

Modeling of Polariton Propagation in CrSBr

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Introduction

Motivation

Hyperbolic polaritons, existing in select materials, hold the key to fascinating phenomena. Highly confined propagation direction and wavelength contraction are features of these quasiparticles that are ideal for applications in nanophotonic devices. Chromium Sulfide Bromide (CrSBr) is one such material that hosts these exotic light-matter interactions. Energy propagation has been a key question within recent experiments, but there is a lack of theoretical development. We seek to fill this gap and model the behavior via a transfer matrix and Green's function Methodology.

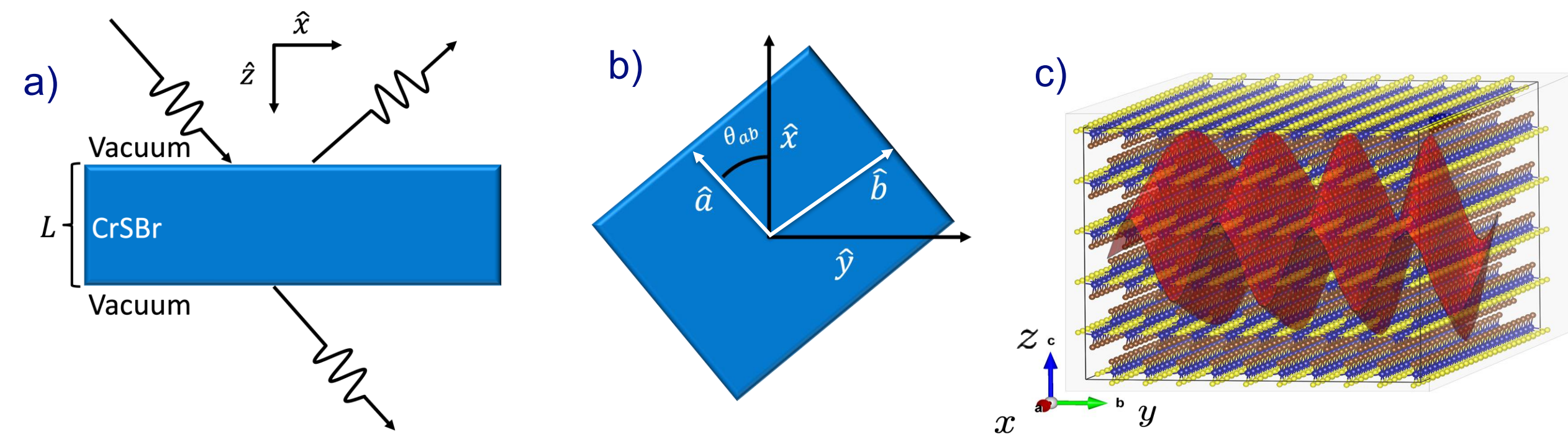


Fig 1. Description of system setup. a) Propagation vector, k , is incident in the x - z plane. b) CrSBr slab (thickness L) is rotated about the z -axis by an angle, θ_{ab} . c) Depiction of layered CrSBr flakes with polariton propagation

Methods

- Derive a **transfer matrix** from Maxwell's equations and boundary conditions [1]
- Use this matrix to extract the reflectivity (**dispersion**) yielding:
 - The polariton branches (angle cross section) and
 - Polariton hyperbolicity (energy cross section)
- Extract the **waveguide modes**
 - Require no incoming light $\rightarrow$ poles of dispersion
 - Solve for corresponding coefficients and polarization
- Construct a Green's function using these modes to calculate **propagation of $\vec{E}$** from an initial source
 - Consider the exciton-polariton as the source
 - Obtain the resulting spectrum, $S(\omega)$

Results

Dispersion Relation

- Calculate the material's reflectivity, R_{pp} , giving the dispersion
- Repeat for various angle rotations

$\theta_{ab} = 0$	Pure TM mode	No polariton interaction
$\theta_{ab} \neq \frac{n\pi}{2}$	Mixed TE/TM modes	Some interaction

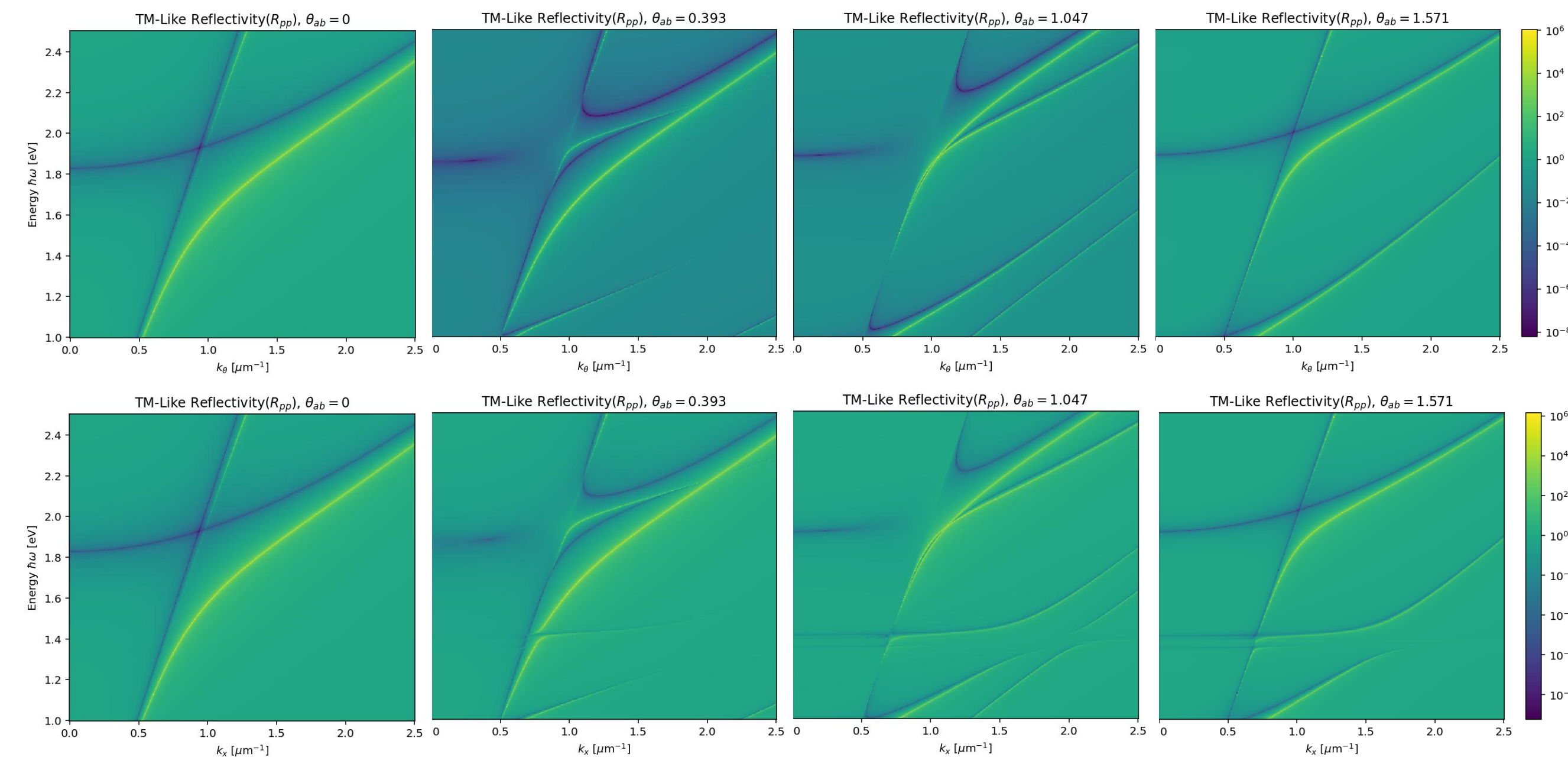


Fig 2. Dispersion relations for 100nm CrSBr slab without and with the exciton, calculated using pyGTM [2]. Due to its anisotropy, these modes interpolate between TM and TE as the slab is rotated.

Hyperbolic Polaritons

- Plot the isofrequency (k_x vs. k_y) contours
- Observe **changes in branch geometry** with $\epsilon_{yy}(\omega)$

$\epsilon_{yy} \gg 0$	Elliptical polaritons
$\epsilon_{yy} > 0$, decreasing	Ellipse stretches out
$\epsilon_{yy} = 0$	Ellipse breaks into two "arms"
$\epsilon_{yy} < 0$	Hyperbolic polaritons

- Change in **propagation behavior** [3]
 - Elliptical $\rightarrow$ No direction restrictions
 - Hyperbolic $\rightarrow$ High directional confinement

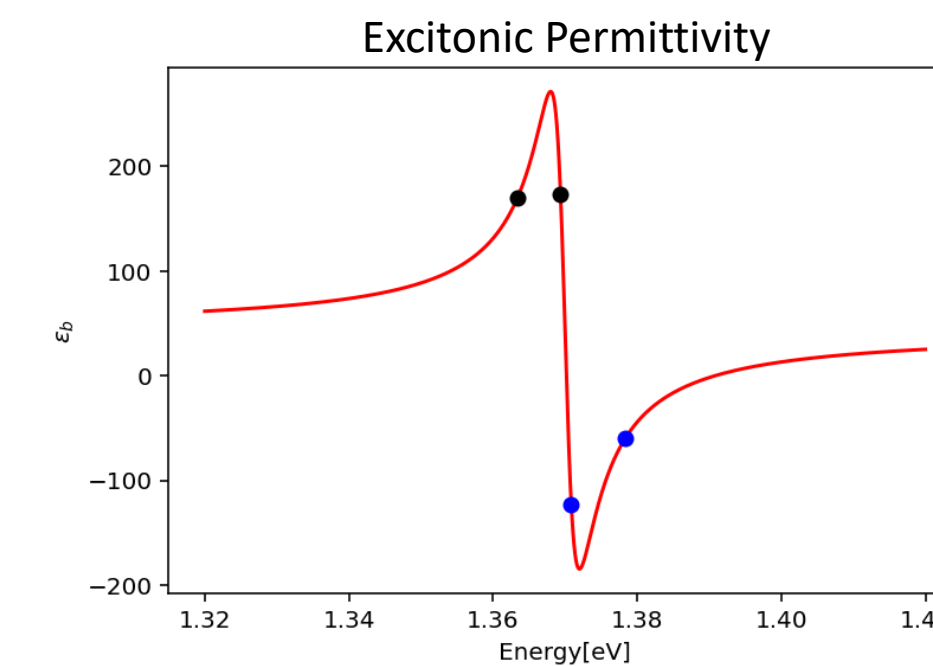


Fig 3. $\text{Re}(\epsilon_{yy})$ parameterized by the Lorentzian Oscillator model [4]

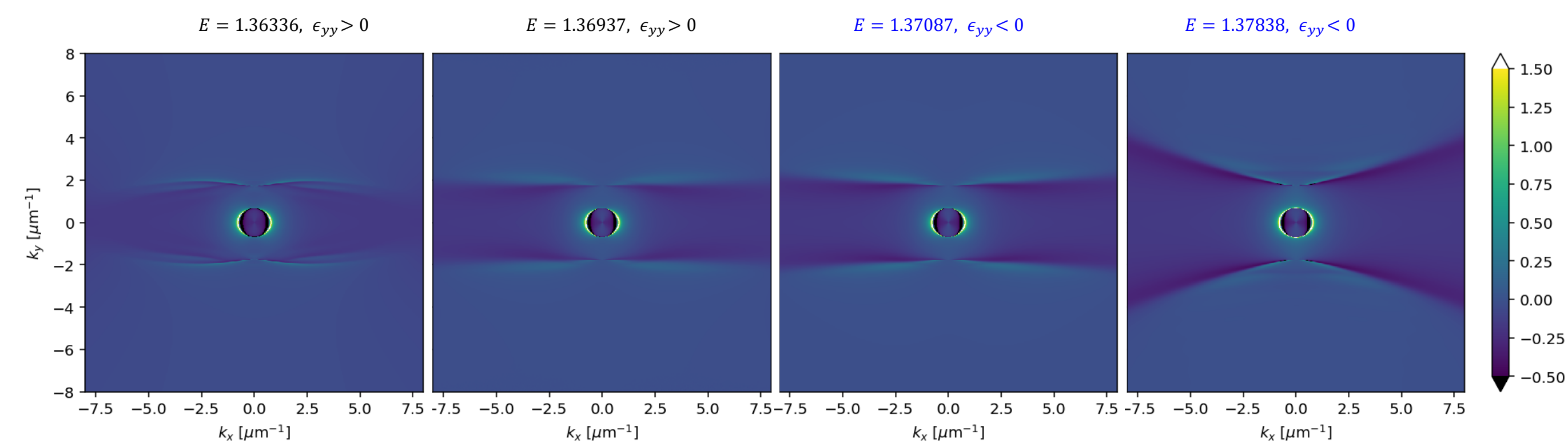


Fig 4. Energy cross sections of slab dispersion, showing geometry of the polariton branches. As ϵ_{yy} drops we see an ellipse which further stretches out, breaking into two "arms", our hyperbola.

Green's Function Approach to Slab Propagation

- Green's function uses slab modes to propagate sources ($\vec{j}$)
 - $\vec{G}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\beta} \sum_{pol} \frac{w_{\beta}(z) \otimes w_{\beta}(z')}{\sum_{jj'} \gamma_{jj'}^2 \tilde{\epsilon}_{jj'}(\omega) - \frac{\omega^2}{c^2} \tilde{\epsilon}_{jj'}(\omega)} e^{i\beta(x-x')}$
 - $\vec{E}(\mathbf{r}) = \int \vec{G}(\mathbf{r}, \mathbf{r}') \cdot \vec{j}(\mathbf{r}') d\mathbf{r}'$

- w-modes are the characteristic modes of the slab
 - No incoming light $\rightarrow$ poles of dispersion
 - Must be normalized
- Consider the exciton as the source

$$\vec{j}(\mathbf{r}) = \frac{f_x}{E^2 - E_x^2 - i\Gamma E} \delta(x) [\Theta(0) - \Theta(L)] \hat{b}$$

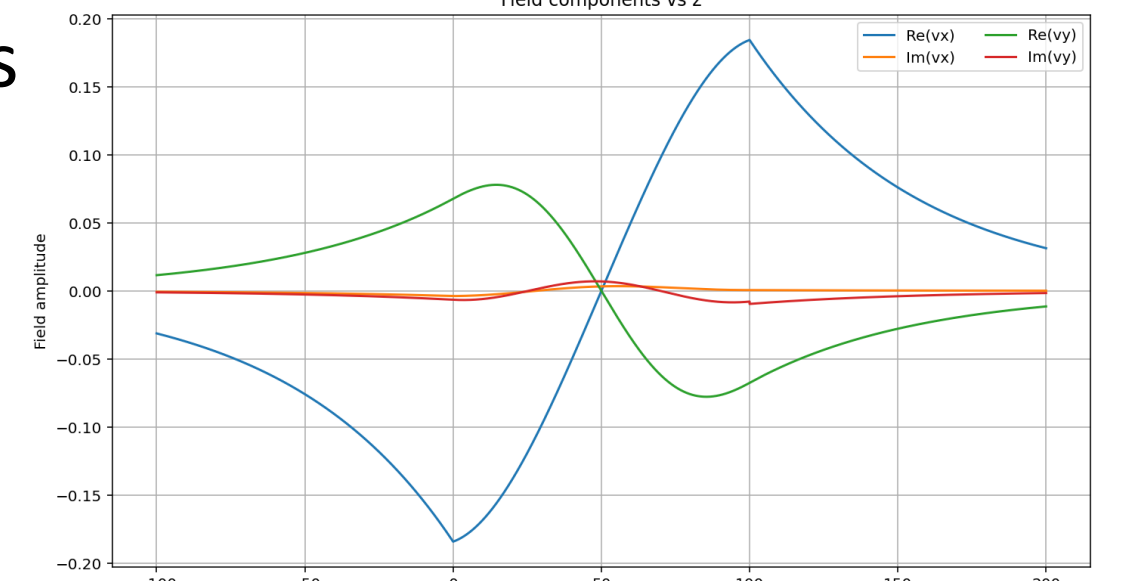


Fig 5. Example Electric Field Mode

Propagation Expectations, Pending Results

- After calculation of $\vec{E}$, we need the spectrum:
 - $S(\omega) = \vec{E} \times \vec{H}$
- Expect to see a peak around excitonic energy
- Experimental results show interference pattern

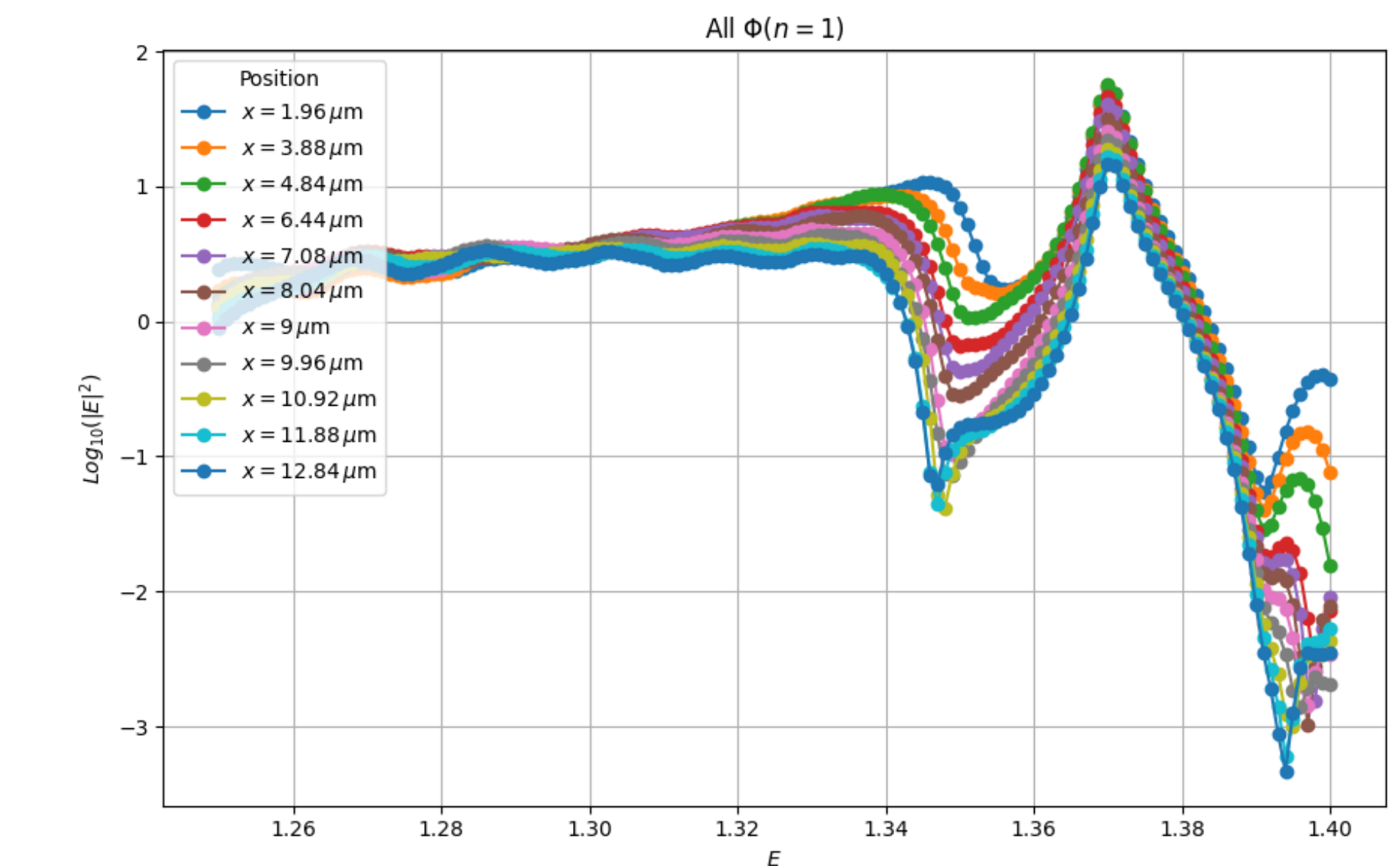


Fig 6. Preliminary Green's function results. Electric Field propagated from the exciton source for individual distances.

Discussion

Current Conclusions

We have been able to calculate several key features of the CrSBr slab purely through the transfer matrix formalism. By deriving the dispersion relation, we revealed both the branch splitting and hyperbolic nature of the polaritons. We also calculated the eigenmodes of the slab, which allow us to mathematically derive the propagation of sources throughout the slab via the Green's function. Finalized results of this propagation are forthcoming.

Acknowledgements

We are working closely with the CINT experimental group led by Dr. Htoon in order to compare theoretical results.

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