf{H}_j(\mathbf{r}) = \mathbf{H}_{0,j}\psi_j(\mathbf{r}),$$

where j is some mode index, and $|\psi(\mathbf{r})|_{\max} = 1$. The mode volume for the mode j is then

$$V_j = \int |\psi_j(\mathbf{r})|^2 d\mathbf{r}$$

The expression so far is fine. However, directly evaluating the mode volume by an expansion as the paper attempts to do in equation (19)

$$V_m = \sum_{n',\mathbf{q}'} \sum_{n,\mathbf{q}} a^{(m)*}_{n',\mathbf{q}'} a^{(m)}_{n,\mathbf{q}} \langle \psi_{n',\mathbf{q}'}(\mathbf{r}) | \psi_{n,\mathbf{q}}(\mathbf{r}) \rangle + c.c.$$

is in fact not so straightforward, and unfortunately incorrect. The corresponding normalization constant $\mathbf{H}_{0,m}$ for the mode m cannot be determined without first doing the summation. Using equation (14) as the expansion for the target mode implies:

$$\begin{aligned} \mathbf{H_m}(\mathbf{r}) &= \sum_n \sum_{\mathbf{q}\in BZ} a^{(m)}_{n,\mathbf{q}} \mathbf{H}_{n,\mathbf{q}}(\mathbf{r}) && \text{(D.6)} \\ &= \mathbf{H_{0,m}}(\mathbf{r})\psi_m(\mathbf{r}) && \text{(D.7)} \end{aligned}$$

Eqn. (D.7) explicitly shows equation (19) is incorrect because

$$\psi_m(\mathbf{r}) \neq \sum_n \sum_{\mathbf{q}\in BZ} a^{(m)}_{n,\mathbf{q}} \psi_{n,\mathbf{q}}(\mathbf{r}) \qquad \text{(D.8)}$$

A simple example that illustrates the error is to choose any basis that has all of its basis functions max 1 normalized, such as the plane wave basis. In such a basis, the RHS of eqn. (D.8) is identically $\mathbf{H_m}(\mathbf{r})$, which is clearly not max 1 normlized in general (hence it cannot equal $\psi_m(\mathbf{r})$ by definition). All equation (19) represents is in fact $\int |\mathbf{H}'_m(\mathbf{r})|^2 d\mathbf{r}$, for some unnormalized mode $\mathbf{H}'_m$, uncorrelated with the actual mode volume. The physical meaning of this term as written in the paper is unclear, but it does skew the optimized mode with some completely undesired effect.

As it turns out, formulating the mode volume minimization is actually unnecessary in this case. By imposing an energy constraint to the optimization, a maximized E field will necessarily have minimum mode volume. If we think about this carefully, it is clear since the point of minimizing mode volume is to maximize the electric field strength per photon. An energy constraint can be imposed by normalizing the expansion coefficients. Obviously in the E field maximization step, this is already done, otherwise by scaling the coefficients, we can increase $\mathbf{E}(\mathbf{0})$ without bound. In other applications where one cannot avoid dealing with the mode volume directly, it would be prudent to exercise more caution in its treatment.

A final comment about the optimization procedure concerns the weighting factors (β's). At the conclusion of Section III-C, it talks about optimizing over the β_i coeffi-

cients, and the idea presented is to nest the inverse equation (equation (24)) within an outer β_i optimization loop. However, a performance metric for the β_i's is not provided (not even a qualitative comment on what makes a set of β better than another set.) If it is just to maximize the $\mathcal{I}$ function (i.e. the total objective function shown in equation (8)) over all combinations of β's, then that seems to defeat the purpose of having those coefficients in the first place. These coefficients enforce the fact that there are tradeoffs between the different properties. $\mathcal{I}$ can be made large if one sets $\beta_V = 0$, effectively removing the requirement for having small mode volume. We simply could not ascertain as to what exactly the algorithm was optimizing. Section III-E and III-F explain that a conjugate-gradient algorithm is used for the optimization with the inverse problem nested within it. No explanations were presented as to why this nesting was necessary, nor how it would be accomplished. For example, how is the solution of the inverse problem (eqn. (24)) used in the subsequent iteration? One would expect that it involves evaluating the gradient of the matrix D with respect to β somehow, but eqn. (24) depends on β implicitly through the mode expansion coefficients $a_{n,q}$. Eqn. (23) shows us that the $a_{n,q}$'s are eigenvectors to an eigenvalue problem parameterized in part by the β's. The study of the rotation of eigenvectors due to perturbations to its operator is not a simple matter [78], so it is not obvious or clear how one might evaluate the gradient.

D.3 Inversion Errors

The second step of the design algorithm involved inverting the Helmholtz equation using the bulk modes as a basis in the paper. From the discussion of the Q factor optimization in section D.2, it is clear that the bulk mode basis is not a natural basis for this problem. As we saw in chapter 6, inverting the equation in the plane wave basis (the natural basis for Q factor type considerations) actually gives a very simple and concise result. Treatment in the bulk mode basis was unnecessarily messy and convoluted, further complicated by the decision to sum over multiple Brillouin zones. Consequently, the derivation gave rise to terms that include $\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})$. The

term $\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})$ is actually rather awkward to interpret, since the purpose of the band index is to reduce all $\mathbf{k}$-vectors into the first Brillouin zone. It is ambiguous what is really meant to run the $\mathbf{k}$-vectors through the entire $\mathbf{k}$-space and still have a band index. Ignoring the strange notation and continuing to expand the bulk mode shows that the assumed orthogonality relation in equation (A2)

$$\int_{V_N} \mathbf{H}^*_{n',\mathbf{k}'}(\mathbf{r})\mathbf{H}_{n,\mathbf{k}}(\mathbf{r})d\mathbf{r} = \delta_{n,n'} \sum_{\mathbf{G}} \delta_{\mathbf{k}',\mathbf{k}+\mathbf{G}}$$

is invalid and therefore misused in the derivation of the inversion equations. A casual examination of this relation would lead us to believe that it appears correct, save for the missing normalization factor of N for repeating the summation over multiple Brillouin zones (see corrected equation (A2) on page 145). However, if we really try to rigorously write down what this notation is supposed to mean, the subtle errors turn out to be quite significant. I will use an example to illustrate.

First, let us revisit the concept of the band index and the $\mathbf{q}$'s in the first Brillouin zone. The number of bands is equivalent to the number of Brillouin zones (BZ) in $\mathbf{k}$-space, which is the same as the number $\mathbf{G}$-vectors we keep. For a truncated $\mathbf{k}$-space, this implies that the total number of $\mathbf{k}$-points in the computational domain is equal to $N_G \times N_q$, where N_G is the number of $\mathbf{G}$-vectors and N_q is the number of wavevectors in the first BZ. Therefore, the label $\{n, q\}$ can be mapped to k by the relation $\mathbf{k}_{n,q} = \mathbf{q} + \mathbf{G}_n$. We explicitly label $\mathbf{k}$ with the subscripts to help us designate where it comes from. This implies that the term

$$\begin{aligned} \mathbf{H}_{n,\mathbf{k}} &= \mathbf{H}_{n,\mathbf{k}_{n',q}} \\ &= \mathbf{H}_{n,\mathbf{q}+\mathbf{G}_{\mathbf{n}'}} \\ &= \mathbf{H}_{n'',\mathbf{q}} \\ \text{where } \mathbf{G}_{n''} &= \mathbf{G}_n + \mathbf{G}_{n'} \end{aligned}$$

Of course, there are no guarantees as to whether $\mathbf{G}_{n''}$ is within the truncated set or not. The reader can refer to appendix C for proper and improper ways of handling

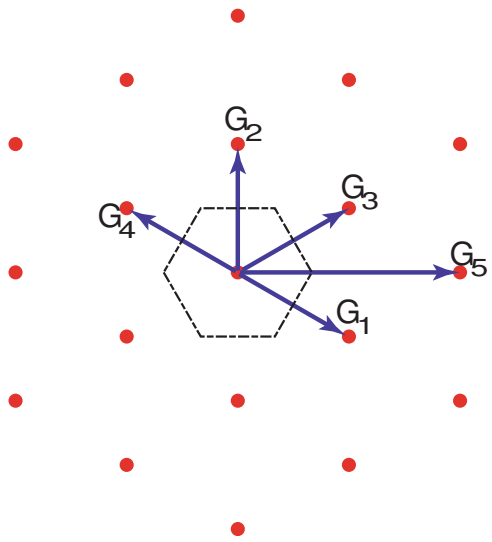

Figure D.1: The dotted line outlines the first Brillouin zone of the defect free bulk photonic lattice in **k**-space, and the red dots are the lattice sites of the reciprocal lattice. As shown above, $\mathbf{G}_3 = \mathbf{G}_1 + \mathbf{G}_2 = \mathbf{G}_4 + \mathbf{G}_5$.

these terms, as this is not addressed in the paper. There are problems even if we do not exceed the truncation domain. Suppose we have a set of $\mathbf{G}$ such that $\mathbf{G}_1 + \mathbf{G}_2 = \mathbf{G}_4 + \mathbf{G}_5 = \mathbf{G}_3$ as illustrated in figure D.1, and consider

$$\mathbf{H}^*_{n_1,\mathbf{k_1}}\mathbf{H}_{n_2,\mathbf{k_2}} = \mathbf{H}^*_{n_1,\mathbf{k}_{n_1',q}}\mathbf{H}_{n_2,\mathbf{k}_{n_2',q}} = \mathbf{H}^*_{n_1'',\mathbf{q}}\mathbf{H}_{n_2'',\mathbf{q}}$$

Let

$$\begin{aligned} n_1 &= 1, \qquad n_1' = 2 \\ n_2 &= 4, \qquad n_2' = 5 \\ \therefore n_1'' &= n_2'' = 3 \end{aligned}$$

So $\mathbf{H}_{n_1,\mathbf{k_1}} = \mathbf{H}_{n_2,\mathbf{k}_2}$, but according to equation (A2), these are orthogonal to each other since $n_1 \neq n_2$. The other scenario would be if we choose $n_1 = n_2$, but $n_1' \neq n_2'$ such that $n_1'' \neq n_2''$. The two modes should actually be orthogonal, but the RHS of equation (A2) would still sum to 1. Getting this orthogonality condition wrong will lead to an incorrect set of inversion equations.

Of course, we have already shown that the better way to do the inversion is to stay in the plane wave basis. However, to show that the derivation in Geremia 2002 is indeed incorrect, we will now rederive the inversion equation in the bulk mode basis, but done properly with the right orthogonality condition. As a final comment, it should be pointed out that besides the fact that the plane wave basis is the natural basis for Q factor considerations, it turns out that from a computation point of view, formulating the inversion problem in the bulk mode basis is also significantly less efficient. Geremia 2002 reports a N^5 scaling for forming the D matrix, whereas in the plane wave basis, forming our inversion matrix scales as a more reasonable N^2. There appears to be no apparent advantage nor any compelling reason to use the bulk mode basis for any of this work.

D.3.1 Correct derivation in the bulk mode basis

We start with Maxwell's equation, but separate out the defect dielectric from the unperturbed lattice:

$$\nabla \times \eta_0(\mathbf{r}) \nabla \times \mathbf{H}_m(\mathbf{r}) + \nabla \times \delta\eta(\mathbf{r}) \nabla \times \mathbf{H}_m(\mathbf{r}) = \frac{\omega_m^2}{c^2} \mathbf{H}_m(\mathbf{r}) \tag{D.9}$$

$$\nabla \times \eta_0(\mathbf{r}) \nabla \times \mathbf{H}_m(\mathbf{r}) - \frac{\omega_m^2}{c^2} \mathbf{H}_m(\mathbf{r}) = -\nabla \times \delta\eta(\mathbf{r}) \nabla \times \mathbf{H}_m(\mathbf{r}) \tag{D.10}$$

We recall that $\delta\eta(\mathbf{r})$ and $\mathbf{H}_m(\mathbf{r})$ can be expanded as:

$$\mathbf{H}_m(\mathbf{r}) \equiv \sum_B a_B \mathbf{H}_B(\mathbf{r}) \tag{D.11}$$

$$\delta\eta(\mathbf{r}) \equiv \sum_{\mathbf{k}} \delta\eta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{D.12}$$

The a_B are the expansion coefficients of the defect mode in the bulk mode basis, $\mathbf{H}_B(\mathbf{r})$ are the bulk modes of the perfect lattice, and the $\mathbf{k}$ points used in the summation are the ones consistent with the specified Born-von Karman boundary conditions (i.e. geometry of the supercell.) The series is truncated with a finite number of reciprocal lattice vectors used to tile the reciprocal superlattice, identical to the truncation in

calculating the band structure of the bulk lattice. The bulk modes are computed in the plane wave basis, and we recall the properties of the bulk modes for a defect-free lattice. The notation that is used here is slightly different than the usual one, so we will elaborate slightly for the sake of clarity. For a defect-free bulk photonic crystal, the usual notation labels all modes by a band index n and a wave vector in the First Brillouin zone $\mathbf{q}$, and the bulk mode label B replaces the $\{n, q\}$ notation. Bulk modes of different bands and/or different $\mathbf{q}$ are orthogonal to one another. In the plane wave expansion method, each $\mathbf{q}$ yields an independent $N_G \times N_G$ eigenvalue problem of the form

$$\widehat{\mathbf{\Theta}}_{\mathbf{q}}\mathbf{h}_{n,\mathbf{q}} = \frac{\omega_{n,\mathbf{q}}}{c^2}\mathbf{h}_{n,\mathbf{q}} \tag{D.13}$$

$$\mathbf{H}_{B_{n,q}}(r) \equiv \mathbf{H}_{n,\mathbf{q}}(r) = \sum_{\mathbf{G}} \mathbf{h}_{n,\mathbf{q}+\mathbf{G}} e^{i(\mathbf{q}+\mathbf{G})\cdot r} \tag{D.14}$$

with the components of the eigenvectors acting as the expansion coefficient for the associated mode. In the supercell method, the Brillouin zone of the superlattice is reduced so that it contains only a single $\mathbf{k}$ point, and in fact, the $\{\mathbf{k}\}$ become the reciprocal lattice vectors (i.e. $\{\mathbf{G}\}$ in the bulk scenario) for the supercell. The eigenvalue problem now involves all $\mathbf{k}$ vectors, and there is only a single $\mathbf{q} = \mathbf{0}$. For a defect-free lattice in the supercell description, the independence of the bulk modes imply that the operator can be expressed in block diagonal form

$$\widehat{\mathbf{\Theta}}^{supercell}_{\mathbf{q=0}} = \widehat{\mathbf{\Theta}}_{\mathbf{q_1}} \oplus \widehat{\mathbf{\Theta}}_{\mathbf{q_2}} \oplus \widehat{\mathbf{\Theta}}_{\mathbf{q_3}} \oplus \cdots \oplus \widehat{\mathbf{\Theta}}_{\mathbf{q_n}} \tag{D.15}$$

if the $\mathbf{k}$ are ordered such that

$$\{\mathbf{k_1}, \ldots, \mathbf{k_N}, \mathbf{k_{N+1}}, \ldots, \mathbf{k_{2N}}, \ldots, \mathbf{k_{n\times N}}\}$$

correspond to

$$\{\mathbf{q_1} + \mathbf{G_1}, \ldots, \mathbf{q_1} + \mathbf{G_N}, \mathbf{q_2} + \mathbf{G_1}, \ldots, \mathbf{q_2} + \mathbf{G_N}, \ldots, \mathbf{q_n} + \mathbf{G_N}\}$$

Therefore, our plane wave expansion of the bulk modes will be expressed as

$$\mathbf{H}_B(\mathbf{r}) = \sum_{\mathbf{k}} h_{B,\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

The orthogonality relation is therefore

$$\int_{s.c.} \mathbf{H}^*_B(\mathbf{r})\mathbf{H}_{B'}(\mathbf{r})dr = N\delta_{B,B'} \tag{D.16}$$

where the area of the supercell is N times that of the bulk unit cell.

We left multiply equation (D.5) by $\mathbf{H}^*_{B''}(\mathbf{r})$ and integrate to obtain for the LHS:

$$\begin{aligned}
& \int \mathbf{H}^*_{B''}(\mathbf{r}) \left[\nabla \times \eta_0(\mathbf{r})\nabla \times \mathbf{H}_m(\mathbf{r}) - \frac{\omega_m^2}{c^2}\mathbf{H}_m(\mathbf{r})\right] dr \\
= & \int \mathbf{H}^*_{B''}(\mathbf{r}) \left[-\frac{\omega_m^2}{c^2} + \nabla \times \eta_0(\mathbf{r})\nabla\times\right] \sum_{B'} a_{B'}\mathbf{H}_{B'}(\mathbf{r}) \\
= & \sum_{B'} a_{B'} \left(\frac{\omega_{B'}^2 - \omega_m^2}{c^2}\right) \int \mathbf{H}^*_{B''}\mathbf{H}_{B'} dr \\
= & N\left(a_{B''}\frac{\omega_{B''}^2 - \omega_m^2}{c^2}\right)
\end{aligned}$$

The right hand side becomes:

$$\begin{aligned}
& -\int \mathbf{H}^*_{B''}(\mathbf{r}) \left[\nabla \times \delta\eta(\mathbf{r})\nabla \times \mathbf{H}_m(\mathbf{r})\right] dr \\
= & -\int \mathbf{H}^*_{B''}(\mathbf{r}) \left[\sum_{\mathbf{k},B} a_B \nabla \times \delta\eta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla \times \mathbf{H}_B(\mathbf{r})\right] dr \\
= & -\int \mathbf{H}^*_{B''}(\mathbf{r}) \left[\sum_{\mathbf{k},\mathbf{k}',B} a_B \nabla \times \delta\eta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla \times h_{B,\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r}}\right] dr \\
= & -\int \mathbf{H}^*_{B''}(\mathbf{r}) \left[\sum_{\mathbf{k},\mathbf{k}',B} a_B \delta\eta_{\mathbf{k}} h_{B,\mathbf{k}'} (\mathbf{k}+\mathbf{k}')\cdot(\mathbf{k}') e^{i\mathbf{k}\cdot\mathbf{r}}\right] dr \\
= & -\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}'',B} h^*_{B'',\mathbf{k}''} a_B \delta\eta_{\mathbf{k}} h_{B,\mathbf{k}'} (\mathbf{k}+\mathbf{k}')\cdot(\mathbf{k}') \int e^{i(\mathbf{k}+\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{r}} dr \\
= & -N \sum_{\mathbf{k},\mathbf{k}'',B} a_B \delta\eta_{\mathbf{k}} h^*_{B'',\mathbf{k}''} h_{B,\mathbf{k}''-\mathbf{k}} (\mathbf{k}'')\cdot(\mathbf{k}''-\mathbf{k})
\end{aligned}$$

where on the last line we have chosen to collapse $\mathbf{k}'$ onto $\mathbf{k}'' - \mathbf{k}$.

Equation (D.10) then becomes

$$\begin{aligned}\sum_{\mathbf{k}} \left(\sum_{\mathbf{k}'',B} a_B h^*_{B'',\mathbf{k}''} h_{B,\mathbf{k}''-\mathbf{k}}(\mathbf{k}'') \cdot (\mathbf{k}'' - \mathbf{k}) \right) \delta\eta_{\mathbf{k}} &= a_{B''} \frac{\omega_m^2 - \omega_{B''}^2}{c^2} \\ \sum_{\mathbf{k}} \mathbf{D}_{B'',\mathbf{k}} \delta\eta_{\mathbf{k}} &= a_{B''} \frac{\omega_m^2 - \omega_{B''}^2}{c^2}\end{aligned}$$

$$\text{where} \qquad \mathbf{D}_{B'',\mathbf{k}} \equiv \sum_{\mathbf{k}'',B} a_B h^*_{B'',\mathbf{k}''} h_{B,\mathbf{k}''-\mathbf{k}}(\mathbf{k}'') \cdot (\mathbf{k}'' - \mathbf{k}) \tag{D.17}$$

D.3.2 Compare with PRE derivation

We are finally ready to compare our results here with the previously obtained expression. We will need to translate our notation again so that a valid comparison of the inversion matrix $\mathbf{D}$ can be made. The sum over the bulk modes B is equivalent to all $(n, \mathbf{q})$ pairs in the original notation, while the sum over $\mathbf{k}''$ will be converted to a double sum over $(\mathbf{q}', \mathbf{G})$ with $\mathbf{k}'' = \mathbf{q}' + \mathbf{G}$. Therefore, equation (D.17) can be rewritten as:

$$\mathbf{D}_{n'',\mathbf{q}'';\mathbf{k}''} = \sum_{\mathbf{q}',\mathbf{G},\mathbf{q},n} a_{n\mathbf{q}} h^*_{n''\mathbf{q}'',\mathbf{q}'+\mathbf{G}} h_{n\mathbf{q},\mathbf{q}'+\mathbf{G}-\mathbf{k}}(\mathbf{q}' + \mathbf{G}) \cdot (\mathbf{q}' + \mathbf{G} - \mathbf{k}) \tag{D.18}$$

Relabelling the indices $\{n, \mathbf{q}\} \to \{n', \mathbf{q}'\}$, $\{\mathbf{q}' \to \mathbf{q}''\}$, and $\{n'', \mathbf{q}''\} \to \{n, \mathbf{q}\}$ produces

$$\mathbf{D}_{n,\mathbf{q};\mathbf{k}} = \sum_{\mathbf{q}'',\mathbf{G},n',\mathbf{q}'} a_{n'\mathbf{q}'} h^*_{n\mathbf{q},\mathbf{q}''+\mathbf{G}} h_{n'\mathbf{q}',\mathbf{q}''+\mathbf{G}-\mathbf{k}}(\mathbf{q}'' + \mathbf{G}) \cdot (\mathbf{q}'' + \mathbf{G} - \mathbf{k}) \tag{D.19}$$

$$\neq \mathbf{D}_{n,\mathbf{q};\mathbf{k}} = \sum_{n',\mathbf{G},\mathbf{q}'} a_{n'\mathbf{q}'} h^*_{n\mathbf{q}+\mathbf{G}} h_{n',\mathbf{q}+\mathbf{G}-\mathbf{k}}(\mathbf{q} + \mathbf{G}) \cdot (\mathbf{q} + \mathbf{G} - \mathbf{k}) \tag{D.20}$$

where equation (D.20) is the old expression. The $\mathbf{q}''$ does not appear in the old expression, so we will have to look more closely at certain terms to reveal what the index is actually doing. We note that in equation (D.19),

$$h^*_{n\mathbf{q},\mathbf{q}''+\mathbf{G}} = 0 \quad \text{if} \quad \mathbf{q} \neq \mathbf{q}''$$

since the indices $(n, \mathbf{q})$ represent the bulk mode obtained from the $\mathbf{q}$ eigenvalue problem, independent of all other $\{\mathbf{q}''\}$'s. Therefore,

$$h^*_{n\mathbf{q},\mathbf{q}''+\mathbf{G}} = h^*_{n\mathbf{q},\mathbf{q}''+\mathbf{G}}\delta_{\mathbf{q},\mathbf{q}''}$$

and the sum over $\mathbf{q}''$ in equation (D.19) collapses to produce

$$\mathbf{D}_{n,\mathbf{q};\mathbf{k}} = \sum_{n',\mathbf{G},\mathbf{q}'} a_{n'\mathbf{q}'} h^*_{n\mathbf{q},\mathbf{q}+\mathbf{G}} h_{n'\mathbf{q}',\mathbf{q}+\mathbf{G}-\mathbf{k}} (\mathbf{q}+\mathbf{G}) \cdot (\mathbf{q}+\mathbf{G}-\mathbf{k}) \tag{D.21}$$

Examining the two equations closely, the discrepancy is in the factor $h_{n'\mathbf{q}',\mathbf{q}+\mathbf{G}-\mathbf{k}}$. In the new expression, $h_{n'\mathbf{q}',\mathbf{q}+\mathbf{G}-\mathbf{k}}$ has an associated delta function that collapses the sum over $\mathbf{q}'$ to a single $\mathbf{q_0}$ which is the $\mathbf{q}+\mathbf{G}-\mathbf{k}$ vector translated back into the First Brillouin zone. In the old expression, this requirement is not present. The n' index specifies the 'band' of interest, and in general, the expansion coefficients for $\mathbf{q_0}$ will not be zero for some given band. This is the manifestation of the incorrect orthogonality expression.

D.3.3 Solving the inverse equation

When it comes to finally solving the inverse equation

$$\sum_{\mathbf{k}} D^{(m)}_{n,\mathbf{q};\mathbf{k}'} \delta\eta_{\mathbf{k}} = a^{(m)}_{n,\mathbf{q}} \frac{\omega_m^2 - \omega_{n,\mathbf{q}}^2}{c^2}$$

the paper never discussed how one actually goes about solving this set of (incorrect) linear equations. The end of Section III-D suggested using approximate methods for solving linear systems of equations and referenced a book by Golub and Van Loan [89] that focusses on numerical implementation of standard linear algebra routines. From chapter 3, we now know that standard linear algebra techniques will not work because the problem is ill-conditioned. The essential tool to use for this type of problem is regularization, but that is somehow omitted in the paper. Regardless, we can use the regularization technique to solve the h_1 defect mode problem, as was done in

chapter 6, but using equation (24) from the paper. We perform our proof of principle calculation as in section 6.4. No amount of regularization enabled the recovery of the nominal h_1 geometry, and this is without the addition of any noise term.

D.4 Results Errors

We end this appendix with a discussion of the results presented in the paper. There is a slight misnomer with the term *radially symmetric defect*, since the defect introduced is not *radially* symmetric, but rather it retains the rotational symmetry of the hexagonal lattice. (An *additive* radially symmetric perturbation cannot produce a displacement of holes surrounding the defect without changing the dielectric between the holes at the same radius.) The details are again somewhat vague, but private communications with the first author confirmed that it indeed was radial symmetry that was enforced in the calculation. It was mentioned that it made the problem easier since it essentially became a 1D problem (solve for $\eta(|r|)$ rather than $\eta(\mathbf{r})$). It is not clear how one can actually use this bulk mode expansion formulation (or even PWE) to enforce radial symmetry, but rotational symmetry can in principle be enforced by selecting only the $\mathbf{k}$-vectors that preserve the desired symmetry. We will assume that in fact, the paper meant defects with hexagonal rotation symmetry. If it is the hexagonal symmetry that is enforced, then the target mode would need to have been expanded in terms of the reduced set of $\mathbf{k}$-vectors, and thus have hexagonal symmetry. The mode shown in figure 1(b) does not have the correct symmetry. Of course, working in the bulk mode basis, it is still unclear which bulk modes should be kept to preserve that symmetry. Even in the plane wave basis, working out the proper symmetry transformations in the inversion matrix is not trivial. That will be left as an exercise for the reader.

To demonstrate the Q factor optimization, figure 3 (and also figure 5 for the asymmetric defect) shows the bulk mode contribution using a dispersion diagram to indicate significant contributors to the mode as an attempt to show the removal of leaky modes. The number of $\mathbf{k}$-points taken in the expansion along the $\Gamma - X$ line

is much greater than 5, which is inconsistent and incompatible with the specified supercell geometry (5 layers surrounding the central defect). There is a discussion in Section III-D about the dimension required of the matrix D. Specifically, it claimed that the number of G's must equal the number of q's, which is incorrect. Briefly, the number of G's dictate the real-space resolution one can achieve, while the number of q's is determined by the size of the supercell. One can have many layers using poor resolution or vice versa. Appendix C explains how to discretize **k**-space appropriately, given the specified boundary conditions.

The smoothed dielectric function that is given by the solution to eqn. (24) (with the defect-free geometry added) is shown in figure 2, and according to Sec. III-E, the nominal structure was extracted from this function by taking a contour plot along $(\eta_{max} + \eta_{min})/2$. According to the text and in figure 1, the holes surrounding the central defect had a reduced radii, and were displaced radially from the original lattice positions. However, the reduction in hole radii and radial displacement are not observed in the 3D view of the dielectric function in figure 2. In addition, none of the surrounding holes exceed the threshold for a valid contour as defined above. For $\eta_{max} = 1$ and $\eta_{min} > 0$, this gives $\overline{\eta} > 0.5$, while figure 2 shows the surrounding regions have η less than 0.5. Again, it is hard to be quantitative given only these contour plots, but it is still worth contemplating the following: What does $\delta\eta$ need to look like in order to actually get these small displacements to the hole locations (as shown in the paper) without distorting the circular shape? And, and for the asymmetric defect, what is the $\delta\eta$ required to stretch and displace these circular holes into elliptical ones so the design has these fractional edge dislocation like features?

Neither solution includes a comparison of Q, V and $E(0)$ of the actual obtained mode with those from the original optimized target mode. One is left to assume that whatever solution was obtained, it perfectly gave back what was designed. We now know that when one regularizes, the solution rarely matches exactly what you had designed. One can only hope that the solution is 'close' in some relevant sense. Unfortunately, these crucial comparisons, as well as other important details were omitted.