Sub-Wavelength Plasmonic Crystals: Dispersion Relations and Effective Properties

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Abstract. We obtain a convergent power series expansion for the first branch of the dispersion relation for subwavelength plasmonic crystals consisting of plasmonic rods with frequency-dependent dielectric permittivity embedded in a host medium with unit permittivity. The expansion parameter is $\eta = 2\pi d/\lambda$, where λ is a fixed wavelength and d is the period of the crystal, and the plasma frequency scales inversely to d, making the dielectric permittivity in the rods large and negative. The expressions for the series coefficients (a.k.a., dynamic correctors) and the radius of convergence in η are explicitly related to the solutions of higher-order cell problems and the geometry of the rods. We obtain radii of convergence on the order of 10^{-2} so that, within this range, we can compute the dispersion relation and the fields and define dynamic effective properties in a mathematically rigorous manner. Explicit error estimates show that a good approximation to the true dispersion relation is obtained using only a few terms of the expansion. The convergence proof requires the use of properties of the Catalan numbers to show that the series coefficients are exponentially bounded in the H^1 Sobolev norm.

Key words. Meta-material, Plasmonic crystal, Dispersion relation, Catalan numbers, Series solutions

Contents

1 Introduction

Sub-wavelength plasmonic crystals are a class of *meta-material* that possesses a microstructure consisting of a periodic array of plasmonic inclusions embedded within a dielectric host. The term "sub-wavelength" refers to the regime in which the period of the crystal is smaller than the wavelength of the electromagnetic radiation traveling inside the crystal. Many recent investigations into the behavior of meta-materials focus on phenomena associated with the *quasi-static limit* in which the ratio of the period cell size to wavelength tends to zero. Sub-wavelength micro-structured composites are known to exhibit effective electromagnetic properties that are not available in naturally-occurring materials. Investigations over the past decade have explored a variety of meta-materials, including arrays of micro-resonators, wires, high-contrast dielectrics, and plasmonic components. The first two, especially in combination, have been shown to give rise to unconventional bulk electromagnetic response at microwave frequencies [28, 24, 23] and, more recently, at optical frequencies [25], including negative effective dielectric permittivity and/or negative effective magnetic permittivity. An essential ingredient in creating this response are local resonances contained within each period due to extreme properties, such as high conductivity and capacitance in split-ring resonators [24].

In the case of plasmonic crystals, the dielectric permittivity ϵ_{p} of the inclusions is frequency dependent and negative for frequencies below the plasma frequency ω_{p},

$$\epsilon_{\mathrm{p}}(\omega) = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega^2}. \tag{1.1}$$

Shvets and Urzhumov [26, 27] have investigated plasmonic crystals in which ω_p *is inversely proportional to the period of the crystal* and for which both inclusion and host materials have unit magnetic permeability. They have proposed that simultaneous negative values for both an effective ϵ and μ arise at sub-wavelength frequencies that are quite far from the quasi-static limit, that is, $\eta = 2\pi d/\lambda$ is not very small, where d is the period of the crystal and λ the wavelength.

In this work, we present rigorous analysis of this type of plasmonic crystal by establishing the existence of convergent power series in η for the electromagnetic fields and the associated dispersion relation. The effective permittivity and permeability defined according to Pendry, *et. al.*, [24], are shown to be positive for all η within the radius of convergence R, and,

r	0.1	0.2	0.3	0.4	0.45
R_m	1/60	1/68	1/88	1/96	1/340

Table 1: Lower bounds on the radii of convergence R for circular inclusions of radii rd.

r	0.1	0.2	0.3	0.4	0.45
λ_m	$38\,\mu m$	$43\,\mu m$	$56\,\mu m$	$73\,\mu m$	$214\,\mu m$
k_M	$1.6 \cdot 10^5\,m^{-1}$	$1.4 \cdot 10^5\,m^{-1}$	$1.1 \cdot 10^6\,m^{-1}$	$1.0 \cdot 10^5\,m^{-1}$	$3.0 \cdot 10^4\,m^{-1}$

Table 2: Values of λ_m and k_M for circular inclusions of radii rd when $d = 10^{-7}m$.

in this regime, *the extreme property of the plasma produces no resonance in the effective permittivity or permeability.*

The analysis shows that the radii of convergence of the power series R is at least R_m which is not too small, as shown in Table 1, which contains values of R_m for circular inclusions of various radii rd. For a fixed choice of cell size d, the lower bound on the convergence radius corresponds to propagating waves with wavelengths greater than λ_m and wave numbers less than k_M respectively. Table 2 presents values of λ_m and k_M when $d = 10^{-7}m$. The wavelengths λ_m are seen to lie in the infrared range. The plasma frequency for $d = 10^{-7}m$ is $\omega_{\rm p} = 10^{15}\,\sec^{-1}$.

The governing family of differential equations for the magnetic field is the Helmholtz equation with a rapidly oscillating coefficient

$$-\nabla \cdot (A(x/d)\nabla u) = \frac{\omega^2}{c^2} u\,, \tag{1.2}$$

in which A is the matrix defined on the unit period of the crystal given by

$$A(y) = \begin{cases} \epsilon_{\rm p}(\omega)^{-1} I & \text{in the plasmonic phase,} \\ \epsilon_{\bar{\rm p}}^{-1} I & \text{in the host phase,} \end{cases}$$

and I is the identity matrix. Since $\epsilon_{\rm p}$ is negative in the regime of interest $\omega_{\rm p} > \omega$, this coefficient is not coercive.

It is precisely the appearence of negative $\epsilon_{\rm p}$ that allows us to obtain a *convergent* power-series expansion of the electromagnetic field and the frequency ω for a fixed Bloch wavevec-

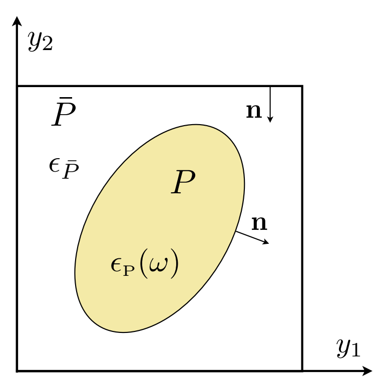

Figure 1: Unit cell with plasmonic inclusion.

tor $\mathbf{k} = k\hat{\kappa}$ with $|\hat{\kappa}| = 1$. The expansion of ω^2 yields a dispersion relation

$$\omega^2 = \omega_\eta^2 = W_\eta^2(\mathbf{k}) = k^2\omega_0^2(\hat{\kappa}) + k^4\eta^2\omega_2^2(\hat{\kappa}) + \ldots, \tag{1.3}$$

in which ω_n^2 is homogeneous of degree $n+2$ in $\hat{\kappa}$, see corollary (5.1). This, in turn, gives rise to a convergent power series for an effective index of refraction n_{eff} defined through

$$n_{\text{eff}}^2 = \frac{c^2k^2}{\omega^2}. \tag{1.4}$$

The effective property n_{eff} is defined for $\eta > 0$ and is not phenomenological in origin but instead follows from first principles using the power series expansion. Interpreting the first term of this series as the quasi-static index of refraction n_{qs}^2, the remaining terms then provide the dynamic correctors of all orders. In section 6, we define the effective permeability and permittivity μ_{eff} and ϵ_{eff} and prove that n_{eff} and μ_{eff} are positive for η in some interval $(0, \eta_0]$ and that an effective magnetic response emerges for the homogenized composite, even though the component materials are non-magnetic ($\mu_{\bar{P}} = \mu_P = 1$). In fact, μ_{eff} is less than unity and is very close to 1 for circular inclusions. The fact that both n_{eff} and μ_{eff} are positive then implies that ϵ_{eff} is also positive. Thus, one has a solid basis on which to assert that plasmonic crystals function as materials of positive index of refraction in which both the effective permittivity and permeability are positive. The method developed here is general and can be applied to other types of frequency-dependent dielectric media including polaratonic crystals. From a physical perspective this work provides the first explicit description of Bloch wave solutions associated with the first propagation band inside nanoscale plasmonic crystals.

To emphasize the difference between effective properties defined for meta-material structures where the crystal period d is fixed and effective properties defined in the quasistatic limit, i.e., k fixed and $d \to 0$, we refer to the latter as quasistatic effective properties and denote these with the subscript qs. The situation considered in this paper contrasts with the case in which $\epsilon \approx d^{-2}$ in the inclusion and is large and positive, investigated by Bouchitté and Felbacq [3]. In that case for $\eta \to 0$, $\mu_{\text{qs}}(\omega)$ has poles at Dirichlet eigenvalues of the inclusion and therefore is negative in certain frequency intervals (see also [4, 12, 11]). In fact, what allows us to prove convergence of the power series in the plasmonic case is precisely the absence, due to negative ϵ_{p}, of these internal Dirichlet resonances.

We focus on harmonic H-polarized electromagnetic waves in a lossless composite medium consisting of a periodic array of plasmonic rods that possess rectangular symmetry, that is, that are invariant under rotation by 180° about the center of the unit cell, embedded in a non-magnetic frequency-independent dielectric host material. Each period can contain multiple parallel rods with different cross-sectional shapes. The regime of interest for this investigation is that in which

1. the plasma frequency ω_{p} is high,
2. the ratio of the cell width to the wavelength is small ($\eta \ll 1$).

A high plasma frequency ω_{p} gives rise to a *large and negative dielectric permittivity* ϵ_{p} in the plasmonic inclusions (see [27, 14]),

$$\epsilon_{\text{p}} = 1 - \frac{\omega_{\text{p}}^2}{\omega^2}. \tag{1.5}$$

In the sub-wavelength regime, we take the point of view that the wave length λ, and hence also the wave number $k = 2\pi/\lambda$, are fixed and that the expansion parameter η is proportional to the period-cell length d:

$$\eta = kd = 2\pi\frac{d}{\lambda}. \tag{1.6}$$

Following [27], the plasma frequency is related to the cell size by

$$\omega_{\mathrm{p}} = \frac{c}{d}. \tag{1.7}$$

This results in the relation

$$\epsilon_{\mathrm{p}} = 1 - \frac{1}{\xi^2\eta^2}, \tag{1.8}$$

in which ξ is a dimensionless frequency

$$\xi = \frac{\omega}{ck}, \tag{1.9}$$

that identifies the in-vacuo frequency ck with unity. Here the wave vector associated with a Bloch wave is written as $k\hat{\kappa}$ where $\hat{\kappa}$ is a unit vector giving the direction of propagation.

For the regime of interest, ϵ_{p} is negative and large, thus the perturbation methods used for describing Bloch waves in heterogeneous media developed in Odeh and Keller [21], Conca [9], and Bensoussan Lions and Papanicolaou [2] cannot be applied. Our analysis instead makes use of the fact that ϵ_{p} is negative and large for sub-wavelength crystals and develops high-contrast power series solutions for the nonlinear eigenvalue problem that describes the propagation of Bloch waves in plasmonic crystals. Our convergence analysis takes advantage of the iterative structure appearing in the series expansion and is inspired by a technique of Bruno [6] developed for series solutions to quasi-static field problems. We prove that the series converges to a solution of the harmonic Maxwell system for ratios of cell size to wavelength that are not too small. Indeed for typical values of the plasma frequency ω_{p} the analysis delivers convergent series solutions for nano scale plasmonic rods at infrared wavelengths.

In section 6.3 we compute the first two terms of the dispersion relation for circular inclusions [26, 27] and provide explicit bounds on the relative error comitted upon replacing the full series with its first two terms. The error is seen to be less than 3% for values of η up to 20% of the convergence radius, so that the two-term approximation provides a numerically fast and accurate approximation to the dispersion relation.

The high contrast in ϵ gives rise to effective constants ϵ_{eff} and μ_{eff}. In the bulk relation

$$B_{\mathrm{eff}} = \mu_{\mathrm{eff}} H_{\mathrm{eff}}, \tag{1.10}$$

B_{eff} is the average over the the period cell (a flux), whereas H_{eff} is the average of H_3 over line segments in the matrix parallel to the rods. Taking the ratio of $B_{\mathrm{eff}}/H_{\mathrm{eff}}$ delivers an effective magnetic permeability and one recovers magnetic activity from meta-materials made from non-magnetic materials. This phenomenon was understood by Pendry, *et. al.*, [24] and has been made rigorous in the quasistatic limit through two-scale analysis in several cases. These include the two-dimensional arrays of inclusions in which ϵ scales as d^{-2} [3, 4, 12, 11, 24], two dimensional arrays of ring resonators whose surface conductivity scales as d^{-1} [16], as well as three-dimensional arrays of split-ring wire resonators in which the conductivity scales as d^{-2} [5]. This "non-standard" homogenization has been understood for some decades in problems of porous media and imperfect interface [8, 1, 19, 10, 31], and recently has given rise to interesting effects in composites of both high contrast and high anisotropy [7, 30].

The two-scale analysis in these cases relies on the coercivity of the underlying partial differential equations. The problem of plasmonic inclusions, however, is not coercive because ϵ is negative in the plasma—but it is precisely this negative index that underlies the convergence of the homogenization power series. As we shall see, the uniqueness of the solution of the Dirichlet problem for $\triangle u - u = 0$ in the plasmonic inclusion gives exponential bounds on the coefficients of the series, which allows us to prove that it converges to a solution of the differential equation (1.2). This result implies homogenization in all orders, in other words, by considering a finite number of terms in the series, one has an approximation of the true solution, to any desired algebraic order of convergence. The formal power series of correctors has been shown to be an asymptotic series in certain cases under the hypothesis that the coefficient A is coercive [29, 15, 22].

2 Mathematical Formulation and Background

We introduce the nonlinear eigenvalue problem describing the propagation of Bloch waves inside a plasmonic crystal and provide the context for the power series approach to its solution.

For points $\mathbf{x} = (x_1, x_2)$ in the x_1x_2-plane, the d-periodic dielectric coefficient of the crystal is denoted by $\epsilon(\omega, \mathbf{x})$, where

$$\epsilon(\omega, \mathbf{x}) = \begin{cases} \epsilon_{\mathrm{p}}(\omega) & \text{for } \mathbf{x} \in P, \\ \epsilon_{\bar{\mathrm{p}}} & \text{for } \mathbf{x} \in \overline{P}. \end{cases}$$

Both materials are assumed to have unit magnetic permeability, $\mu_{\mathrm{p}} = \mu_{\bar{\mathrm{p}}} = 1$.

We assume a Bloch-wave form of the field, where $\hat{\kappa} = (\kappa_1, \kappa_2)$ is the unit vector along the direction of the traveling wave and $k = 2\pi/\lambda$ is the wave number for a wave of length λ. The magnetic and electric fields are denoted by $\mathbf{H} = (H_1, H_2, H_3)$ and $\mathbf{E} = (E_1, E_2, E_3)$ respectively. For H-polarized time-harmonic waves, the non-vanishing field components are

$$\begin{aligned} H_3 &= H_3(\mathbf{x}) e^{ik\hat{\kappa}\cdot\mathbf{x} - i\omega t} & (2.1) \\ E_1 &= E_1(\mathbf{x}) e^{ik\hat{\kappa}\cdot\mathbf{x} - i\omega t}, & (2.2) \\ E_2 &= E_2(\mathbf{x}) e^{ik\hat{\kappa}\cdot\mathbf{x} - i\omega t}, & (2.3) \end{aligned}$$

in which the fields $H_3(\mathbf{x})$, $E_1(\mathbf{x})$, and $E_2(\mathbf{x})$ are continuous and d-periodic in both x_1 and x_2. The Maxwell equations take the form (1.2), in which substitution of $u = H_3(\mathbf{x})e^{ik\hat{\kappa}\cdot\mathbf{x}-i\omega t}$ gives

$$-(\nabla + ik\hat{\kappa})\epsilon_p(\omega)^{-1}(\nabla + ik\hat{\kappa})H_3 = \frac{\omega^2}{c^2} H_3 \quad \text{in the rods,} \qquad (2.4)$$

$$-(\nabla + ik\hat{\kappa})\epsilon_{\overline{p}}^{-1}(\nabla + ik\hat{\kappa})H_3 = \frac{\omega^2}{c^2} H_3 \quad \text{in the host material,} \qquad (2.5)$$

where H_3 satisfies the transmission conditions on the interface between the rods and host material given by

$$\mathbf{n} \cdot (\epsilon_p(\omega)^{-1}(\nabla + ik\hat{\kappa})H_3)_{|_p} = \mathbf{n} \cdot (\epsilon_{\overline{p}}^{-1}(\nabla + ik\hat{\kappa})H_3)_{|_{\overline{p}}}. \qquad (2.6)$$

Here, the subscripts indicate the side of the interface where the quantities are evaluated and $\mathbf{n}$ is the unit normal vector to the interface pointing into the host material. We denote the unit vector pointing along the x_3 direction by $\mathbf{e}_3$, and the electric field component of the wave is given by

$$\mathbf{E} = \frac{-ic}{\omega\epsilon(\omega, \mathbf{x})}\mathbf{e}_3 \times \nabla H_3. \tag{2.7}$$

For each value of k and $\hat{\kappa}$ equations (2.4, 2.5, 2.6) provide a nonlinear eigenvalue problem for the solution of H_3 and ω. One of the main results of this work is to show that this problem is well posed by explicitly constructing solutions using power series expansions. In order to develop the appropriate expansions we rewrite (2.4, 2.5, 2.6) in terms of η, $k\hat{\kappa}$, ξ, and a dimensionless variable $\mathbf{y}$ in $\mathbb{R}^2$ that normalizes a period cell to the unit square $Q = [0, 1]^2$,

$$\mathbf{x} = \mathbf{y}d = \mathbf{y}\frac{\eta}{k}. \tag{2.8}$$

With a slight abuse of notation we continue to denote the part of the unit square occupied by plasmonic material by P and the part occupied by host material by $\overline{P}$. We define the Q-periodic function

$$h(\mathbf{y}) = H_3(d\mathbf{y}) \tag{2.9}$$

and set

$$\epsilon(\xi, \mathbf{y}) = \begin{cases} \epsilon_{\mathrm{p}}(ck\xi) & \text{for } \mathbf{y} \in P, \\ \epsilon_{\bar{\mathrm{p}}} & \text{for } \mathbf{y} \in \overline{P}. \end{cases} \tag{2.10}$$

to arrive at the *nonlinear eigenvalue problem* that requires the pair $h(\mathbf{y})$ and ξ^2 to be a solution of our master system

$$\begin{cases} -(\nabla_{\mathbf{y}} + i\eta\hat{\kappa})\epsilon(\xi, \mathbf{y})^{-1}h(\mathbf{y})(\nabla_{\mathbf{y}} + i\eta\hat{\kappa}) = \eta^2\xi^2 h(\mathbf{y}) & \text{for } \mathbf{y} \in P \cup \overline{P}, \\ \mathbf{n} \cdot \epsilon_{\mathrm{p}}(\xi)^{-1}(\nabla_{\mathbf{y}} + i\eta\hat{\kappa})h(\mathbf{y})|_{\mathrm{p}} = \mathbf{n} \cdot \epsilon_{\bar{\mathrm{p}}}^{-1}(\nabla_{\mathbf{y}} + i\eta\hat{\kappa})h(\mathbf{y})|_{\bar{P}} & \text{for } \mathbf{y} \in \partial P. \end{cases} \tag{2.11}$$

The solution of this eigenvalue problem determines the magnetic field $h(\mathbf{y})$ and normalized frequency ξ. We prove in Theorem 5.2 that this eigenvalue problem can be solved by constructing explicit convergent power series solutions. Here the power series that delivers $h(\mathbf{y})$ is shown to converge with respect to the norm on the standard Sobolev space $H^1(Q)$. The power series expansion for ξ is shown to converge and delivers the dispersion relation describing the first pass band.

The power series method introduced in this paper is developed in the next sections. The development is as follows. In section 3 the power series expansion is introduced and the associated boundary-value problems necessary for determining each term in the series are obtained. The boundary value problems are given by a strongly coupled infinite system of linear partial differential equations. The existence and uniqueness of the solution to this infinite system is proved under fairly general hypotheses in section 4. Because the system is coupled through convolution products, the convergence analysis is delicate. The convolutions are handled through estimates involving sequences of Catalan numbers whose convolution products determine the next element of the sequence. The Catalan numbers and their relevant properties are discussed and used to derive bounds on the Sobolev norm of each term of the series expansion in section 5. These bounds are then used to establish the radius of convergence for the power series representations of the field and frequency (the dispersion relation), which solve the nonlinear eigenvalue problem (2.11). Section 6 deals with the computation of error bounds for finite-term approximations of the magnetic field and the dispersion relation.

3 Power Series Expansions

Let us take η to be the expansion parameter for the field $h(\mathbf{y})$,

$$h(\mathbf{y}) = h_\eta(\mathbf{y}) = h_0(\mathbf{y}) + \eta h_1(\mathbf{y}) + \eta^2 h_2(\mathbf{y}) + \dots, \tag{3.1}$$

in which all coefficients h_m are periodic with period cell Q. For a fixed Bloch wavevector $k\hat{\kappa}$, the nonlinear eigenvalue problem (2.11) imposes a restriction on ξ^2, and we write

$$\xi^2 = \xi_\eta^2 = \xi_0^2 + \eta\xi_1^2 + \eta^2\xi_2^2 + \dots. \tag{3.2}$$

In our calculations, we take $\epsilon_{\bar{\mathrm{p}}} = 1$. The nonlinear eigenvalue problem (2.11) is rewritten as

$$\begin{cases} (\Delta + 2i\eta\hat{\kappa}\cdot\nabla - \eta^2)h_\eta(\mathbf{y}) = -\eta^2\xi_\eta^2 h_\eta(\mathbf{y}) & \text{for } \mathbf{y} \in \bar{P}, \\ (\Delta + 2i\eta\hat{\kappa}\cdot\nabla - \eta^2)h_\eta(\mathbf{y}) = (1 - \eta^2\xi_\eta^2)h_\eta(\mathbf{y}) & \text{for } \mathbf{y} \in P, \\ (\eta^2\xi_\eta^2 - 1)(\nabla + i\eta\hat{\kappa})h_\eta(\mathbf{y})|_{\bar{P}} \cdot \mathbf{n} = \eta^2\xi_\eta^2(\nabla + i\eta\hat{\kappa})h_\eta(\mathbf{y})|_{\mathrm{p}} \cdot \mathbf{n} & \text{for } \mathbf{y} \in \partial P, \end{cases} \tag{3.3}$$

and, identifying coefficients of the right- and left-hand sides yields the equations

$$\begin{cases} \Delta h_m + 2i\hat{\kappa}\cdot\nabla h_{m-1} - h_{m-2} = -\xi_\ell^2 h_{m-2-\ell} & \text{in } \bar{P}, \\ \Delta h_m + 2i\hat{\kappa}\cdot\nabla h_{m-1} - h_{m-2} = h_m - \xi_\ell^2 h_{m-2-\ell} & \text{in } P, \\ (\nabla(\xi_\ell^2 h_{m-2-\ell}) - \nabla h_m - ih_{m-1}\hat{\kappa})|_{\bar{P}} \cdot \mathbf{n} = \nabla(\xi_\ell^2 h_{m-2-\ell})|_{\mathrm{p}} \cdot \mathbf{n} & \text{on } \partial P, \end{cases} \tag{3.4}$$

for $m = 0, 1, 2, \dots$, in which $h_m \equiv 0$ and $\xi_m^2 = 0$ for $m < 0$ and the terms involving the subscript ℓ are convolutions written according to the following summation conventions,

$$a_\ell b_{n-\ell} = \sum_{\ell=0}^{n} a_\ell b_{n-\ell}\,, \qquad a_\ell b_{n-\ell}^{(\ell<\ell_2)} = \sum_{\ell=0}^{\ell_2-1} a_\ell b_{n-\ell}$$

$$a_\ell b_{n-\ell}^{(\ell_1<\ell<\ell_2)} = \sum_{\ell=\ell_1+1}^{\ell_2-1} a_\ell b_{n-\ell}\,, \qquad a_\ell b_{n-\ell}^{(\ell\,\mathrm{even})} = \sum_{\ell=0}^{[n/2]} a_{2\ell} b_{n-2\ell}\,.$$

Now, h_0 is necessarily equal to a constant $\bar{h}_0$ in $\bar{P}$ and for $\mathbf{y}$ in $\overline{P}$ we write $h_0(\mathbf{y}) = \bar{h}_0$. It is convenient to express the equations (3.4) in terms of the functions ψ_m defined through $h_m(\mathbf{y}) = \bar{h}_0 i^m \psi_m(\mathbf{y})$. Arranging terms we obtain an infinite system which the sequences $\{\psi_m(\mathbf{y})\}_{m=0}^\infty$ and $\{\xi_m^2\}_{m=0}^\infty$ must satisfy. The system is written in terms of a Poisson equation in $\bar{P}$ with Neumann boundary data and a Helmholtz equation in P with Dirichlet boundary data. The system is given by

$$\begin{cases} \Delta\psi_m = G_m & \text{in } \bar{P}, \\ \nabla\psi_m|_{\bar{P}} \cdot \mathbf{n} = F_m & \text{on } \partial P, \end{cases} \tag{3.5}$$

and

$$\begin{cases} \Delta\psi_m = \psi_m + G_m & \text{in } P, \\ \psi_m|_{\mathrm{P}} = \psi_m|_{\bar{P}} & \text{on } \partial P, \end{cases} \tag{3.6}$$

where

$$\begin{cases} G_m = (-i)^\ell \xi_\ell^2 \psi_{m-2-\ell} - 2i\hat{\kappa}\cdot\nabla\psi_{m-1} - \psi_{m-2} \\ F_m = \nabla((-i)^\ell \xi_\ell^2 \psi_{m-2-\ell})|_{\mathrm{P}} \cdot \mathbf{n} - (\nabla((-i)^\ell \xi_\ell^2 \psi_{m-2-\ell}) - \psi_{m-1}\hat{\kappa})|_{\bar{P}} \cdot \mathbf{n}, \end{cases} \tag{3.7}$$

where $\psi_m|_{\bar{P}}$ and $\psi_m|_{\mathrm{P}}$ indicate the trace of ψ_m on the $\bar{P}$ and P sides of the interface ∂P separating the two materials. The Neumann boundary value problem (3.5) is subject to the standard *solvability condition* given by

$$\langle G_m \rangle_{\bar{P}} + \langle F_m \rangle_{\partial P} = 0. \tag{3.8}$$

Here the area integral over the domain $\overline{P}$ is denoted by $\langle\cdot\rangle_{\overline{P}}$, the area integral over P is denoted by $\langle\cdot\rangle_P$, and the line integral over the interface ∂P separating the two materials is denoted by $\langle\cdot\rangle_{\partial P}$. It is easily seen that the infinite system is highly coupled through the convolution terms appearing in (3.5), (3.6), and (3.7).

The iterative algorithm for solving the system is as follows. First note from the definition of ψ_0 it follows that that $\psi_0 = 1$ for $\mathbf{y}$ in $\overline{P}$. The function ψ_0 is determined inside P by solving (3.6) with Dirichlet boundary data $\psi_0|_{\mathrm{P}} = \psi_0|_{\bar{P}} = 1$ on ∂P. Then ψ_1 on $\overline{P}$ is the solution of (3.5) with Neumann data $\nabla\psi_1|_{\bar{P}} \cdot \mathbf{n} = -\psi_0|_{\overline{P}}\hat{\kappa} \cdot \mathbf{n}$ on ∂P. The process then continues with the boundary values on ∂P of ψ_m in $\bar{P}$ providing the Dirichlet data for ψ_m in P which, in turn, provides the Neumann data for ψ_{m+1} in $\bar{P}$, up to an additive constant. The term ξ_{m-2}^2 is determined by the consistency condition (3.8) and an inductive argument can be used to show that it is a monomial of degree m in $\hat{\kappa}$. The equations satisfied by $\psi_0, \dots, \psi_4$ inside $\bar{P}$, P, and ∂P are listed in Table 3 below.

$\bar{P}$	P	∂P
$\psi_0 = 1$	$\Delta\psi_0 = \psi_0$	$\nabla\psi_0\|_{\bar{\mathrm{P}}} \cdot \mathbf{n} = 0$
$\Delta\psi_1 + 2\hat{\kappa}\cdot\nabla\psi_0 = 0$	$\Delta\psi_1 + 2\hat{\kappa}\cdot\nabla\psi_0 = \psi_1$	$(\nabla\psi_1 + \psi_0\hat{\kappa})\|_{\bar{\mathrm{P}}} \cdot \mathbf{n} = 0$
$\Delta\psi_2 + 2\hat{\kappa}\cdot\nabla\psi_1 + \psi_0 = \xi_0^2\psi_0$	$\Delta\psi_2 + 2\hat{\kappa}\cdot\nabla\psi_1 + \psi_0 = \psi_2 + \xi_0^2\psi_0$	$(\nabla(\xi_0^2\psi_0) + \nabla\psi_2 + \psi_1\hat{\kappa})\|_{\bar{\mathrm{P}}} \cdot \mathbf{n}$ $= \nabla(\xi_0^2\psi_0)\|_{\mathrm{P}} \cdot \mathbf{n}$
$\Delta\psi_3 + 2\hat{\kappa}\cdot\nabla\psi_2 + \psi_1 = \xi_0^2\psi_1$	$\Delta\psi_3 + 2\hat{\kappa}\cdot\nabla\psi_2 + \psi_1 = \psi_3 + \xi_0^2\psi_1$	$(\nabla(\xi_0^2\psi_1) + \nabla\psi_3 + \psi_2\hat{\kappa})\|_{\bar{\mathrm{P}}} \cdot \mathbf{n}$ $= \nabla(\xi_0^2\psi_1)\|_{\mathrm{P}} \cdot \mathbf{n}$
$\Delta\psi_4 + 2\hat{\kappa}\cdot\nabla\psi_3 + \psi_2 = \xi_0^2\psi_2 - \xi_2^2\psi_0$	$\Delta\psi_4 + 2\hat{\kappa}\cdot\nabla\psi_3 + \psi_2$ $= (\xi_0^2\psi_2 - \xi_2^2\psi_0) + \psi_4$	$(\nabla(\xi_0^2\psi_2 - \xi_2^2\psi_0) + \nabla\psi_4 + \psi_3\hat{\kappa})\|_{\bar{\mathrm{P}}} \cdot \mathbf{n}$ $= \nabla(\xi_0^2\psi_2 - \xi_2^2\psi_0)\|_{\mathrm{P}} \cdot \mathbf{n}$

Table 3: Table of PDEs for ψ_m from the expansion in η.

Note in the table that $\xi_{odd}^2 = 0$ (meaning $\xi_\ell^2 = 0$ for $\ell = 1, 3, 5, \dots$). In the next section we identify a large class of shapes for the plasmonic rod cross sections for which the sequences $\{\psi_m(\mathbf{y})\}_{m=0}^\infty$ and $\{\xi_m^2\}_{m=0}^\infty$ satisfy the infinite system (3.5, 3.6, 3.7, 3.8) and $\langle\psi_m\rangle_{\overline{P}} = 0$, $m = 1, 2, \dots$. The mean zero property of ψ_m on $\overline{P}$ provides a tractable scenario for proving the convergence of the resulting power series. This topic is discussed further in section 4.

In what follows we will make use of the equivalent weak form of the infinite system. To introduce the weak form we introduce the space of complex valued square integrable functions with square integrable derivatives $H^1(Q)$. For u and v in $H^1(Q)$ the inner product is defined by

$$(u,v)_{H^1(Q)} = \left(\int_Q u\overline{v}\,d\mathbf{y} + \int_Q \nabla u\cdot\nabla\overline{v}\,d\mathbf{y}\right), \tag{3.9}$$

and the norm is given by $\|v\|_{H^1(Q)} = (v,v)^{1/2}_{H^1(Q)}$. The H^1 inner products and norms over P and $\overline{P}$ are defined similarly.

The weak form of the infinite system is given in terms of the space $H^1(Q)_{per}$ of functions in $H^1(Q)$ that take the same boundary values on opposite faces of Q. The weak form of the system (3.5, 3.6, 3.7, 3.8) is given by

$$\begin{aligned}\langle[\nabla\sigma'_{m-2}+\hat\kappa\sigma'_{m-3}]\cdot\nabla\bar v-[\hat\kappa\cdot\nabla\sigma'_{m-3}-\sigma'_{m-2}-\sigma''_{m-4}+\sigma'_{m-4}]\bar v\rangle_P +\\ +\langle[\nabla\sigma'_{m-2}+\hat\kappa\sigma'_{m-3}]\cdot\nabla\bar v-[\hat\kappa\cdot\nabla\sigma'_{m-3}-\sigma'_{m-2}-\sigma''_{m-4}+\sigma_{m-4}]\bar v\rangle_{\bar P} +\\ +\langle[\nabla\psi_m+\hat\kappa\psi_{m-1}]\cdot\nabla\bar v-[\hat\kappa\cdot\nabla\psi_{m-1}+\psi_{m-2}]\bar v\rangle_{\bar P}=0,\end{aligned} \tag{3.10}$$

for all $v\in H^1_{per}(Q)$, where $\sigma'_m = (-i)^\ell\xi^2_\ell\psi_{m-\ell}$ and $\sigma''_m = (-i)^\ell\psi_{m-\ell}\xi^2_{\ell-j}\xi^2_j$. The equivalence between (3.5, 3.6, 3.7) and the weak form follows from integration by parts and the solvability condition (3.8) follows from (3.10) on choosing the test function $v=1$ in (3.10).

4 Solutions of the Infinite System for Plasmonic Domains with Rectangular Symmetry

The goal here is to identify solutions of the infinite system for which one can prove convergence of the associated power series with a minimum of effort. Looking ahead we note that the convergence proof is expedited when one can apply the Poincare inequality to the restriction of ψ_m on $\overline{P}$ for m greater than some fixed value. To this end we seek a solution $(\{\psi_m(\mathbf{y})\}_{m=0}^\infty, \{\xi^2_m\}_{m=0}^\infty)$ such that for $m\geq 1$ one has $\langle\psi_m\rangle_{\overline{P}}=0$ and the sequences satisfy satisfy (3.5, 3.6, 3.7, 3.8) or equivalently satisfy (3.10). We show that we can find such solutions for the class of plasmonic domains P with rectangular symmetry. Here we suppose that the unit period cell is centered at the origin and the class of rectangular symmetric domains is given by the set of all shapes invariant under 180^o rotations about the origin. This class includes simply connected domains such as rectangles and ellipses as well as multiply connected domains. For these geometries and for each $m=1,2,3\ldots$ it is demonstrated that one can add an arbitrary constant to the restriction of the function ψ_m on $\overline{P}$ with out affecting the solvability condition (3.8).

Under the assumption of rectangular symmetry we will show that there exists an infinite sequence of functions $\{\psi_m\}_{m=1}^\infty$ in the space of $H^1(Q)$-periodic *real-valued* functions *with zero average in* $\bar P$ satisfying (3.10). For brevity, we denote this space by $H^1_*(Q)$.

We now record the symmetries necessarily satisfied by any solution $\psi_m\in H^1_*(Q)$ to (3.5, 3.6, 3.7) for plasmonic domains with rectangular symmetry. We denote the dependence of ψ_m on the unit vector $\hat\kappa$ by writing $\psi^{\hat\kappa}_m$, so that we have

(i) $\psi^{-\hat\kappa}_m(y) = (-1)^m\psi^{\hat\kappa}_m(y)$, $\forall y\in Q$ (homogeneity in $\hat\kappa$)

(ii) $\psi_m^{-\hat{\kappa}}(-y) = \psi_m^{\hat{\kappa}}(y)$, $\forall y \in Q$ (rectangular symmetry).

Statement (i) is true for inclusions of arbitrary shape, while statement (ii) is true only for inclusions with rectangular symmetry. Taking sums and differences of (i) and (ii) gives

$$\psi_m^{\hat{\kappa}}(-y) = (-1)^m \psi_m^{\hat{\kappa}}(y).$$

Thus the function $\psi_m^{\hat{\kappa}}$ is even or odd in Q according as the index m is even or odd. From its definition, $\psi_0 \equiv 1$ in $\overline{P}$ and trivially satisfies the solvability condition (3.8). The solvability of ψ_m when $m \geq 1$ is proved by induction on m using the weak form (3.10). We have the following theorem.

Theorem 4.1. *For each $\hat{\kappa}$, there exists a sequence of functions $\{\psi_m\}_{m=1}^{\infty}$, $\psi_m \in H_*^1(Q)$, and a sequence of real numbers $\{\xi_m^2\}$, with $\xi_{odd}^2 = 0$, solving the weak form (3.10) for each integer m.*

Proof. The proof is divided into the base case ($m = 1$ and $m = 2$) and the inductive step.

Base case:

The solvability for ψ_1 and ψ_2 can be established without the need to restrict to rectangular symmetric inclusions. This restriction will be necessary only in the inductive step. Setting $m = 1$ and $v \equiv 1$ in (3.10), we see that the left-hand side of (3.10) vanishes. This establishes the solvability for ψ_1. If we then take $\langle \psi_1 \rangle_{\bar{P}} = 0$, we have a solution $\psi_1 \in H_*^1(Q)$. Setting $m = 2$ and $v \equiv 1$ in (3.10), we obtain

$$\langle \sigma_0' \rangle_P + \langle \sigma_0' \rangle_{\bar{P}} - \langle \hat{\kappa} \cdot \nabla \psi_1 + \psi_0 \rangle_{\bar{P}} = 0.$$

Since $\langle \psi_0 \rangle_Q > 0$ (see Appendix) and $\langle \sigma_0' \rangle_P + \langle \sigma_0' \rangle_{\bar{P}} = \xi_0^2 \langle \psi_0 \rangle_Q$, this is one equation in one unknown ξ_0^2. Solving for ξ_0^2 then gives

$$\xi_0^2 = \frac{\langle \hat{\kappa} \cdot \nabla \psi_1 + \psi_0 \rangle_{\bar{P}}}{\langle \psi_0 \rangle_Q}. \tag{4.1}$$

Choosing this value for ξ_0^2 and also taking $\langle \psi_2 \rangle_{\bar{P}} = 0$, we have a solution $\psi_2 \in H_*^1(Q)$.

Inductive step:

Let $2n$ be an even positive integer and assume that (3.10) has solutions $\psi_m \in H_*^1(Q)$ for $m = 1, 2, ..., 2n$, with $\xi_{m-2}^2 \in \mathbb{R}$ and $\xi_{odd}^2 = 0$. Then (3.10) has solutions ψ_{2n+1}, $\psi_{2n+2} \in H_*^1(Q)$ for $m = 2n+1, 2n+2$ with $\xi_{2n-1}^2 = 0$ and $\xi_{2n}^2 \in \mathbb{R}$.

The solvability condition for ψ_{2n+1} is obtained by setting $v = 1$ and $m = 2n+1$ in the weak form, namely

$$\begin{aligned} &\langle [\hat{\kappa} \cdot \nabla \sigma_{2n-2}' - \sigma_{2n-1}' - \sigma_{2n-3}'' + \sigma_{2n-3}'] \rangle_P + \\ &+ \langle [\hat{\kappa} \cdot \nabla \sigma_{2n-2}' - \sigma_{2n-1}' - \sigma_{2n-3}'' + \sigma_{2n-3}'] \rangle_{\bar{P}} + \\ &\qquad + \langle [\hat{\kappa} \cdot \nabla \psi_{2n} + \psi_{2n-1}] \rangle_{\bar{P}} = 0. \end{aligned}$$

The hypothesis $\xi_{odd}^2 = 0$, $odd \leq 2n-2$, will imply that the convolutions σ_m, $m \leq 2n-2$, have the same even/odd property as the functions ψ_m. Indeed, wrting out σ_{2n-3}, we have

$$\begin{aligned} \sigma_{2n-3}' &= (-1)^\ell \xi_\ell^2 \psi_{2n-3-\ell} \\ &= (-1)^\ell \xi_\ell^2 \psi_{2n-3-\ell}^{(\ell \text{ even})}. \end{aligned}$$

Since $2n-3-\ell$ is odd when ℓ is even, it follows that σ'_{2n-3} is a linear combination of odd functions and is, therefore, an odd function. The same reasoning applies to all the other convolutions of index $\leq 2n-2$. Moreover, $\hat{\kappa}\cdot\nabla\sigma'_{2n-2}$ is an odd function, since σ'_{2n-2} is even. Thus, all integrals in the consistency condition above vanish (for the integrals in $\bar{P}$ we can also use the fact that all functions belong to $H^1_*(Q)$), except that

$$\langle\sigma'_{2n-1}\rangle_P + \langle\sigma'_{2n-1}\rangle_{\bar{P}} \;\; = \;\; (-i)^{2n-1}\xi^2_{2n-1}\langle\psi_0\rangle_Q.$$

Since $\langle\psi_0\rangle_Q > 0$ (see Appendix), the solvability condition for ψ_{2n+1} is simply $\xi^2_{2n-1} = 0$. We thus take $\xi^2_{2n-1} = 0$ to establish the existence of $\psi_{2n+1} = 0$. Moreover, since ψ_m and ξ_{m-2} are real by the induction hypothesis, $0 \leq m \leq 2n$, it follows that ψ_{2n+1} is real-valued. Thus, taking $\langle\psi_{2n+1}\rangle_{\bar{P}} = 0$, we have a solution $\psi_{2n+1} \in H^1_*(Q)$. Also, ψ_{2n+1} is an odd function since its index is odd. We now proceed to the solvability of ψ_{2n+2}, namely

$$\begin{aligned}\langle[\hat{\kappa}\cdot\nabla\sigma'_{2n-1} - \sigma'_{2n-2} - \sigma''_{2n-2} + \sigma'_{2n}]\rangle_P +\\ +\langle[\hat{\kappa}\cdot\nabla\sigma'_{2n-1} - \sigma'_{2n-2} - \sigma''_{2n-2} + \sigma'_{2n}]\rangle_{\bar{P}} +\\ +\langle[\hat{\kappa}\cdot\nabla\psi_{2n+1} + \psi_{2n}]\rangle_{\bar{P}} = 0.\end{aligned}$$

All terms in the above equation are real numbers, since we assumed ψ_m and ξ^2_{m-2} real for $0 \leq m \leq 2n$, with $\xi^2_{odd} = 0$, and we just took $\xi^2_{2n-1} = 0$ and ψ_{2n+1} is real-valued. Thus, this equation contains the only one undetermined term $(-i)^{2n}\xi^2_{2n}\langle\psi_0\rangle_Q$. Thus, we have one real equation with one real variable, so that taking ξ^2_{2n} to be such as to solve this equation and also taking $\langle\psi_{2n+2}\rangle_{\bar{P}} = 0$, we complete the proof of the inductive step. □

5 Convergence Proof

In this section we show that the power series $\sum_{m=0}^{\infty}\bar{p}_m\eta^m$, $\sum_{m=0}^{\infty}p_m\eta^m$ and $\sum_{m=0}^{\infty}\xi^2_m\eta^m$, where $\bar{p}_m = \|\psi_m\|_{H^1(\bar{P})}$ and $p_m = \|\psi_m\|_{H^1(P)}$, converge and provide lower bounds on their radius of convergence. This will then be used to show that the pair $h_\eta = \sum_{m=0}^{\infty}\overline{h}_0 i^m\psi_m\eta^m$ and $\xi^2_\eta = \sum_{m=0}^{\infty}\xi^2_m\eta^m$ is a solution to the non-linear eigenvalue problem (2.11). In subsection 5.1, we present the Catalan Bound theorem, which is used to provide a lower bound on the radius of convergence of the power series. In subsection 5.2, we derive inequalities which bound $\bar{p}_m$, p_m and ξ^2_m in terms of lower index terms. In subsection 5.3, we present the properties of the Catalan numbers relevant for bounding convolutions of the kind appearing in (3.5) and (3.6). In subsection 5.4, we use an inductive argument on the inequalities of subsection 5.2 to prove the Catalan Bound. Finally, in subsection 5.2, we give a proof that the pair h_η and ξ^2_η is a solution to the eigenvalue problem (2.11).

5.1 The Catalan Bound

The following theorem is the main result of this paper

Theorem 5.1. *(Catalan Bound)*
For every integer m, we have that

$$\bar{p}_m,\; p_m,\; |\xi^2_m| \leq \beta C_m J^m \tag{5.1}$$

in which C_m is the m^{th} Catalan number, $\beta = max\{\bar{p}_0,\, p_0,\, |\xi^2_0|\}$ and $J = max\{J_1, J_2\}$, where the numbers J_1 and J_2 are determined as follows: J_1 is the smallest value of J such that

(5.1) *holds for* $m \leq 4$ *and* J_2 *is the smallest value of* J *for which the following polynomials* Q^*, R^*, S^* *in the variable* J^{-1} *are all less than unity*

$$\begin{aligned}Q^* = \Omega_{\bar{P}}[\ & A\{2E(4)\beta J^{-2}1/3 + E(4)\beta J^{-3}5/42 + E(4)\beta J^{-4}1/21 + E^2(4)\beta^2 J^{-4}5/42\}+\\ & + 2E(4)\beta J^{-2}1/3 + 2E(4)\beta J^{-3}5/42 + E(4)\beta J^{-4}1/21 + E^2(4)\beta^2 J^{-4}5/42 + J^{-2}5/42\\ & + 2\Omega_{\bar{P}}(A\{2E(4)\beta J^{-3}5/42 + 2E(4)\beta J^{-4}1/21 + E(4)\beta J^{-5}1/42 + E^2(4)\beta^2 J^{-5}1/21\}+\\ & \qquad + 2E(4)\beta J^{-3}5/42 + 2E(4)\beta J^{-4}1/21 + E(4)\beta J^{-5}1/42+\\ & \qquad\qquad + E^2(4)\beta^2 J^{-5}1/21 + J^{-3}1/21 + 2J^{-2}5/42\ )],\end{aligned}$$

$$R^* = AQ^* + E(4)\beta J^{-2}1/3 + 2J^{-1}1/3 + J^{-2}5/42,$$

$$\begin{aligned}S^* = 4J\{ & \sqrt{\theta_{\bar{P}}}Q^* + \sqrt{\theta_P}(E(4)\beta J^{-2}(1/3) + E^2(4)\beta^2 J^{-3}(1/3) + E(4)\beta J^{-3}(5/42))\\ & + \sqrt{\theta_{\bar{P}}}(E(4)\beta J^{-2}(1/3) + E(4)\sqrt{\theta_{\bar{P}}}\beta J^{-3}(5/42) + \sqrt{\theta_P}J^{-3}(1/21))\} +\\ & + \sqrt{\theta_P}\{(\,|\xi_0^2|R^* + |\xi_2^2|J^{-2}(1/7) + p_2 J^{-2}(1/7)\,) + (0.7976\beta)\}.\end{aligned}$$

The constants A, $\Omega_{\bar{P}}$, β, $\sqrt{\theta_{\bar{P}}}$, $\sqrt{\theta_P}$, $|\xi_0^2|$, $|\xi_2^2|$ *and* p_2 *are determined by the particular choice of inclusion, while* $E(4) = 16C_2/C_5 \leq 0.7619$.

All bounds obtained here are expressed in terms of the Catalan numbers, area fractions and geometric parameters that appear in the Poincare inequality and in an extension operator inequality. We start by listing these parameters and give the background for their description. It is known [20] that any $H^1(\overline{P})$ function ϕ can be extended into P as an $H^1(Q)$ function $E(\phi)$ such that $E(\phi) = \phi$ for $\mathbf{y}$ in $\overline{P}$ and

$$\|E(\phi)\|_{H^1(P)} \leq A\|\phi\|_{H^1(\overline{P})} \tag{5.2}$$

where A is a nonnegative constant and is independent of ϕ depending only on P. For general shapes A can be calculated via numerical solution of a suitable eigenvalue problem. Constants of this type appear[6] for high contrast expansions of the DC fields inside frequency independent dielectric media. The second constant is the Poincare constant $D^2_{\overline{P}}$ given by the reciprocal of the first nonzero Neumann eigenvalue of $\overline{P}$. In what follows we write $\Omega_{\overline{P}} = 1 + D^2_{\overline{P}}$. The last two geometric constants appearing in the bounds are the volume fractions of P and $\bar{P}$ given by θ_P and $\theta_{\bar{P}}$, respectively.

Using that $C_m \leq 4^m$ (see section 5.3), theorem (5.1) shows that $\sum \bar{p}_m \eta^m$, $\sum p_m \eta^m$ and $\sum \xi_m^2 \eta^m$ are convergent for $\eta \leq 1/4J$, so that one may prove the following theorem

Theorem 5.2. *(Solution of the Eigenvalue Problem) Let* $R = 1/4J$*, where* J *is the number prescribed by theorem* (5.1)*. Then* $\sum_{m=0}^{\infty} \xi_m^2 \eta^m$ *converges as a series of real numbers and* $\sum_{m=0}^{\infty} h_m \eta^m$ *converges in the* $H^1(Q)$ *Sobolev norm for* $\eta \leq R$ *and the positive number*

$$\xi = \xi_\eta = \left(\sum_{m=0}^{\infty} \xi_m^2 \eta^m\right)^{1/2}$$

and the function

$$h = h_\eta = \sum_{m=0}^{\infty} h_m \eta^m \in H^1_*(Q)$$

satisfy the eigenvalue problem given by the master system (2.11) *(or by* (1.2)*).*

The expansion for the dispersion relation follows immediately from Theorem 5.2 on writing $\omega_m^2(\mathbf{k}) = c^2k^2\xi_m^2$ and noting that $\xi_m^2 = 0$ for odd values of m and that ξ_0^2 is given by (7.1).

Corollary 5.1. *(The dispersion relation)*

$$\omega^2 = W_\eta^2(\mathbf{k}) = \sum_{m=0}^{\infty} \eta^{2m}\omega_{2m}^2(\mathbf{k}) \tag{5.3}$$

and ω_0^2 *is given by*

$$\omega_0^2 = \omega_{qs}^2(\mathbf{k}) = \frac{c^2k^2}{n_{qs}^2} \tag{5.4}$$

where the quasi static index of refraction is defined by

$$n_{qs}^{-2} = \frac{\langle \hat{\kappa}\cdot\nabla\psi_1 + \psi_0\rangle_{\overline{P}}}{\langle\psi_0\rangle_Q}. \tag{5.5}$$

We discuss the notions of effective properties and quasistatic properties in section 6.

5.2 The $\bar{p}_m$, p_m and ξ_m^2 Inequalities—Stability Estimates

We now derive the inequalities which bound $\bar{p}_m$, p_m and ξ_m^2 in terms of lower index terms. These inequalities follow from stability estimates for (3.5, 3.6, 3.7).

Theorem 5.3. *Let $m \geq 0$ be an integer. Then*

$$\begin{aligned}
\bar{p}_m &\leq \Omega_{\bar{P}}[A\{2q'_{m-2} + 2q'_{m-3} + q'_{m-4} + q''_{m-4}\} + 2\bar{q}'_{m-2} + 2\bar{q}'_{m-3} + \bar{q}'_{m-4} \\
&\quad + \bar{q}''_{m-4} + \bar{p}_{m-2} + 2\,\Omega_{\bar{P}}(A\{2q'_{m-3} + 2q'_{m-4} + q'_{m-5} + q''_{m-5}\} \\
&\quad + 2\bar{q}'_{m-3} + 2\bar{q}'_{m-4} + \bar{q}'_{m-5} + q''_{m-5} + \bar{p}_{m-3} + 2\bar{p}_{m-2})] \\
p_m &\leq A\bar{p}_m + q'_{m-2} + 2p_{m-1} + p_{m-2} \\
|\xi_{m-1}^2| &\leq \langle\psi_0\rangle_Q^{-1}\{\sqrt{\theta_P}\,q'^{*}_{m-1} + \sqrt{\theta_{\bar{P}}}\bar{p}_m + \\
&\quad + \sqrt{\theta_P}(q'_{m-2} + q''_{m-3} + q'_{m-3}) + \sqrt{\theta_{\bar{P}}}(\bar{q}'_{m-2} + \bar{q}''_{m-3} + \bar{q}'_{m-3})\},
\end{aligned} \tag{5.6}$$

where the $\bar{p}_m$ inequality holds for $m \geq 2$ only.

Here we have introduced the following notation for the convolution terms

$$\begin{aligned}
q'_m &= |\xi_\ell^2|p_{m-\ell} \\
q''_m &= p_{m-\ell}|\xi_{\ell-j}^2||\xi_j^2| \\
\bar{q}'_m &= |\xi_\ell^2|\bar{p}_{m-\ell} \\
\bar{q}''_m &= \bar{p}_{m-\ell}|\xi_{\ell-j}^2||\xi_j^2| \\
q'^{*}_{m-1} &= |\xi_\ell^2|p_{m-1-\ell}^{(\ell<m-1)}.
\end{aligned}$$

Proof. We start by proving the p_m inequality. Recalling that (3.6) is satisfied by ψ_m in P gives

$$\begin{cases} \Delta\psi_m = \psi_m + G_m, & \text{in } P \\ \psi_m|_{\mathrm{p}} = \psi_m|_{\bar{P}}, & \text{on } \partial P \end{cases}$$

where $G_m = (-i)^\ell \xi_\ell^2 \psi_{m-2-\ell} - 2\hat{\kappa}\cdot\nabla\psi_{m-1} - \psi_{m-2}$. Write the orthogonal decomposition $\psi_m = u_m + v_m$, where

$$\begin{cases} \Delta u_m = u_m, & \text{in } P \\ u_m = \psi_m, & \text{on } \partial P \end{cases} \tag{5.7}$$

and

$$\begin{cases} \Delta v_m = v_m + G_m, & \text{in } P \\ v_m = 0, & \text{on } \partial P. \end{cases}$$

We then have by the triangle inequality that

$$\|\psi_m\|_{H_1(P)} \leq \|u_m\|_{H_1(P)} + \|v_m\|_{H_1(P)}. \tag{5.8}$$

The term $\|u_m\|_{H_1(P)}$ is bounded using (5.2) and

$$\|u_m\|_{H_1(P)} \leq \|E(\psi_m)\|_{H^1(P)} \tag{5.9}$$

to obtain

$$\|u_m\|_{H_1(P)} \leq A\|\psi_m\|_{H_1(\bar{P})}. \tag{5.10}$$

Here (5.9) follows from the fact that the solution of (5.7) minimizes the $H^1(P)$ norm over all functions with the same trace on ∂P. The term $\|v_m\|_{H_1(P)}$ can be bounded using a direct integration by parts on the BVP for v_m

$$\|v_m\|_{H_1(P)} \leq \|G_m\|_{L_2(P)}. \tag{5.11}$$

Now,

$$\begin{aligned} \|G_m\|_{L_2(P)} &= \|(-i)^\ell \xi_\ell^2 \psi_{m-2-\ell} - 2\hat{\kappa}\cdot\nabla\psi_{m-1} - \psi_{m-2}\|_{L_2(P)} \\ &\leq |\xi_\ell^2|\|\psi_{m-2-\ell}\|_{L_2(P)} + 2|\hat{\kappa}|\||\nabla\psi_{m-2}|^2\|_{L_2(P)} + \|\psi_{m-2}^2\|_{L_2(P)} \\ &\leq |\xi_\ell^2| p_{m-2-\ell} + 2p_{m-1} + p_{m-2}, \end{aligned}$$

where $p_m = \|\psi_m\|_{H_1(P)}$. Using (5.10) and (5.11) in (5.8) gives

$$p_m \leq A\bar{p}_m + p_{m-2-\ell}|\xi_\ell^2| + 2p_{m-1} + p_{m-2},$$

or

$$p_m \leq A\bar{p}_m + q'_{m-2} + 2p_{m-1} + p_{m-2}. \tag{5.12}$$

and the p_m inequality is established. We now prove the $\bar{p}_m$ inequality. In the weak form (3.10), set $v = \psi_m$ in $\bar{P}$ and $v = u_m$ in P to obtain

$$\begin{aligned} &\langle[\nabla\sigma'_{m-2} + \hat{\kappa}\sigma'_{m-3}]\cdot\nabla\psi_m - [\hat{\kappa}\cdot\nabla\sigma'_{m-3} - \sigma'_{m-2} - \sigma''_{m-4} + \sigma'_{m-4}]\psi_m\rangle_{\bar{P}} + \\ &+\langle[\nabla\sigma'_{m-2} + \hat{\kappa}\sigma'_{m-3}]\cdot\nabla u_m - [\hat{\kappa}\cdot\nabla\sigma'_{m-3} - \sigma'_{m-2} - \sigma''_{m-4} + \sigma'_{m-4}]u_m\rangle_P + \\ &+\langle[\nabla\psi_m + \hat{\kappa}\psi_{m-1}]\cdot\nabla\psi_m - [\hat{\kappa}\cdot\nabla\psi_{m-1} + \psi_{m-2}]\psi_m\rangle_{\bar{P}} = 0, \end{aligned}$$

We now use the Cauchy-Schwarz inequality on the product of integrals appearing in each individual term. For the convolutions, we obtain

$$
\begin{aligned}
|\langle \nabla\sigma'_{m-2}\cdot\nabla u_m\rangle_P| &= |\langle \nabla((-i)^{\ell}\psi_{m-2-\ell}\xi_\ell^2)\cdot\nabla u_m\rangle_P| \\
&= |(-i)^{\ell}\xi_\ell^2\langle \nabla\psi_{m-2-\ell}\cdot\nabla u_m\rangle_P| \\
&\le |\xi_\ell^2|\bar{p}_{m-2-\ell}A\bar{p}_m, \\
&= q'_{m-2}A\bar{p}_m
\end{aligned}
$$

where we used that $\|u_m\|_{H_1(P)} \le A\bar{p}_m$. For the double-convolutions, we obtain

$$
\begin{aligned}
|\langle \sigma''_{m-4}u_m\rangle_P| &= |\langle((-i)^{\ell}\psi_{m-2-\ell}\xi_{\ell-j}^2\xi_j^2)u_m\rangle_P| \\
&= |(-i)^{\ell}\xi_{\ell-j}^2\xi_j^2\langle \nabla\psi_{m-2-\ell}\cdot\nabla u_m\rangle_P| \\
&\le |\xi_{\ell-j}^2||\xi_j^2|\bar{p}_{m-2-\ell}A\bar{p}_m \\
&= q''_{m-2}A\bar{p}_m
\end{aligned}
$$

Proceeding similarly with the other terms, we obtain

$$
\begin{aligned}
\langle \nabla\psi_m\cdot\nabla\psi_m\rangle_{\bar{P}} \le\; & \bar{p}_m(\,A\{2q'_{m-2}+2q'_{m-3}+q'_{m-4}+q''_{m-4}\}+ \\
& +2\bar{q}'_{m-2}+2\bar{q}'_{m-3}+\bar{q}'_{m-4}+\bar{q}''_{m-4}+2\bar{p}_{m-1}+\bar{p}_{m-2}).
\end{aligned} \tag{5.13}
$$

Since the functions ψ_m have zero average in $\overline{P}$, we have the Poincare inequality

$$
\langle \psi_m^2\rangle_{\bar{P}} \le D_{\overline{P}}^2\langle \nabla\psi_m\cdot\nabla\psi_m\rangle_{\bar{P}}, \tag{5.14}
$$

where the constant $D_{\overline{P}}$ can be computed from the Rayleigh quotient characterization of the first positive eigenvalue for the free membrane problem in $\overline{P}$. A simple computation using (5.14) then gives

$$
\bar{p}_m^2 \le \Omega_{\bar{P}}\langle \nabla\psi_m\cdot\nabla\psi_m\rangle_{\bar{P}}, \tag{5.15}
$$

where $\Omega_{\bar{P}} = D_{\bar{P}}^2+1$. Using this inequality (5.13) gives:

$$
\begin{aligned}
\bar{p}_m \le\; & \Omega_{\bar{P}}(\,A\{2q'_{m-2}+2q'_{m-3}+q'_{m-4}+q''_{m-4}\}+ \\
& +2\bar{q}'_{m-2}+2\bar{q}'_{m-3}+\bar{q}'_{m-4}+\bar{q}''_{m-4}+\bar{p}_{m-2}+2\bar{p}_{m-1}).
\end{aligned} \tag{5.16}
$$

It will turn out to be to our advantage to apply (5.16) to the last term $2\bar{p}_{m-1}$ in (5.16) so as to replace it with

$$
\begin{aligned}
\bar{p}_{m-1} \le\; & \Omega_{\bar{P}}(\,A\{2q'_{m-3}+2q'_{m-4}+q'_{m-5}+q''_{m-5}\}+ \\
& +\bar{q}'_{m-3}+2q'_{m-4}+\bar{q}'_{m-5}+\bar{q}''_{m-5}+\bar{p}_{m-3}+2\bar{p}_{m-2}).
\end{aligned} \tag{5.17}
$$

Using (5.17) in (5.16) yields the $\bar{p}_m$ inequality in (5.6), valid for $m \ge 2$ (for $m = 1$, use (5.16)):

Last we establish the ξ_{m-1}^2 inequality. Setting $v = 1$ in the weak form (3.10) we obtain

$$
\begin{aligned}
& \langle \hat{\kappa}\cdot\nabla\sigma'_{m-3}-\sigma'_{m-2}-\sigma''_{m-4}+\sigma'_{m-4}\rangle_P+ \\
& +\langle \hat{\kappa}\cdot\nabla\sigma'_{m-3}-\sigma'_{m-2}-\sigma''_{m-4}+\sigma'_{m-4}\rangle_{\bar{P}}+ \\
& \qquad +\langle \hat{\kappa}\cdot\nabla\psi_{m-1}+\psi_{m-2}\rangle_{\bar{P}} = 0.
\end{aligned} \tag{5.18}
$$

(recall that for m odd, each term on the left-hand side of the above equation vanishes individually). Solving for ξ^2_{m-2} we then obtain

$$\begin{aligned} -(-i)^{m-2}\xi^2_{m-2}\langle\psi_0\rangle_Q = \langle\hat\kappa\cdot\nabla\sigma'_{m-3} - \sigma'^{\,*}_{m-2} - \sigma''_{m-4} + \sigma'_{m-4}\rangle_P + \\ +\langle\hat\kappa\cdot\nabla\sigma'_{m-3} - \sigma'^{\,*}_{m-2} - \sigma''_{m-4} + \sigma'_{m-4}\rangle_{\bar P} + \\ +\langle\hat\kappa\cdot\nabla\psi_{m-1} + \psi_{m-2}\rangle_{\bar P}. \end{aligned} \tag{5.19}$$

We shall be using this equality for $m \geq 5$ only, so that $\langle\sigma'^{\,*}_{m-2}\rangle_{\bar P} = 0$ and $\langle\psi_{m-2}\rangle_{\bar P} = 0$. Moreover, using the inequality

$$\langle|\psi_m|\rangle_P \leq \sqrt{\theta_P\langle|\psi_m|^2\rangle_P} \tag{5.20}$$

and similarly for $\bar P$, where θ_P and $\theta_{\bar P}$ denote the volume fractions of the regions P and $\bar P$ ($\theta_p + \theta_{\bar p} = 1$), we have that $\langle\psi_m\rangle_P \leq \sqrt{\theta_P}\, p_m$ and $\langle\psi_m\rangle_{\bar P} \leq \sqrt{\theta_{\bar P}}\,\bar p_m$. Thus, proceeding with (5.19) as we did in the previous stability estimates, we obtain

$$\begin{aligned} |\xi^2_{m-2}| \;\leq\; & \langle\psi_0\rangle_Q^{-1}\{\sqrt{\theta_P}\,p_{m-2-\ell}|\xi^2_\ell|^{\ell<m-2} + \sqrt{\theta_{\bar P}}\bar p_{m-1} + \sqrt{\theta_P}(q'_{m-3} + q''_{m-4} + q'_{m-4}) + \\ & +\sqrt{\theta_{\bar P}}(\bar q'_{m-3} + \bar q''_{m-4} + \bar q'_{m-4})\}. \end{aligned} \tag{5.21}$$

Since the iteration scheme at each step involves p_m and $\overline{p}_m$ and ξ^2_{m-1} we adjust subscripts in (5.21) to obtain

$$\begin{aligned} |\xi^2_{m-1}| \;\leq\; & \langle\psi_0\rangle_Q^{-1}\{\sqrt{\theta_P}\,q'^{*}_{m-1} + \sqrt{\theta_{\bar P}}\bar p_m + \sqrt{\theta_P}(q'_{m-2} + q''_{m-3} + q'_{m-3}) + \\ & +\sqrt{\theta_{\bar P}}(\bar q'_{m-2} + \bar q''_{m-3} + \bar q'_{m-3})\} \end{aligned} \tag{5.22}$$

and the ξ^2_{m-1} inequality is established. □

5.3 The Catalan Numbers

We briefly present some facts about the Catalan numbers which will be used in the sequel and indicate with a simple example why they are necessary in the proof. The Catalan numbers C_m are defined algebraically through the recursion

$$C_{m+1} = C_{m-\ell}C_\ell, \quad C_0 = 1. \tag{5.23}$$

They are named after E. Catalan and are one of the special integers that arise in many combinatorial contexts [18] as well as in the study of random processes [13]. By computing their generating function [18], it can be shown that

$$C_m = \frac{1}{m+1}\binom{2m}{m}$$

and a simple computation gives their ratio

$$\frac{C_{m+1}}{C_m} = 4 - \frac{6}{m+2} \quad \text{and} \quad \frac{C_m}{C_{m+1}} = \frac{1}{4} + \frac{3}{8m+6}, \tag{5.24}$$

so that we have the exponential bound

$$C_m \leq 4^m. \tag{5.25}$$

It will be convenient to introduce the following notation

$$\rho_m^k = \frac{C_{m-k}}{C_m}. \tag{5.26}$$

From (5.24), it is clear that ρ_m^k is decreasing in both m and k. In section 5.4 we shall make use of the following table of values for ρ_5^k

k	0	1	2	3	4
ρ_5^k	1	1/3	5/42	1/21	1/42

Table 4: Values of ρ_5^k.

We end this section with a short discussion on how the Catalan numbers will be used to prove exponential bounds on the sequences $\bar{p}_m$, p_m, ξ_m^2. Recall the many convolutions appearing in (5.6) and suppose that we wish to prove inductively that certain positive numbers $\{b_\ell\}_{\ell=0}^\infty$ are bounded exponentially,

$$b_\ell \leq b_0 r^\ell, \tag{5.27}$$

using the information that they are bounded by the convolution of the previous terms,

$$b_{m+1} \leq b_\ell b_{m-\ell}. \tag{5.28}$$

Assuming (5.27) for $0 \leq \ell \leq m$, inequality (5.28) gives

$$b_{m+1} \leq (b_0 r^\ell)(b_0 r^{n-\ell}) \leq m\frac{b_0^2}{r} r^{m+1}$$

The factor m will grow with each iteration of this estimate, giving super-exponential growth. If we use instead the induction hypothesis

$$b_\ell \leq b_0 r^\ell \ell!, \tag{5.29}$$

we obtain

$$\begin{aligned} b_{m+1} &\leq b_\ell b_{m-\ell} \\ &\leq b_0^2 r^m \ell!(m-\ell)!. \end{aligned} \tag{5.30}$$

The convolution $\ell!(m-\ell)!$ has $m+1$ terms, the largest of which is $m!$. Thus, inequality (5.30) gives

$$b_{m+1} \leq \frac{b_0^2}{r} r^{m+1}(m+1)!, \tag{5.31}$$

and the induction is successful for $r \geq b_0$. Of course, bound (5.30) does not give exponential growth, but its proof suggests that factorials work well with convolutions. Indeed, there is a special combination of factorials which does give exponential growth, namely the Catalan number C_m. If we assume that

$$b_\ell \leq b_0 r^\ell C_\ell, \tag{5.32}$$

then

$$\begin{aligned} b_{m+1} &\leq b_\ell b_{m-\ell} \\ &\leq b_0^2 r^m C_\ell C_{m-\ell} \\ &= \frac{b_0^2}{r} r^{m+1} C_{m+1}, \end{aligned}$$

and using that $C_m \leq 4^m$, an exponential bound is obtained.

5.3.1 The Even Part of the Catalan Convolution

The fact that $\xi_{odd}^2 = 0$ needs to be taken into account in order to provide a suitable upper estimate on the incomplete convolution term q'^{*}_{m-1} appearing in the ξ_{m-1}^2 inequality in (5.6). Thus we consider the convolution $C_{n-\ell}C_\ell$ with the odd values of the index ℓ omitted and denote it by $C_{n-\ell}C_\ell^{(\ell\ even)}$. We then define the even part $E(n)$ by

$$E(n) = \frac{C_{n-\ell}C_\ell^{(\ell\ even)}}{C_{n-\ell}C_\ell}. \tag{5.33}$$

The following lemma gives the estimate $E(n) \leq E(4)$, $n \geq 4$.

Lemma 5.1.

(**i**) $E(2m)$*is a decreasing sequence*

(**ii**) $E(2m+1) = 1/2$.

Thus, for all $m \geq 4$, *we have that* $E(m) \leq max\{E(4), 1/2\} = E(4)$.

Proof. Statement (ii) is actually just an observation, as one can see by writing out the sum $C_{n-\ell}C_\ell$, e.g., for $n = 7$

$$\begin{aligned} C_{7-\ell}C_\ell &= C_7C_0 + C_6C_1 + C_5C_2 + C_4C_3 + C_3C_4 + C_2C_5 + C_1C_6 + C_0C_7 \\ &= 2(C_7C_0 + C_5C_2 + C_3C_4 + C_1C_6) \\ &= 2C_{7-\ell}C_\ell^{(\ell\ even)}. \end{aligned}$$

Statement (ii) can be deduced from the following identity [17]

$$C_{2m-2\ell}C_{2\ell} = 4^m C_m.$$

Indeed, dividing both sides of the identity by C_{2m+1}, we obtain

$$\begin{aligned} E(2m) &= \frac{4^m C_m}{C_{2m+1}} \\ &= \frac{1}{4}\frac{4C_m}{C_{m+1}}\frac{4C_{m+1}}{C_{m+2}} \cdots \frac{4C_{2m}}{C_{2m+1}}. \end{aligned}$$

From 5.24, each of the above fractions $4C_m/C_{m+\ell}$, $\ell = 1, 2, ..., m+1$, is a decreasing sequence in m so that their product is also decreasing in m. This completes the proof. ☐

5.4 Proof of the Catalan Bound

Before proceeding to the proof, we note that the numerical value of the radius of convergence is affected only by J and not by β, which affects the error term in approximating the full series by a finite series (see Appendix for values of J for circular inclusions).

Proof. (Catalan Bound, theorem (5.1)) Fix the values of the geometric parameters A, $\mathbf{\Omega_{\bar{P}}}$, θ_P and $\theta_{\bar{P}}$ in (5.6). Using (5.6) recursively, we can then determine J_1 such that

$$\bar{p}_m,\, p_m,\, |\xi^2_m| \leq \beta C_m J_1^m, \quad 0 \leq m \leq 4.$$

In the appendix, we have written explicitly the bounds a recursive use of (5.6) gives for $m \leq 4$. We now proceed inductively: assume that

$$\bar{p}_n,\, p_n,\, |\xi^2_n| \leq \beta C_n J^n, \quad n \in \{0, 1, 2, \ldots, m-1\}, \tag{5.34}$$

where $m \geq 5$. We then get for the single convolutions

$$\begin{aligned}
q'_{m-k} &= p_{m-k-\ell}|\xi^2_\ell| \\
&\leq (\beta C_{m-k-\ell} J^{m-k-\ell})(\beta C_\ell J^\ell)^{(\ell \text{ } even)} \\
&= \beta^2 J^{m-k} C_{m-k-\ell} C_\ell^{(\ell \text{ } even)} \\
&\leq E(4)\beta^2 J^{m-k} C_{m-k-\ell} C_\ell \\
&= E(4)\beta J^{-k} \left(\frac{C_{m+1-k}}{C_m}\right) \beta J^m C_m \\
&= E(4)\beta J^{-k} \rho_m^{k-1}\, \beta J^m C_m.
\end{aligned} \tag{5.35}$$

where $\rho_m^k = C_{m-k}/C_m$ and lemma (5.1) was used to introduce the factor $E(4)$. Similarly, for double convolutions we get

$$\begin{aligned}
q''_{m-k} &= p_{m-k-\ell}|\xi^2_{\ell-j}||\xi^2_j| \\
&\leq (\beta C_{m-k-\ell} J^{m-k-\ell})(\beta C_{\ell-j} J^{\ell-j})^{(\ell-j \text{ } even)}(\beta C_j J^j)^{(j \text{ } even)} \\
&= \beta^3 J^{m-k} C_{m-k-\ell} C_{\ell-j}^{(\ell-j \text{ } even)} C_j^{(j \text{ } even)} \\
&\leq E^2(4)\beta^3 J^{m-k} C_{m-k-\ell} C_{\ell-j} C_j \\
&= E^2(4)\beta^3 J^{m-k} C_{m-k-\ell} C_{\ell+1} \\
&\leq E^2(4)\beta^3 J^{m-k} C_{m+2-k} \\
&= E^2(4)\beta^2 J^{-k} \left(\frac{C_{m+2-k}}{C_m}\right) \beta J^m C_m \\
&= E^2(4)\beta^2 J^{-k} \rho_m^{k-2}\, \beta J^m C_m
\end{aligned} \tag{5.36}$$

where the factor $E(4)^2$ comes from using lemma (5.1) twice. For the non-convolution terms

$$\begin{aligned}
p_{m-k} &\leq \beta J^{m-k} C_{m-k} \\
&= J^{-k} \left(\frac{C_{m-k}}{C_m}\right) \beta J^m C_m \\
&= J^{-k} \rho_m^k\, \beta J^m C_m.
\end{aligned} \tag{5.37}$$

The same bounds hold for the terms $\bar{p}_{m-k}$, $\bar{q}'_{m-k}$ and $\bar{q}''_{m-k}$ so that we have

$$\begin{array}{rcl} \bar{p}_{m-k},\, p_{m-k} & \leq & J^{-k}\rho_m^k\,\beta J^m C_m \\ \bar{q}'_{m-k},\, q'_{m-k} & \leq & E(4)\beta J^{-k}\rho_m^{k-1}\,\beta J^m C_m \\ \bar{q}''_{m-k},\, q''_{m-k} & \leq & E^2(4)\beta^2 J^{-k}\rho_m^{k-2}\,\beta J^m C_m. \end{array} \tag{5.38}$$

The proof now essentially consists of applying these bounds to all terms in inequalities (5.6). The factor J^{-k} appearing on the right-hand side of each inequality is the workhorse of the proof: by taking J sufficiently large, it will allow us to close the induction argument. The incomplete convolution term q'^{*}_{m-1} presents special difficulties, since attempting a bound of the type (5.38) for this term does not produce a factor of J^{-k} (actually, it produces $J^0 = 1$).

Recall the $\bar{p}_m$ inequality from (5.6)

$$\begin{aligned} \bar{p}_m \leq \Omega_{\bar{P}}[A\{2q'_{m-2} + 2q'_{m-3} + q'_{m-4} + q''_{m-4}\} + & \\ + 2\bar{q}'_{m-2} + 2\bar{q}'_{m-3} + \bar{q}'_{m-4} + \bar{q}''_{m-4} + \bar{p}_{m-2} + & \\ + 2\,\Omega_{\bar{P}}(A\{2q'_{m-3} + 2q'_{m-4} + q'_{m-5} + q''_{m-5}\} + & \\ + 2\bar{q}'_{m-3} + 2\bar{q}'_{m-4} + \bar{q}'_{m-5} + q''_{m-5} + \bar{p}_{m-3} + 2\bar{p}_{m-2})] & \end{aligned}$$

Using (5.38) on this inequality gives

$$\bar{p}_m \leq Q_m\,\beta J^m C_m, \tag{5.39}$$

where Q_m is the following polynomial in J^{-1}

$$\begin{aligned} Q_m = \Omega_{\bar{P}}[\; & A\{2E(4)\beta J^{-2}\rho_m^1 + E(4)\beta J^{-3}\rho_m^2 + E(4)\beta J^{-4}\rho_m^3 + E^2(4)\beta^2 J^{-4}\rho_m^2\} + \\ & + 2E(4)\beta J^{-2}\rho_m^1 + 2E(4)\beta J^{-3}\rho_m^2 + E(4)\beta J^{-4}\rho_m^3 + E^2(4)\beta^2 J^{-4}\rho_m^2 + J^{-2}\rho_m^2 + \\ & + 2\Omega_{\bar{P}}(A\{2E(4)\beta J^{-3}\rho_m^2 + 2E(4)\beta J^{-4}\rho_m^3 + E(4)\beta J^{-5}\rho_m^4 + E^2(4)\beta^2 J^{-5}\rho_m^3\} + \\ & + 2E(4)\beta J^{-3}\rho_m^2 + 2E(4)\beta J^{-4}\rho_m^3 + E(4)\beta J^{-5}\rho_m^4 + E^2(4)\beta^2 J^{-5}\rho_m^3 + J^{-3}\rho_m^3 + 2J^{-2}\rho_m^2\;)]. \end{aligned}$$

Since we shall be using this inequality for $m \geq 5$ only, table 5.3 can be used to bound the numbers ρ_m^k, so that we may write $Q_m \leq Q^*$, where

$$\begin{aligned} Q^* = \Omega_{\bar{P}}[\; & A\{2E(4)\beta J^{-2}1/3 + E(4)\beta J^{-3}5/42 + E(4)\beta J^{-4}1/21 + E^2(4)\beta^2 J^{-4}5/42\} + \\ & + 2E(4)\beta J^{-2}1/3 + 2E(4)\beta J^{-3}5/42 + E(4)\beta J^{-4}1/21 + E^2(4)\beta^2 J^{-4}5/42 + J^{-2}5/42 \\ & + 2\Omega_{\bar{P}}(A\{2E(4)\beta J^{-3}5/42 + 2E(4)\beta J^{-4}1/21 + E(4)\beta J^{-5}1/42 + E^2(4)\beta^2 J^{-5}1/21\} + \\ & + 2E(4)\beta J^{-3}5/42 + 2E(4)\beta J^{-4}1/21 + E(4)\beta J^{-5}1/42 + \\ & + E^2(4)\beta^2 J^{-5}1/21 + J^{-3}1/21 + 2J^{-2}5/42\;)]. \end{aligned} \tag{5.40}$$

The strategy now is to determine similar polynomials R_m and S_{m-1} for the other two inequalities, that is

$$\begin{array}{rcl} p_m & \leq & R_m\,\beta J^m C_m \\ |\xi^2_{m-1}| & \leq & S_{m-1}\,\beta J^{m-1} C_{m-1}, \end{array}$$

and then take J large enough that all three polynomials are less than unity, allowing us to complete the induction argument. Having obtained Q_m, it is straightforward to obtain R_m. Indeed, using (5.38) and (5.39), the p_m inequality in (5.6) yields

$$p_m \leq R_m \, \beta J^m C_m,$$

where

$$R_m = AQ_m + E(4)\beta J^{-2}\rho^1_m + 2J^{-1}\rho^1_m + J^{-2}\rho^2_m.$$

Thus, $R_m \leq R^*$, where

$$R^* = AQ^* + E(4)\beta J^{-2}1/3 + 2J^{-1}1/3 + J^{-2}5/42. \tag{5.41}$$

The ξ^2_{m-1} inequality requires a little more care due to the presence of the incomplete convolution term ${q'}^*_{m-1}$. For the remaining terms, we proceed as we did with the previous inequalities:

$$\begin{aligned}\sqrt{\theta_{\bar{P}}}\bar{p}_m + \sqrt{\theta_P}({q'}_{m-2} + {q''}_{m-3} + {q'}_{m-3}) + \sqrt{\theta_{\bar{P}}}(\bar{q}'_{m-2} + \sqrt{\theta_{\bar{P}}}|\xi^2_\ell \xi^2_{m-3-\ell}| + \sqrt{\theta_P}|\xi^2_{m-3}|) \quad \leq \\ \{\sqrt{\theta_{\bar{P}}}Q_m + \sqrt{\theta_P}(0.5\beta J^{-2}\rho^1_m + 0.25\beta^2 J^{-3}\rho^1_m + 0.5\beta J^{-3}\rho^2_m) \\ +\sqrt{\theta_{\bar{P}}}(0.5\beta J^{-2}\rho^1_m + 0.5\sqrt{\theta_{\bar{P}}}\beta J^{-3}\rho^2_m + J^{-3}\rho^3_m)\}\,\beta J^m C_m.\end{aligned}$$

since this is an upper bound on $|\xi^2_{m-1}|$, we must replace the term $\beta J^m C_m$ with $\beta J^{m-1}C_{m-1}$ as follows:

$$\begin{aligned}\beta J^m C_m &= J\left(\frac{C_m}{C_{m-1}}\right)\beta J^{m-1}C_{m-1} \\ &\leq 4J\,\beta J^{m-1}C_{m-1}.\end{aligned}$$

Using this replacement and the bounds 5.3 on the numbers ρ^k_m, we obtain the upper bound

$$\begin{aligned}4J\{\sqrt{\theta_{\bar{P}}}Q^* + \sqrt{\theta_P}(E(4)\beta J^{-2}(1/3) + E^2(4)\beta^2 J^{-3}(1/3) + E(4)\beta J^{-3}(5/42)) \\ +\sqrt{\theta_{\bar{P}}}(E(4)\beta J^{-2}(1/3) + E(4)\sqrt{\theta_{\bar{P}}}\beta J^{-3}(5/42) + \sqrt{\theta_P}J^{-3}(1/21))\}\,\beta J^{m-1}C_{m-1}\end{aligned} \tag{5.42}$$

It remains to deal with ${q'}^*_{m-1}$. We proceed as follows:

$$\begin{aligned}{q'}^*_{m-1} &= p_{m-1-\ell}|\xi^2_\ell|^{\ell<m-1} &(5.43)\\ &= p_{m-1}|\xi^2_0| + p_{m-3}|\xi^2_2| + p_2|\xi^2_{m-3}| + p_{m-1-\ell}|\xi^2_\ell|^{2<\ell<m-3}. &(5.44)\end{aligned}$$

The non-convolution terms then give

$$\begin{aligned}&p_{m-1}|\xi^2_0| + p_{m-3}|\xi^2_2| + p_2|\xi^2_{m-3}| \\ &\qquad \leq \left(|\xi^2_0|R_{m-1} + |\xi^2_2|J^{-2}\frac{C_{m-3}}{C_{m-1}} + p_2 J^{-2}\frac{C_{m-3}}{C_{m-1}}\right)\beta J^{m-1}C_{m-1} \\ &\qquad\qquad \leq (\,|\xi^2_0|R^* + |\xi^2_2|J^{-2}(1/7) + p_2 J^{-2}(1/7)\,)\,\beta J^{m-1}C_{m-1},\end{aligned} \tag{5.45}$$

since $C_{m-3}/C_{m-1} \le C_2/C_4 = 1/7$, if $m \ge 5$. The remaining term $p_{m-1-\ell}|\xi_\ell^2|^{2<\ell<m-3}$ is treated in a completely different manner:

$$\begin{aligned}
p_{m-1-\ell}|\xi_\ell^2|^{2<\ell<m-3} &= p_{m-5}|\xi_4^2| + p_{m-7}|\xi_6^2| + \cdots + p_6|\xi_{m-8}^2| + p_4|\xi_{m-5}^2| \\
&\le (C_{m-5}C_4 + C_{m-7}C_6 + \cdots + C_6C_{m-7} + C_4C_{m-5})\,\beta^2 J^{m-1} \\
&\le (C_{m-1-\ell}C_\ell^{(\ell\ even)} - 2C_2C_{m-3} - 2C_0C_{m-1})\,\beta^2 J^{m-1} \\
&= (E(4)C_{m-1-\ell}C_\ell - 2C_2C_{m-3} - 2C_0C_{m-1})\,\beta^2 J^{m-1} \\
&= (E(4)C_m - 2C_2C_{m-3} - 2C_0C_{m-1})\,\beta^2 J^{m-1} \\
&= \left(\beta\frac{E(4)C_m - 2C_2C_{m-3} - 2C_0C_{m-1}}{C_{m-1}}\right)\beta J^{m-1}C_{m-1} \\
&\le \beta(E(4)4 - 1/4 - 2)\,\beta J^{m-1}C_{m-1}, \\
&\le (0.7976\beta)\,\beta J^{m-1}C_{m-1},
\end{aligned} \tag{5.46}$$

Thus, adding (5.42), (5.45) and (5.46), we set

$$\begin{aligned}
S^* = 4J\{&\sqrt{\theta_{\bar P}}Q^* + \sqrt{\theta_P}(E(4)\beta J^{-2}(1/3) + E^2(4)\beta^2 J^{-3}(1/3) + E(4)\beta J^{-3}(5/42)) \\
&+\sqrt{\theta_{\bar P}}(E(4)\beta J^{-2}(1/3) + E(4)\sqrt{\theta_{\bar P}}\beta J^{-3}(5/42) + \sqrt{\theta_P}J^{-3}(1/21))\} + \\
&+\sqrt{\theta_P}\{(\,|\xi_0^2|R^* + |\xi_2^2|J^{-2}(1/7) + p_2J^{-2}(1/7)\,) + (0.7976\beta)\}.
\end{aligned} \tag{5.47}$$

Thus, taking J_2 such that $Q^*(J_2)$, $R^*(J_2)$, $S^*(J_2) \le 1$ and $J = \max\{J_1,\, J_2\}$, we have shown that the induction hypothesis (5.34) implies

$$\bar p_m,\, p_m,\, |\xi_m^2| \le \beta C_m J^m, \tag{5.48}$$

so that in fact (5.48) holds for every integer m. □

Remark: The Catalan bound could turn out to be a very crude estimate, for every time the triangle inequality is used in the above proof, no cancellation is taken into consideration.

5.5 Proof of Theorem 5.2: Solution of the Eigenvalue Problem

Proof. The weak form of the master system is

$$\int_Q \left[\epsilon_\eta^{-1}(\nabla + i\eta\hat\kappa)h_\eta(y)\cdot(\nabla - i\eta\hat\kappa)\bar v(y) - \eta^2\xi_\eta^2 h_\eta(y)\bar v(y)\right] = 0 \quad \text{for all } v \in H^1_{\text{per}}(Q). \tag{5.49}$$

Using that $\epsilon_\eta^{-1} = \eta^2\xi_\eta^2/(\eta^2\xi_\eta^2 - 1)$ in P and $\epsilon_\eta = 1$ in $\bar P$, and multiplying by $(\eta^2\xi_\eta^2 - 1)$, gives the equivalent system

$$a_\eta(h, \xi^2; v) = 0 \quad \text{for all } v \in H^1_{\text{per}}(Q),$$

in which

$$\begin{aligned}
a_\eta(h,\xi^2;v) = -\int_{\bar P}&(\nabla + i\eta\hat\kappa)h\cdot(\nabla - i\eta\hat\kappa)\bar v + \\
&+\int_Q\left[\eta^2\xi^2(\nabla + i\eta\hat\kappa)h\cdot(\nabla - i\eta\hat\kappa)\bar v - (\eta^2\xi^2 - 1)\eta^2\xi^2 h\bar v\right].
\end{aligned}$$

This form can be expanded in powers of η,

$$a_\eta(h,\xi^2;v) = a_0(h;v) - i\eta a_1(h;v) - \eta^2 a_2(h,\xi^2;v) + i\eta^3 a_3(h,\xi^2;v) + \eta^4 a_4(h,\xi^2;v) \quad (5.50)$$

in which the a_m are real forms

$$\begin{aligned}
a_0(h;v) &= -\int_{\bar{P}} \nabla h \cdot \nabla \bar{v}, \\
a_1(h;v) &= \int_{\bar{P}} (h\hat{\kappa} \cdot \nabla \bar{v} - \nabla h \cdot \hat{\kappa}\bar{v}), \\
a_2(h,\xi^2;v) &= \int_{\bar{P}} h\bar{v} - \xi^2 \int_Q (\nabla h \cdot \nabla \bar{v} + h\bar{v}), \\
a_3(h,\xi^2;v) &= \xi^2 \int_Q (h\hat{\kappa} \cdot \nabla \bar{v} - \nabla h \cdot \hat{\kappa}\bar{v}), \\
a_4(h,\xi^2;v) &= \xi^2 \int_Q (1-\xi^2) h\bar{v}.
\end{aligned}$$

Define the partial sums

$$\begin{aligned}
\xi_\eta^{2,N} &= \sum_{m=0}^{N} \eta^m \xi_m^2, \\
h_\eta^N &= \sum_{m=0}^{N} \eta^m h_m.
\end{aligned}$$

For $\eta < R$, the sequence $\{\xi_\eta^{2,N}\}$ converges to a number ξ_η^2 and the sequence $\{h_\eta^N\}$ converges in H_*^1 to a function h_η; thus

$$a_j(h_\eta^N, \xi_\eta^{2,N}; v) \to a_j(h_\eta, \xi_\eta^2; v) \quad \text{for all } v \in H^1_{\text{per}}(Q) \text{ and } i = 0, \ldots, 4.$$

Therefore, $a_j(h_\eta, \xi_\eta^2; v)$, $j = 1, \ldots, 4$, has a convergent series representation in powers of η, in which the m^{th} coefficient is related to the coefficients ξ_ℓ and h_ℓ by

$$\begin{aligned}
&(j=0) \quad \int_{\bar{P}} -\nabla h_m \cdot \nabla \bar{v}, \\
&(j=1) \quad \int_{\bar{P}} \left(h_m \hat{\kappa} \cdot \nabla \bar{v} - \nabla h_m \cdot \hat{\kappa}\bar{v}\right), \\
&(j=2) \quad \int_{\bar{P}} h_m \bar{v} - \int_Q \left(\nabla(\xi_\ell^2 h_{m-\ell}) \cdot \nabla \bar{v} + (\xi_\ell^2 h_{m-\ell})\bar{v}\right), \\
&(j=3) \quad \int_Q \left((\xi_\ell^2 h_{m-\ell})\hat{\kappa} \cdot \nabla \bar{v} - \nabla(\xi_\ell^2 h_{m-\ell}) \cdot \hat{\kappa}\bar{v}\right), \\
&(j=4) \quad \int_Q \left(\xi_\ell^2 h_{m-\ell} - \xi_j^2 \xi_{\ell-j}^2 h_{m-\ell}\right) \bar{v}.
\end{aligned}$$

¿From these, one obtains the m^{th} coefficient of $a_\eta(h_\eta, \xi_\eta^2; v)$ (see 5.50), which, by means of the relations

$$\begin{aligned}
h_m &= h_0 i^m \psi_m, \\
\xi_\ell^2 h_{m-\ell} &= h_0 i^m \sigma'_m, \\
\xi_j^2 \xi_{\ell-j}^2 h_{m-\ell} &= h_0 i^m \sigma''_m,
\end{aligned}$$

is seen to be equal to the $-i^m h_0$ times the right-hand side of equation (3.10). All these coefficients are therefore equal to zero, and we conclude that

$$a_\eta(h_\eta, \xi_\eta^2; v) = 0.$$

This proves that the function h_η, together with the frequency $\sqrt{\xi_\eta}$ solve the weak form (5.49) of the master system. □

6 Effective Properties, Error Bounds and the Dispersion Relation

In this section we start by identifying a new type of effective property that follows directly from the dispersion relations. We then discuss the relation between effective properties and quasistatic properties. Next we provide explicit error bounds for finite-term approximations to the first branch of the dispersion relation for nonzero values of η. The error bounds show that numerical computation of the first two terms of the power series delivers an accurate and inexpensive numerical method for calculating dispersion relations for sub-wavelength plasmonic crystals.

6.1 The Effective Index of Refraction - Quasistatic Properties and Homogenization

The identification of an effective index of refraction valid for $\eta > 0$ follows directly from the dispersion relation given by Corollary 5.1. Indeed the effective refractive index n_{eff} is defined by expressing the dispersion relation as

$$\omega^2 = \frac{c^2 k^2}{n_{\text{eff}}^2} \tag{6.1}$$

and it follows immediately from (5.3) that the effective refractive index has the convergent power series expansion given by

$$n_{\text{eff}}^{-2} = n_{\text{qs}}^{-2} + \sum_{m=1}^{\infty} \eta^{2m} \xi_{2m}^2. \tag{6.2}$$

We emphasize that this effective index of refraction follows directly from the dispersion relation and is obtained from first principles.

We now discuss the relationship between the effective index of refraction and the quasistatic effective properties seen in the $d \to 0$ limit with k fixed. Having established that $h_\eta(\mathbf{y}) e^{i\eta\hat{\kappa}\cdot\mathbf{y}}$ is the solution to the unit cell problem, we can undo the change of variable $\mathbf{y} = k\mathbf{x}/\eta$ to see that the function

$$\hat{h}_\eta\left(\frac{k\mathbf{x}}{\eta}\right) e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_\eta t)}, \tag{6.3}$$

where $\hat{h}_\eta$ is the Q-periodic extension of h_η to all of $\mathbb{R}^2$, is a solution of

$$\nabla_{\mathbf{x}} \cdot (\epsilon_\eta^{-1} \nabla_{\mathbf{x}} \hat{h}_\eta) = \frac{1}{c^2} \partial_{tt} \hat{h}_\eta, \quad \mathbf{x} \in \mathbb{R}^2, \tag{6.4}$$

for every η in the radius of convergence.

We investegate the quasistatic limit directly using the power series (6.3). Here we wish to describe the average field as $d \to 0$. To do this we introduce the three-dimensional period cell for the crystal $[0, d]^3$. The base of the cell in the x_1x_2 plane is denoted by $Q_d = [0, d]^2$ and is the period of the crystal in the plane transverse to the rods. We apply the definition of B_{eff} and H_{eff} given in [24] which in our context is

$$(B_3)_{\text{eff}} = \frac{1}{d^2} \int_{Q_d} \hat{h}_\eta \left(\frac{k\mathbf{x}}{\eta} \right) e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_\eta t)} dx_1 dx_2 \tag{6.5}$$

and

$$(H_3)_{\text{eff}} = \frac{1}{d} \int_{(0,0,0)}^{(0,0,d)} \hat{h}_\eta \left(\frac{k\mathbf{x}}{\eta} \right) e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_\eta t)} dx_3. \tag{6.6}$$

Taking limits for k fixed and $d \to 0$ in (6.3) gives

$$\lim_{d\to 0} (B_3)_{\text{eff}} = \langle \psi_0 \rangle_Q \bar{h}_0 e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_{\text{qs}} t)} \quad \text{and} \quad \lim_{d\to 0} (H_3)_{\text{eff}} = \bar{h}_0 e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_{\text{qs}} t)},$$

in which $\omega_{\text{qs}}^2 = \frac{c^2 k^2}{n_{\text{qs}}^2}$. These are the same average fields that would be seen in a quasistatic magnetically active effective medium with index of refraction n_{qs} and μ_{qs} that supports the plane waves

$$(B_3)_{\text{qs}} = \mu_{qs} \bar{h}_0 e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_{\text{qs}} t)} \quad \text{and } (H_3)_{\text{qs}} = \bar{h}_0 e^{i(k\hat{\kappa}\cdot\mathbf{x} - \omega_{\text{qs}} t)},$$

where $\mu_{\text{qs}} = \langle \psi_0 \rangle_Q$. It is evident that these fields are solutions of the homogenized equation

$$\frac{n_{\text{qs}}^2}{c^2} \partial_{tt} u = \Delta u \tag{6.7}$$

This quasistatic interpretation provides further motivation for the definition of n_{eff} for nonzero η given by 6.2.

Now we apply the definition of effective permeability μ_{eff} given in [24], together with n_{eff} to define an effective permeability ϵ_{eff} for $\eta > 0$. The relationships between the effective properties and quasistatic effective properties are used to show that plasmonic crystals function as meta-materials of positive index of refraction in which both the effective permittivity and permeability are positive for $\eta > 0$.

The effective refraction index n_{eff} can be rewritten in the equivalent form by the equation $n_{\text{eff}}^2 = 1/\xi_\eta^2$. By setting $v = h_\eta$ in the weak form of the master system (5.49), it is easily seen that $\xi_\eta^2 > 0$ for all η within the radius of convergence, so that $n_{\text{eff}}^2 > 0$ for those values of η. Following Pendry et. al. [24], see also [16], we define the effective permeability by

$$\mu_{\text{eff}} = \frac{(B_3)_{\text{eff}}}{(H_3)_{\text{eff}}}, \tag{6.8}$$

and we then define ϵ_{eff} through the equation

$$n_{\text{eff}}^2 = \epsilon_{\text{eff}} \mu_{\text{eff}}. \tag{6.9}$$

The quasi-static effective properties are recovered by passing to the limits

$$\begin{aligned} n^2_{\text{qs}} &= \lim_{\eta\to 0} n^2_{\text{eff}} \\ \mu_{\text{qs}} &= \lim_{\eta\to 0} \mu_{\text{eff}} \\ \epsilon_{\text{qs}} &= \lim_{\eta\to 0} \epsilon_{\text{eff}}. \end{aligned}$$

An easy calculation shows that $\mu_{\text{qs}} = \langle\psi_0\rangle_Q > 0$ (see appendix for proof that $\langle\psi_0\rangle_Q > 0$). Hence, we have that $\mu_{\text{eff}} > 0$ for η in a neighborhood of the origin, so that $\epsilon_{\text{eff}} > 0$ for these values of η, since $n^2_{\text{eff}} > 0$ for all η in the radius of convergence. Thus, *one has a solid basis on which to assert that plasmonic crystals function as materials of positive index of refraction in which both the effective permittivity and permeability are positive.*

6.2 Absolute Error Bounds

The Catalan bound provides simple estimates on the size of the tails for the series ξ^2_η and h_η,

$$\begin{aligned} E_{m_0,\xi} &= \sum_{m=m_0+1}^{\infty} \xi^2_{2m}\eta^{2m} \\ E_{m_0,h} &= \sum_{m=m_0+1}^{\infty} h_m\eta^m. \end{aligned}$$

We have established convergence for $\eta \le 1/4J$, so that we may write $\eta = \alpha/4J$, $0 \le \alpha \le 1$. Then, using that $|\xi^2_{2m}| \le \beta C_{2m}J^{2m}$, $C_{2m} \le 4^{2m}$ and $4J\eta = \alpha$, we have

$$\begin{aligned} |E_{m_0,\xi}| &= \left|\sum_{m=m_0+1}^{\infty} \xi^2_{2m}\eta^{2m}\right| \\ &\le \beta \sum_{m=m_0+1}^{\infty} C_{2m}J^{2m}\eta^{2m} \\ &\le \beta \sum_{m=m_0+1}^{\infty} (4J\eta)^{2m} \\ &\le \beta \sum_{m=m_0+1}^{\infty} \alpha^{2m} \\ &= \beta\frac{\alpha^{2m_0+2}}{1-\alpha^2}. \end{aligned} \tag{6.10}$$

Similarly, for h_η we have that

$$\|E_{m_0,h}\|_{H^1(Q)} \le 2\beta|h_0|\frac{\alpha^{m_0+1}}{1-\alpha}. \tag{6.11}$$

6.3 Relative Error Bounds

- **The Field:**
  In this section, we use the absolute error bound (6.11) with $m_0 = 1$ to obtain a relative

error bound for the particular case of a circular inclusion of radius $r = 0.45$ [26]. The first term approximation to h_η is

$$h_\eta = h_0\psi_0 + ih_0\psi_1\eta + E_{1,h}. \tag{6.12}$$

For a circular inclusion of radius $r = 0.45$, we have

$$\begin{aligned} &J \le 85, \quad \beta \le 0.79, \\ &\|\psi_0\| = 0.97, \\ &\|\psi_1\| = 0.02, \end{aligned}$$

where $\|\cdot\| = \|\cdot\|_{H^1(Q)}$. Thus, using bound (6.11), the relative error $R_{1,h}$ is bounded by

$$\begin{aligned} |R_{1,h}| &= \frac{|E_{1,h}|}{\|h_0 + ih_0\psi_1\eta\|} &(6.13)\\ &\le \frac{1.58\frac{\alpha^2}{1-\alpha}}{\|h_0\| - \|h_0\psi_1\||\eta|} &(6.14)\\ &\le \frac{1.58\frac{\alpha^2}{1-\alpha}}{0.97 - 0.02\frac{\alpha}{340}}, &(6.15) \end{aligned}$$

so that for $\alpha \le 0.2$ the relative error is less than 8.2%. The graphs of ψ_0 and ψ_1 can be found in the Appendix.

- **The Frequency ξ^2:**
The first term approximation to ξ_η^2 is

$$\xi_\eta^2 = \xi_0^2 + \xi_2^2\eta^2 + E_{1,\xi}. \tag{6.16}$$

In the Appendix we indicate how the tensors ξ_m^2 may be computed. For an inclusion of radius $r = 0.45$, we have

$$\xi_0^2 = 0.36, \;\; \xi_2^2 = -0.14.$$

Thus, using bound (6.10), the relative error $R_{1,\xi}$ is bounded by

$$\begin{aligned} |R_{1,\xi}| &= \frac{|E_{1,\xi}|}{|\xi_0^2\psi_0 + \xi_2^2\eta^2|} \\ &\le \frac{\beta\frac{\alpha^4}{1-\alpha^2}}{|\xi_0^2 + \xi_2^2\eta^2|} \\ &\le \frac{0.79\frac{\alpha^4}{1-\alpha^2}}{|0.36 - 0.14\frac{\alpha^2}{340^2}|}, \end{aligned}$$

so that for $\alpha \le 0.3$ the relative error is less than 2%.

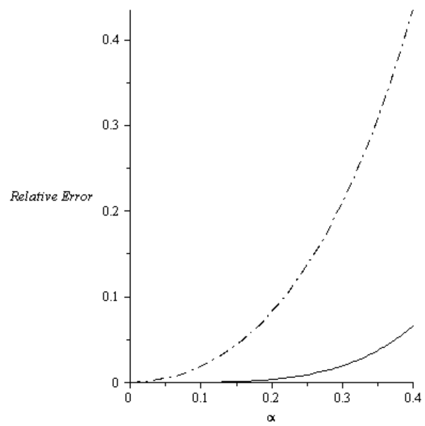

Figure 2: Solid curve is $R_{1,\xi}$ and dotdash curve is $R_{1,h}$.

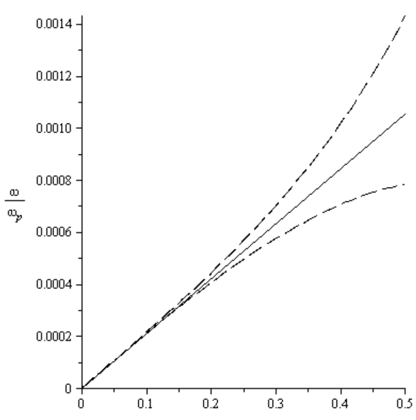

Figure 3: Graph of the first branch of the dispersion relation. Dashed curves represent error bars.

r	0.1	0.2	0.3	0.4	0.45
A	1.058	1.293	1.907	3.956	4.840
$\mathbf{\Omega_{\bar{P}}}$	1.0	1.0	1.0	1.0	1.0
J_1	3	4	8	25	85
J_2	15	17	22	29	62
J	15	17	22	29	85

Table 5: Table of parameters for circular inclusions of radii rd.

7 Appendix

7.1 Table of Values of A, $\mathbf{\Omega_{\bar{P}}}$ and J for Circular Inclusions

7.2 Explicit Expressions for Tensors

The tensors ξ_0^2 and ξ_2^2 were calculated using the weak form (3.10), as follows. Setting $m = 2$ and $v \equiv 1$ in (3.10) and solving for ξ_0^2 gives

$$\xi_0^2 = \frac{\langle \hat{\kappa} \cdot \nabla \psi_1 + \psi_0 \rangle_{\bar{P}}}{\langle \psi_0 \rangle_Q}. \tag{7.1}$$

Setting $m = 4$ and $v \equiv 1$ and solving for ξ_2^2 gives

$$\xi_2^2 = \frac{-\xi_0^2 \langle \hat{\kappa} \cdot \nabla \psi_1 \rangle_Q + \xi_0^2 \langle \psi_2 \rangle_P + \xi_0^2 \xi_0^2 \langle \psi_0 \rangle_Q + \xi_0^2 \langle \psi_0 \rangle_Q - \langle \hat{\kappa} \cdot \nabla \psi_3 \rangle_{\bar{P}}}{\langle \psi_0 \rangle_Q}. \tag{7.2}$$

All integrals appearing in (7.1) and (7.2) were then computed using the program COMSOL.

7.3 Bounds on $\bar{p}_m$, p_m and $|\xi_{m-1}^2|$, $m = 0, 1, 2, 3$

In this section we present the bounds which (5.6) give for $\bar{p}_m$, p_m and ξ_{m-1}^2, $1 \le m \le 3$, starting with estimates on $\bar{p}_0$, p_0 and ξ_0^2. We write the bounds as polynomials in the two "variables" $\Omega_{\bar{P}}$ and A. In practice, it is rather unwieldy to use these polynomials, so that one may use some computer program such as MAPLE to compute the iterations for any particular choice of problem parameters.

- **m=0:**

$$\begin{aligned} \bar{p}_0 &= \theta_{\bar{P}} \\ p_0 &\le \sqrt{\theta_P} \\ |\xi_0^2| &\le 1 \end{aligned}$$

  These initial estimates are obtained as follows: we have $\psi_0 \equiv 1$ in $\bar{P}$, so that $\bar{p}_0 = \theta_{\bar{P}}$. Using the BVP for ψ_0 in P one can prove that $0 \le \psi_0(\mathbf{y}) \le 1$, $\forall \mathbf{y} \in P$, and that $p_0^2 = \langle \psi_0 \rangle_P$. These two facts together give the estimate $p_0 \le \sqrt{\theta_P}$. Setting $v = \psi_1$ in the weak form for ψ_1, we get that $\langle \hat{\kappa} \cdot \nabla \psi_1 \rangle_{\bar{P}} = -\langle \nabla \psi_1 \cdot \nabla \psi_1 \rangle_{\bar{P}} < 0$. Using this in expression (7.1) gives $\xi_0^2 < 1$. Since θ_P, $\theta_{\bar{P}} \le 1$, these three estimates allow us to take $\beta \le 1$.

- **m=1:**

$$\begin{array}{rcl}
\bar{p}_1 & \leq & (2\bar{p}_0)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} \\
p_1 & \leq & (2\bar{p}_0)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A}^2 + 2p_0\mathbf{1}
\end{array}$$

- **m=2:**

$$\begin{array}{rcl}
\bar{p}_2 & \leq & (4\bar{p}_0){\mathbf{\Omega}_{\bar{\mathbf{P}}}}^2\mathbf{A} + (2p_0|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} + p_0(1+2|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}} \\
p_2 & \leq & (4\bar{p}_0)\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{2}} + (2p_0|\xi_0^2| + 4\bar{p}_0)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A}^2 + \bar{p}_0(1+2|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} + p_0(1+|\xi_0^2|)\mathbf{1}
\end{array}$$

- **m=3:**

$$\begin{array}{rcl}
\bar{p}_3 & \leq & 4\bar{p}_0\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{3}} + 8\bar{p}_0{\mathbf{\Omega}_{\bar{\mathbf{P}}}}^2\mathbf{A} + 2(p_0+\bar{p}_0)(1+2|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} + 2\bar{p}_0(1+6|\xi_0^2|)\mathbf{1} \\
p_3 & \leq & 4\bar{p}_0\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{4}} + 16\bar{p}_0\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{2}} + (6\bar{p}_0 + 2(p_0+\bar{p}_0)(1+3|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A}^2 + \bar{p}_0(1+2|\xi_0^2|)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} + \\
 & & +2\bar{p}_0(1+6|\xi_0^2|)\mathbf{A} + 3p_0(|\xi_0^2|+1)\mathbf{1} \\
|\xi_2^2| & \leq & 4\bar{p}_0\sqrt{\theta_{\bar{P}}}\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{3}} + 4\sqrt{\theta_P}|\xi_0^2|\bar{p}_0\mathbf{\Omega}^{\mathbf{2}}_{\bar{\mathbf{P}}}\mathbf{A}^{\mathbf{2}} + 8\sqrt{\theta_{\bar{P}}}\bar{p}_0{\mathbf{\Omega}_{\bar{\mathbf{P}}}}^2\mathbf{A} + 2\sqrt{\theta_P}|\xi_0^2|(3\bar{p}_0+p_0)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A}^2 + \\
 & & +(\sqrt{\theta_P}|\xi_0^2|\bar{p}_0(1+2|\xi_0^2|) + \sqrt{\theta_{\bar{P}}}(2(p_0+\bar{p}_0)(1+2|\xi_0^2|) + 2|\xi_0^2|\bar{p}_0)\mathbf{\Omega}_{\bar{\mathbf{P}}}\mathbf{A} + \\
 & & +(\sqrt{\theta_P}|\xi_0^2|p_0(1+|\xi_0^2|) + 2\sqrt{\theta_{\bar{P}}}\bar{p}_0(1+6|\xi_0^2|) + 2\sqrt{\theta_P}|\xi_0^2|p_0 + p_0|\xi_0^2|^2 + p_0|\xi_0^2| + 2\sqrt{\theta_{\bar{P}}}|\xi_0^2|^2\bar{p}_0)\mathbf{1}
\end{array}$$

7.4 Computing the Constant A for Circular Inclusions

Given a function $\psi \in H^1_{\mathrm{per}}(\bar{P})$, let $u \in H^1_P$ satisfy

$$\begin{array}{ll}
\nabla^2 u - u = 0 & \text{in } P, \\
u = \psi & \text{on } \partial P.
\end{array}$$

We seek to compute a number A such that

$$\|u\|^2_{H^1(P)} \leq A\|\psi\|^2_{H^1(\bar{P})}$$

for all ψ. Following [6, Appendix A], we will calculate a value of A for circular inclusions P of radius $r_0 < 0.5$ by restricting ψ to the annulus between P and the circle of unit radius. It suffices to consider real-valued functions ψ that minimize the H^1 norm in the annulus, that is

$$\nabla^2\psi - \psi = 0, \quad r_0 < r < 0.5.$$

A function of this type is given generally by the real part of an expansion

$$\psi(r,\theta) = \sum_{n=0}^{\infty} \left(c_n I_n(r) + d_n K_n(r)\right) e^{in\theta},$$

in which c_n and d_n are complex numbers and I_n and K_n are the "modified" Bessel functions. The continuous continuation of ψ into the disk with $\nabla^2 u - u = 0$ is given by the real part of

$$u(r,\theta) = \sum_{n=0}^{\infty} f_n I_n(r) e^{in\theta}$$

under the relations

$$f_n = c_n + d_n \frac{K_n(r_0)}{K_n(r_0)}. \tag{7.3}$$

One computes that

$$\|\mathrm{Re}\,\psi\|^2 = \frac{1}{2}\|\psi\|^2 \quad \text{and} \quad \|\mathrm{Re}\,u\|^2 = \frac{1}{2}\|u\|^2,$$

so we may work with the complex functions rather than their real parts.

The Helmholtz equation in P and integration by parts yield

$$\|u\|^2_{H^1(P)} = \int_P \left(|\nabla u|^2 + |u|^2\right) dA = \int_{\partial P} \bar{u}\partial_n u,$$

and this provides the representation

$$\|u\|^2_{H^1} = 2\pi r_1 \sum_{n=0}^{\infty} \bar{f}_n I_n(r_1) f_n I_n'(r_1).$$

The analogous representation in the annulus is

$$\begin{aligned}
\|\psi\|^2_{H^1} = & \int_0^{2\pi} (\partial_r \psi(1,\theta)\overline{\psi(1,\theta)}\, d\theta - \int_0^{2\pi} r_0(\partial_r \psi(r_0,\theta)\overline{\psi(r_0,\theta)}\, d\theta \\
= & \; 2\pi \sum_{n=0}^{\infty} \left(\bar{c}_n I_n(0.5) + \bar{d}_n K_n(0.5)\right)\left(c_n I_n'(0.5) + d_n K_n'(0.5)\right) + \\
& - 2\pi r_0 \sum_{n=0}^{\infty} \left(\bar{c}_n I_n(r_0) + \bar{d}_n K_n(r_0)\right)\left(c_n I_n'(r_0) + d_n K_n'(r_0)\right)
\end{aligned}$$

We seek a positive number A such that, for all choices of complex numbers c_n and d_n,

$$0 \leq A\|\psi\|^2 - \|u\|^2.$$

The right-hand-side is a quadratic form in all of the coefficients (c_n, d_n) that depends on A,

$$A\|\psi\|^2 - \|u\|^2 = m_n^{11} c_n \bar{c}_n + m_n^{12} c_n \bar{d}_n + m_n^{21} d_n \bar{c}_n + m_n^{22} d_n \bar{d}_n,$$

in which the m_n^{ij} depend on A and are conveniently expressed in terms of the functions

$$\begin{aligned}
\mathrm{II}_n(r) &= I_n(r) I_n'(r), \\
\mathrm{KK}_n(r) &= K_n(r) K_n'(r), \\
\mathrm{IK}_n(r) &= I_n(r) K_n'(r), \\
\mathrm{KI}_n(r) &= K_n(r) I_n'(r), \\
\mathrm{JJ}_n(r) &= \frac{K_n(r)^2}{I_n(r)} I_n'(r).
\end{aligned}$$

$$
\begin{aligned}
m_n^{11} &= -r_0\mathrm{II}_n(r_0) - Ar_0\mathrm{II}_n(r_0) + A\,\mathrm{II}_n(0.5),\\
m_n^{22} &= -r_0\mathrm{JJ}_n(r_0) - Ar_0\mathrm{KK}_n(r_0) + A\,\mathrm{KK}(0.5),\\
m_n^{12} &= -r_0\mathrm{KI}(r_0) - Ar_0\mathrm{KI}_n(r_0) + A\,\mathrm{KI}_n(0.5),\\
m_n^{21} &= -r_0\mathrm{KI}(r_0) - Ar_0\mathrm{IK}_n(r_0) + A\,\mathrm{IK}_n(0.5).
\end{aligned}
$$

The form m_n^{ij} is Hermitian, as one can show that $m_n^{12} = m_n^{21}$ by using the fact that $r\mathrm{Wron}[I_n, K_n]$ is constant.

We must find $A > 0$ such that $m_n^{11} \geq 0$ and $m_n^{11}m_n^{22} - m_n^{12}m_n^{21} \geq 0$ for all $n = 0, 1, 2, \ldots$. These quantities are equal to

$$
\begin{aligned}
m_n^{11} &= \beta(r_0, 0.5)A - \alpha(r_0),\\
m_n^{11}m_n^{22} - m_n^{12}m_n^{21} &= \epsilon(r_0, 0.5)A^2 - \delta(r_0, 0.5)A,
\end{aligned}
$$

in which

$$
\begin{aligned}
\alpha_n(r) &= r\mathrm{II}_n(r),\\
\beta_n(r,s) &= \mathrm{II}_n(s) - r\mathrm{II}_n(r),\\
\delta_n(r,s) &= rs\left[\mathrm{II}_n(r)\mathrm{KK}_n(s) + \mathrm{II}_n(s)\mathrm{JJ}_n(r) - \mathrm{KI}_n(r)\mathrm{IK}_n(s) - \mathrm{KI}_n(s)\mathrm{KI}_n(r)\right] +\\
&\quad + r^2\left[-\mathrm{II}_n(r)\mathrm{KK}_n(r) - \mathrm{II}_n(r)\mathrm{JJ}(r) + \mathrm{KI}_n(r)\mathrm{IK}_n(r) + \mathrm{KI}_n(r)\mathrm{KI}_n(r)\right],\\
\epsilon_n(r,s) &= rs\left[-\mathrm{II}_n(r)\mathrm{KK}_n(s) - \mathrm{II}_n(s)\mathrm{KK}_n(r) + \mathrm{KI}_n(r)\mathrm{IK}_n(s) + \mathrm{KI}_n(s)\mathrm{IK}_n(r)\right].
\end{aligned}
$$

The numbers $\alpha_n(r)$ and $\beta_n(r,s)$ for $r < s$ are positive; the latter because

$$
(rI_nI_n')' = \frac{1}{r}(r^2 + n^2)I_n^2 + r{I_n'}^2 > 0.
$$

One can show that δ and ϵ are positive. Thus, it is sufficient to find $A > 0$ such that, for all $n = 0, 1, 2, \ldots,$

$$
A \geq \max\left\{\frac{\alpha_n(r_0)}{\beta_n(r_0, 0.5)}, \frac{\delta_n(r_0, 0.5)}{\epsilon_n(r_0, 0.5)}\right\}.
$$

Table 5.3 shows computed values of A for various values of r_0.

7.5 Graphs of ψ_0 and ψ_1

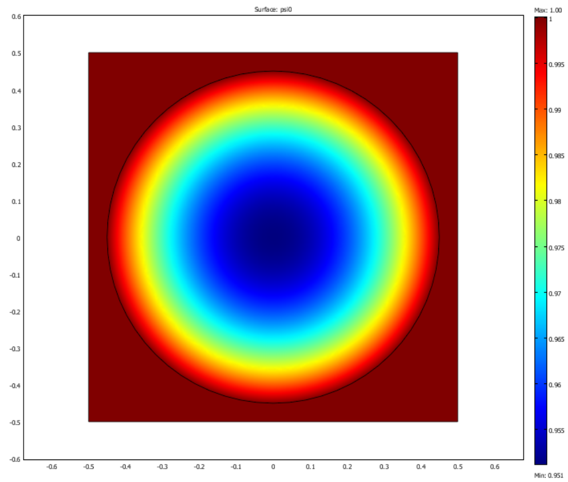

Figure 4: Graph of ψ_0. This function is symmetric about the origin.

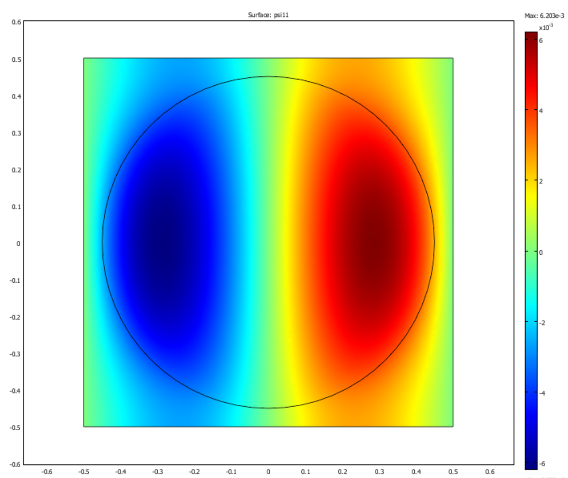

Figure 5: Graph of ψ_1 when $\hat{\kappa} = (1, 0)$. This function is antisymmetric about the origin.

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