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Theory and Computation of Scattering Resonances of Photonic Microstructures

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ABSTRACT. The optical properties of microstructured photonic waveguides are governed, in the scalar approximation, by a Schrödinger equation with a high contrast and oscillatory potential. We outline a scattering resonance perturbation theory for this non-selfadjoint eigenvalue problem. The imaginary parts of the scattering resonance "eigenvalues" correspond to the radiative leakage rates from these photonic waveguides. We implement a multiple scale approach to the study of such waveguides in the scalar approximation. The leading order theory agrees with classical homogenization theory, describing an effective homogeneous medium with dielectric properties given by an appropriate averaging of the refractive index profile. We compute the first non-trivial correction, which takes into account the microstructure, and find that the higher order homogenization expansion gives very good agreement with direct numerical simulations by Fourier and multipole methods. The higher order expansion is crucial for estimation of the leakage rates; in various examples of physical interest the leading order (homogenization) gives a substantial underestimation. We rigorously derive our 2^{nd} order homogenization expansion for the case of $N-$ fold symmetric structures.

CONTENTS

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1. Introduction and outline

The propagation of light in inhomogeneous media is a rich source of physical phenomena and is of huge technological importance. Recent advances in fabrication technology have made possible the fabrication of micro- and nanostructure media. Such media are often called *photonic* micro- or nanostructures, because by variation of the distribution of micrometer, respectively nanometer, scale structures, their individual geometry and material contrasts, one can influence the light propagation properties, linear and nonlinear, by finely tuning *optical* properties such as group velocity, dispersion and loss. Regardless of the characteristic length scale of the individual features, we shall loosely refer to such structures as *photonic microstructures*. Potential applications range from devices for telecommunication networks [**10**] to the exploration of quantum electrodynamics (QED) in microcavities [**19**].

In this paper, we focus on a class of photonic microstructure waveguides which have attracted a great deal of recent interest. Photonic crystal waveguides or "holey" optical fibers are waveguides with novel cross-sections consisting of holes surrounded by glass. The holes may be empty or filled with a material chosen to influence the propagation. The ability to vary the transverse geometry, combined with the large index contrasts possible with such structures, give multiple new degrees of freedom that potentially enable designs with radically different properties than is possible with standard fiber. See [**7**] for a discussion of interesting physical phenomena observed in such waveguides.

Efficient and accurate mathematical modeling of light propagation in microstructured waveguides is clearly necessary for their design and analysis. A feature of most such structures is that they are inherently leaky due to the existence of paths leading from the waveguide "core" to the outer region that avoid the holes and pass only through the background glass. Such structures support no true guided modes (the L^2- spectrum is continuous, corresponding to extended radiation states), but they will have leaky modes characterized by complex-valued propagation constants or effective indexes (scattering resonances); the leakage rate is given by the imaginary part. Physically, this leakage is due to a combination of tunneling through the holes and propagation through the glass surrounding them. The ability to calculate such rates is clearly of fundamental importance. Other quantities of interest include the real parts of the effective indexes, which determine the response of the structure to longitudinal variations such as gratings, and the dispersion relations of the various leaky modes, which may be quite unusual compared to standard waveguides due to the presence of large index contrasts and interference effects.

In the scalar approximation, the leaky modes and effective indexes are obtainable from the solution of the eigenvalue problem for the Schrödinger equation

$$\begin{aligned} H\psi \ = \ (\ -\Delta \ + \ V\ )\,\psi \ = \ E\psi \\ \psi \text{ outgoing as } r = |\mathbf{x}| \to \infty. \end{aligned} \tag{1.1}$$

Formulations of this *scattering resonance problem* are in section 3 and section 4. Here, $\Delta = \Delta_\perp$ denotes the two-dimensional Laplace operator in the transverse plane. (In the following, we shall omit the subscript $\perp$.) Since the outgoing radiation condition at infinity is not self-adjoint, we expect the eigenvalues, E, to be complex. The imaginary parts of the scattering resonance energies, E, determine the leakage rates; see section 2.

We view the potential as consisting of two parts:

$$V(x) \ = \ V_0(x) \ + \ \delta V(x),$$

where in the above waveguide context, V_0 is a slowly varying "average" and $\delta V(x)$ is oscillatory but, possibly, pointwise large, corresponding to a microstructure with high contrast.

We now give a brief description of the results presented in this article.

I. Theory of scattering resonances of the Schrödinger equation for high contrast and oscillatory potentials: In section 4 we formulate the scattering resonance problem with potential V, $SRP(V)$, as an appropriate Lippman-Schwinger equation. We prove that if $SRP(V_0)$ has a scattering resonance pair $(\psi_0, E_0) \in H^1(\chi(x)dx) \times \mathbb{C}$, then $SRP(V_0 + \delta V)$ has a "nearby" scattering resonance pair, which varies smoothly with δV for small δV in appropriate norm $|||\delta V|||$. This norm of the perturbation is small if δV is sufficiently oscillatory. In particular, for a potential $\delta V_N = \delta V(r, N\theta)$, where $\delta V(r,\Theta)$ is 2π periodic in Θ, corresponding to an N-fold symmetric potential, $|||\delta V_N||| = \mathcal{O}(N^{-1})$. In the microstructure waveguide context, smallness of $|||\delta V_N|||$ is implied the smallness of $\lambda^{-2}\ N^{-1}$, where λ denotes the wavelength of light.

II. Multiple scales, higher order homogenization expansion and approximate numerical methods: We develop a multiple scale perturbation theory of a large class of "sufficiently oscillatory" structures suitable for the analytical study and efficient numerical computation of such quantities as leakage rates, group velocities and dispersion. The procedure becomes more accurate as the transverse structure becomes more oscillatory, in a sense which we make precise below. If the transverse structure is invariant under rotation by $2\pi/N$ (*e.g.* in the case of a single ring of N holes uniformly distributed in an annulus) we expand the leaky modes and the effective indexes (scattering resonances) in powers of N^{-1}. The leading order, $\mathcal{O}(N^0)$, term in the expansion is derived from a suitably averaged or homogenized refractive index profile [**4, 12**]. We derive and numerically compute the leading order corrections due to microstructure (which enter at order N^{-2}) of both the real and imaginary parts of the effective indexes of the leaky modes. Since the leading order behavior is given by a homogenized (in angle) effective medium, we refer to this expansion as a homogenization expansion. Results on first-order corrections to homogenized eigenvalues of periodic composite media were obtained in [**16, 14**].

A few of the consequences of the homogenization expansion and numerical implementation that we wish to highlight are:

(1) Computational algorithm: Our analytic theory leads to a natural efficient computational algorithm for the modes and spectral characteristics, *e.g.* leakage rates, dispersion. Multiscale analysis enables us to eliminate the "stiff" aspects of the computation due to the rapidly varying structure. Therefore, one can expect significant reduction in computational effort. This is especially important for increasingly microstructured media, for which the approximation improves, as well as for simulation based optimization of light-guiding characteristics.

(2) Arbitrary geometry and index contrasts: Although we require N-fold symmetry of the structure, the individual microfeatures may have arbitrary geometry and large index contrasts. In our current implementation, we approximate an arbitrary

microfeature by a *simple layered structure*, defined in section 7.2, for which many of the calculations required can be done explicitly.

(3) Very good agreement with full numerical simulation: In section 6 we present results of numerical simulations based on our theory for several waveguides with transverse microstructure. A more extensive discussion of and comparison with other numerical approaches is presented in [**7**]. We focus on the complex effective indexes as they vary with the geometry of the microstructure. We are particularly interested in the imaginary parts of the effective indexes, which correspond to the leakage rates. We present comparisons of our predicted loss rates with results obtained by solving the Helmholtz equation directly by Fourier decomposition algorithm [**15**] and the vector Maxwell equation by multipole methods [**20**]. One expects homogenization theory to be valid when the wavelength of light is long compared with the individual microfeatures. We find very good agreement of our theory with full simulations even in regimes where $\lambda_{\rm fs}/d$, the ratio of wavelength to length scale of microfeatures, is as small as $3/2$. Although, the expansion is derived for N large, with the $N = \infty$ limit being the leading order term, examples of section 6 show agreement in cases where $N = 3$ and $N = 6$. We also observe the expected departure of our approximate methods from the results of full simulations for sufficiently small $\lambda_{\rm fs}/d$.

(4) Sensitivity of leakage rates to microstructure: In section 6 we have used our theory to compute the first two nontrivial terms of the effective indexes (scattering resonances) of the leaky modes. The first term corresponds to an average theory and the second term is a correction due to microstructure. The imaginary parts of the effective indexes, corresponding to the leakage rates, are very sensitive to the introduction of microstructure and their accurate approximation requires both terms. In contrast, as noted above, the real parts of the effective indexes are relatively insensitive to microstructure, and are well captured by the leading order term.

(5) Corrected fields: We find that corrections, due to microstructure, of the mode fields predicted by the averaged structure are compactly supported in space if the microstructure perturbation is compactly supported in space. This is not possible for the true solution of the mathematical model. An additional observation indicating a limitation of the homogenization expansion is seen for a family of structures consisting of two rings of holes, parametrized by the relative phase angle of the arrangement in one ring to another. Since the variation in refractive index in one ring occurs on a set disjoint from that for the second ring, we find the homogenization expansion predicts complex effective indexes that are *independent* of the phase angle. This suggests that in the regime where certain interference effects are important, the expansion of this paper may have limited use. Nevertheless, we have proved in [**6**] (see also section 4) that two-term approximate expansion of modes and effective indexes is valid for sufficiently large N. This rigorous theory gives field corrections which, at any finite N, are not compactly supported.

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2. Maxwell's equations in a wave guide and the scalar approximation

Maxwell's equations in a three dimensional dielectric medium with spatial coordinates, $\mathbf{x} = (x_1, x_2, x_3)$, and time coordinate, t are:

$$\begin{aligned} \nabla \cdot \vec{\mathcal{D}} &= 0 \quad \nabla \wedge \vec{\mathcal{E}} = -\partial_t \vec{\mathcal{B}} \\ \nabla \cdot \vec{\mathcal{B}} &= 0, \quad \nabla \wedge \vec{\mathcal{H}} = \partial_t \vec{\mathcal{D}} \end{aligned} \tag{2.1}$$

$\vec{\mathcal{E}}$ denotes the electric field, $\vec{\mathcal{D}}$ the electric displacement, $\vec{\mathcal{B}}$, the magnetic induction and $\vec{\mathcal{H}}$ the magnetic field. We have assumed no sources of free charge or current. A linear nonmagnetic dielectric medium is characterized by the linear constitutive laws:

$$\vec{\mathcal{D}} = \epsilon \vec{\mathcal{E}}, \quad \vec{\mathcal{H}} = \mu_0^{-1} \vec{\mathcal{B}}.$$

The free space (vacuum) values of ϵ and μ are denoted by ϵ_0 and μ_0. The *speed of light* in a vacuum, c, is given by $(\epsilon_0\mu_0)^{-\frac{1}{2}}$, while that in a general nonmagnetic medium $(\epsilon\mu_0)^{-\frac{1}{2}}$. The *index of refraction* of the medium, $n(\mathbf{x})$, is the ratio of c to the speed of light in the medium:

$$n(\mathbf{x}) = \frac{\sqrt{\epsilon_0\mu_0}}{\sqrt{\epsilon\mu_0}} = \sqrt{\frac{\epsilon_0}{\epsilon}}$$

and therefore

$$\epsilon(\mathbf{x}) = n^2(\mathbf{x})\ \epsilon_0 \tag{2.2}$$

We fix a frequency, ω, and derive the equation of the corresponding modes of the waveguide. Thus, we let

$$\vec{\mathcal{E}} = \vec{\mathcal{E}}(\mathbf{x}, \omega) e^{-i\omega t}, \ \vec{\mathcal{H}} = \vec{\mathcal{H}}(\mathbf{x}, \omega) e^{-i\omega t} \tag{2.3}$$

The relationship between frequency and wavelength in free space is given by

$$\omega = ck = \frac{2\pi c}{\lambda_{\text{fs}}},$$

where λ_{fs} denotes the free space wavelength.

Substitution of (2.3) into (2.1) yields:

$$\vec{\nabla} \wedge \vec{\mathcal{E}} = i\sqrt{\frac{\mu_0}{\epsilon_0}}\ k\ \vec{\mathcal{H}} \tag{2.4}$$

$$\vec{\nabla} \wedge \vec{\mathcal{H}} = -i\sqrt{\frac{\epsilon_0}{\mu_0}}\ k\ n^2\ \vec{\mathcal{E}} \tag{2.5}$$

Apply the curl operator, $\vec{\nabla}\wedge$ to (2.4) and using (2.5) yields the vector Helmholtz wave equation:

$$\vec{\nabla}\left(\vec{\nabla} \cdot \vec{\mathcal{E}}\right) - \Delta\vec{\mathcal{E}} = k^2 n^2 \vec{\mathcal{E}}. \tag{2.6}$$

The condition $\vec{\nabla} \cdot \vec{\mathcal{D}} = 0$ becomes

$$\vec{\nabla} \cdot \left(n^2\ \vec{\mathcal{E}}\right) = 0$$

which can be used in (2.6) to give

$$\Delta\vec{\mathcal{E}} \ + \ k^2 n^2 \ \vec{\mathcal{E}} \ = \ -\vec{\nabla}\left[\ \vec{\mathcal{E}}\cdot\vec{\nabla}\ln n^2\ \right] \tag{2.7}$$

We consider propagation in a waveguide, with x_3 taken to be the longitudinal coordinate and $\mathbf{x}_\perp = (x_1, x_2)$ the transverse coordinates and assume the waveguide has a uniform transverse cross-section (translation invariance in x_3):

$$n(\mathbf{x}) \ = \ n(\mathbf{x}_\perp) \ = \ n(x_1, x_2).$$

It is then natural to seek elementary modes which propagate in the x_3 direction

$$\vec{\mathcal{E}}(\mathbf{x}) \ = \ \vec{e}(\mathbf{x}_\perp)e^{i\beta x_3} \ = \left[\ \vec{e}_\perp(\mathbf{x}_\perp) \ + \ e_{\rm lon}(\mathbf{x}_\perp)\hat{k}\ \right] \ e^{i\beta x_3}$$

where $\hat{k} = (0,0,1)$, $\vec{e}_\perp\cdot\hat{k} = 0$. The vectors $\vec{e}_\perp$ and $e_{\rm lon}$ denote transverse and longitudinal field amplitudes. Substituting into (2.7), we obtain the following equations [**18**]

$$\left(\ \Delta_\perp \ + \ k^2 n^2(\mathbf{x}_\perp) \ - \ \beta^2\ \right) \ \vec{e}_\perp \ = \ \mathcal{V}_1 \ \vec{e}_\perp, \tag{2.8}$$

$$\left(\ \Delta_\perp \ + \ k^2 n^2(\mathbf{x}_\perp) \ - \ \beta^2\ \right) \ e_{\rm lon} = -i\beta\ \vec{e}_\perp\cdot\nabla_\perp\ln n^2, \tag{2.9}$$

where

$$\mathcal{V}_1\vec{e}_\perp \ \equiv \ -\vec{\nabla}_\perp\left(\vec{e}_\perp\cdot\vec{\nabla}_\perp\ln n^2\right)$$

Note that (2.8) is a closed equation for $\vec{e}_\perp$. Therefore, we can first solve for $\vec{e}_\perp$, and then obtain $e_{\rm lon}$ solving (2.9).

We shall work in the *scalar approximation*, which entails neglecting the term $\mathcal{V}_1\ \vec{e}_\perp$ in (2.8) that arises due to the vector nature of the fields. For modes that are localized away from the microstructure, which includes most of the examples in section 6, the vector corrections are expected to be small because the field $\vec{e}_\perp$ is small at the interfaces, which are the only places at which it contributes. However, this will not be true in other examples of interest, and we expect that our methods can be extended to the full vector case. In any case, we will not discuss vector effects further in this work.

In the scalar approximation the components of $\vec{e}_\perp$ satisfy independent scalar Helmholtz equations. We let φ denote either of these transverse components. Then,

$$\left(\ \Delta_\perp \ + k^2 n^2\ \right)\varphi \ = \beta^2\varphi \tag{2.10}$$

where $\Delta_\perp$ denotes the Laplace operator in the transverse variables, $x_\perp = (x_1, x_2)$.

Introducing the notation

$$V \ = \ k^2(n_g^2 - n^2), \quad E \ = \ k^2 n_g^2 - \beta^2, \tag{2.11}$$

the equation for the φ and propagation constant β can be viewed as a Schrödinger equation with potential $V(\mathbf{x}_\perp)$ and energy parameter E:

$$H\varphi \ \equiv \ (-\Delta_\perp \ + \ V)\varphi \ = \ E\ \varphi. \tag{2.12}$$

Corresponding to the physical problem described in section 3 we assume that for some $r_* > 0$,

$$\begin{aligned} V(\mathbf{x}) \quad &\geq \quad 0, \text{for all } \ \mathbf{x} \text{ and} \\ V(\mathbf{x}) \quad &= \quad 0, \text{for } r \geq r_* \end{aligned} \tag{2.13}$$

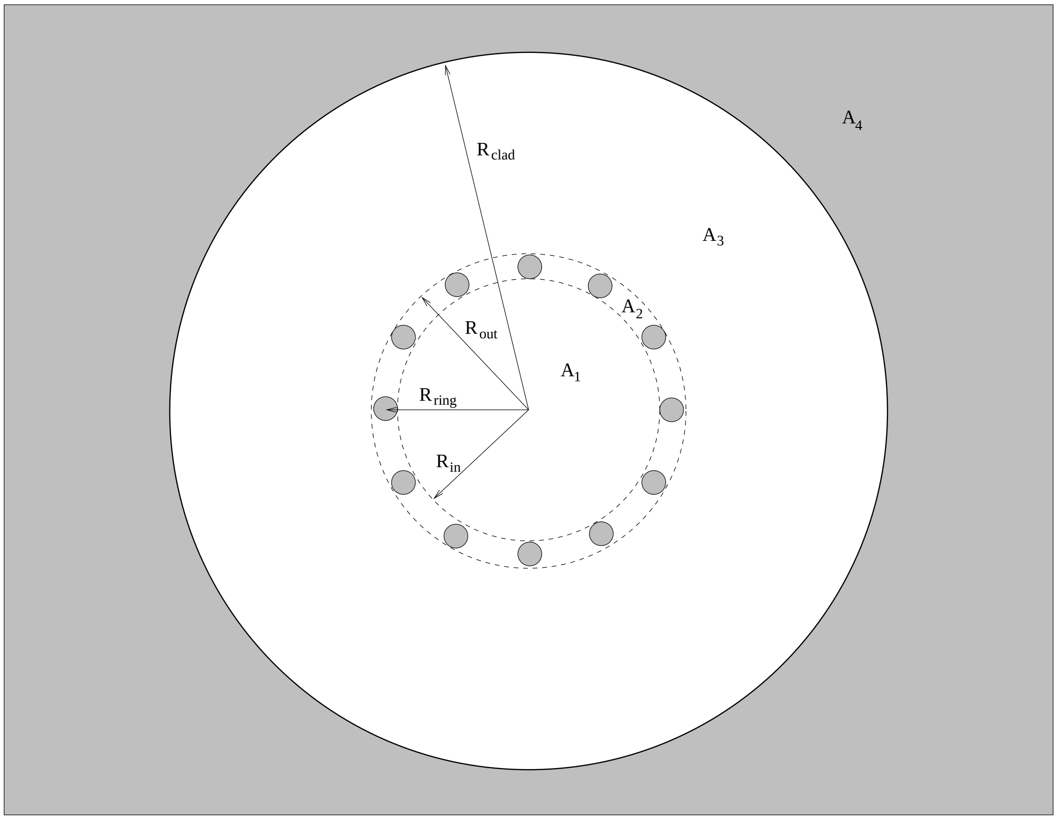


FIGURE 1. A cross section of a microstructured waveguide.

The potential, V, therefore does not support bound states (guided modes) and only has scattering states (radiation modes), along with scattering resonances (leaky modes).

3. The resonance problem for microstructure waveguides

To fix ideas, consider a cylindrical waveguide composed of two materials "g" and "h", with corresponding refractive indexes n_g and n_h. We specify a transverse cross-section of the waveguide in the 2-dimensional plane, with coordinates $\mathbf{x} = (x, y) = (r, \theta)$. In figure 1 we show a schematic picture of a glass waveguide with a single ring of 12 air holes in a solid glass cylinder. Four regions are illustrated:

A_1, the region $|\mathbf{x}| \le R_{\rm in}$, a disc of glass with refractive index n_g;
A_2, the region $R_{\rm in} \le |\mathbf{x}| \le R_{\rm out}$, an annular region with 12 equally spaced air-holes. In A_2, n takes on two values, n_g in the bulk and $n_h \sim 1$ in the holes;
A_3, the region $R_{\rm out} \le |\mathbf{x}| \le R_{\rm clad}$, consisting of a solid glass, $n = n_g$, and finally;
A_4, the region $|\mathbf{x}| \ge R_{\rm clad}$ consisting of air, $n = n_h$.

We are interested in how well light is confined to the core (A_1) region in such microstructured fiber. This structure has actual guided, in addition to leaky, modes, due to the lower refractive index of region A_4. However, we view any propagation of light from A_1 to A_3 as loss. Therefore, the appropriate mathematical problem for our purposes is the mode equation (2.12) posed on the spatial domain: $\{|\mathbf{x}| \le R_{\rm in}\ \} \cup \{R_{\rm in} \le |\mathbf{x}| \le R_{\rm out}\} \cup \{R_{\rm out} \le |\mathbf{x}|\}$, subject to an *outward going radiation condition as* $|\mathbf{x}| \to \infty$. In practice, the glass optical fiber is usually coated with a high index and high loss polymer, so any light that does leak into A_3 is rapidly attenuated, further justifying the use of this boundary condition.

We now present a more general mathematical formulation of the problem.

The scattering resonance problem: *Given a potential (index profile)* $V = V(r, \theta)$ *of compact support, we seek* E *and nonzero* φ *for which*

$$H\varphi \ \equiv \ (-\Delta \ + \ V\ )\,\varphi \ = \ E\varphi \tag{3.1}$$

subject to the outward going radiation condition, as $r \to \infty$*. We call a pair* (φ, E) *a scattering resonance pair.*

A scattering resonance pair is sometimes called a *quasiresonance* [**9**].

In our setting, the radiation condition can be simply described. Because $V(r)$ is identically zero for $r \ge r_*$, equation (2.12) becomes:

$$-\,(\ \Delta_\perp + E\ )\,\varphi \ = \ 0, \quad r \ge r_* \tag{3.2}$$

Solutions of (3.2) can be expanded in a series

$$\varphi \ = \ \sum_{l=-\infty}^{+\infty} \ \Big(\ c_l^{(1)}\ e^{il\theta}\ H_l^{(1)}(\sqrt{E}\ r) \ + \ c_l^{(2)}\ e^{il\theta}\ H_l^{(2)}(\sqrt{E}\ r)\ \Big). \tag{3.3}$$

The functions $H_l^{(1)}$ and $H_l^{(2)}$ are first and second Hankel functions of order l and satisfy the following asymptotic formulae for large arguments [**1**] (page 364, equations 9.2.3 and 9.2.4):

$$H_l^{(1)}(\zeta) \ \sim \ \sqrt{\frac{2}{\pi\zeta}}\ e^{i(\zeta - \frac{1}{2}l\pi - \frac{\pi}{4})}, \quad -\pi < \arg\zeta < 2\pi$$

$$H_l^{(2)}(\zeta) \ \sim \ \sqrt{\frac{2}{\pi\zeta}}\ e^{-i(\zeta - \frac{1}{2}l\pi - \frac{\pi}{4})}, \quad -2\pi < \arg\zeta < \pi \tag{3.4}$$

The functions $H_l^{(1)}$ are interpreted as *outgoing radiation* because, in the time dependent setting, they have outward moving phase fronts for increasing t:

$$e^{-i\omega t} H_l^{(1)}(\zeta) \sim \frac{h_l}{\sqrt{\zeta}} e^{i(\zeta - \omega t)},$$

where h_l is a complex constant. Therefore the requirement that φ be outgoing is equivalent to the vanishing of all coefficients $c_l^{(2)}$ in (3.3):

$$\textit{Outward going radiation} \Longleftrightarrow c_l^{(2)} = 0 \text{ for all } l. \tag{3.5}$$

Therefore, the scattering resonance problem can be formulated as the eigenvalue problem (3.1), (3.5).

Since (3.5) is a non-self adjoint boundary condition at infinity E can be expected to be complex. However, there are constraints on the location of E in the complex plane. For the φ to be oscillatory at infinity, we must have $\Re E > 0$ and, for φ to be outgoing $\Re\sqrt{E} > 0$. Furthermore, $\Im E \le 0$. For, if $\Im E > 0$, then $\Im\sqrt{E} > 0$.

From the series expansion (3.3) with $c_l^{(2)} = 0$ we conclude that φ is exponentially decaying as $r \to \infty$, and therefore a eigenstate of the self-adjoint operator H with non-real eigenvalue. This yields a contradiction. To summarize:

If E is an energy for which there is a solution of the resonance problem, then $\Re E > 0$ and $\Im E \leq 0$ Correspondingly, by (2.11), we have $\Re\beta > 0$ and $\Im\beta > 0$. Since the electric field $\vec{\mathcal{E}}(\mathbf{x}, \omega) = \vec{e}_\perp(\mathbf{x}_\perp)e^{i\beta x_3}$, the complex resonances E correspond to the radiative decay or leakage rates of the structure.

In the following section, section 4, we discuss an alternative formulation of the scattering resonance problem, more amenable to rigorous theory. In section 5 we embark on a multiple scale / homogenization approach, which can be justified using the results of section 4.

4. Scattering resonances of the Schrödinger equation for high contrast and oscillatory potentials

Motivated by a class of problems arising in wave propagation through high contrast microstructures, we now study the scattering resonances for the Schrödinger equation with high contrast and oscillatory potentials. We present an outline of results, specialized to the case of $N-$ fold symmetric potentials. The detailed proofs can be found in [**6**].

Let $H = -\Delta + V$, where V is sufficiently smooth and of compact support. The essential spectrum of H is the postive half-line, $[0, \infty)$. For $E \notin [0, \infty)$, the resolvent $(H - E)^{-1}$ is a well-defined bounded operator on L^2. Restricted to the dense subspace of smooth compactly supported functions, it can be analytically continued across the essential spectrum to the lower half plane, where it defines a meromorphic function, with the poles corresponding to scattering resonances; see, for example, [**5, 17, 3**]. We denote this analytical continuation by $(H - E)_+^{-1}$.

Consider $H = -\Delta$ and dimension $n = 2$. Then, for compactly supported f

$$(-\Delta - E)_+^{-1}\ f \ = \ \frac{i}{4}\int \ H_0^{(1)}(\sqrt{E}|x - y|)\ f(y)\ dy; \tag{4.1}$$

see [**9**], page 165, and [**13**].

In this section we shall work with the following formulation of the scattering resonance problem for the potential V, $SRP(V)$:

Given V a bounded function of compact support, find (E, ψ) such that $\psi \in L^2_{\rm loc}$ and

$$\psi \ = \ -(-\Delta - E)_+^{-1}\ V\psi. \tag{4.2}$$

Equation (4.2) is often called a Lippman-Schwinger equation.

Suppose (E_0, ψ_0) is a solution to $SRP(V_0)$. E_0 is a complex number in the fourth quadrant, and $|\psi_0(x)| \leq e^{\alpha_0|x|}$. Consider the scattering resonance problem $SRP(V_0 + \delta V)$, where $\delta V(x)$ is pointwise large (high contrast) and oscillatory. We next reformulate (4.2), in a manner appropriate for class of perturbations we consider.

We introduce a smooth function, $\chi(x)$, with $\chi(x) \sim e^{-\alpha|x|}$ for large $|x|$, for $\alpha > \alpha_0$ sufficiently large. Define the operators

$$T_V \ = \ \langle D\rangle^{-1}\ \chi^{-1}V\chi^{-1}\ \langle D\rangle^{-1} \tag{4.3}$$

$$T_+(E) \ = \ \langle D\rangle\ \chi\ (-\Delta - E)_+^{-1}\ \chi\ \langle D\rangle \tag{4.4}$$

Finally, define

$$\Psi \ = \ \langle D \rangle \ \chi(x) \ \psi(x), \tag{4.5}$$

where

$$\langle D \rangle \ = \ (\ I - \Delta \ )^{\frac{1}{2}} .$$

Instead of studying (4.2), we shall consider the reformulation

$$(\ I \ + \ T_+(E) T_V \ ) \ \Psi \ = \ 0 \tag{4.6}$$

We shall refer to this as a *preconditioned* Lippman-Schwinger equation. In terms of this formulation, given a nontrivial solution (Ψ_0, E_0) of (4.6), we want to study the solutions $(\Psi_0 + \delta\Psi, E_0 + \delta E)$ of

$$(\ I \ + \ T_+(E_0 + \delta E) T_{V_0 + \delta V} \ ) \ (\Psi_0 + \delta\Psi) \ = \ 0 \tag{4.7}$$

for δV sufficiently "small".

Concerning the definition of Ψ in (4.5), the purpose of multiplication by $\chi(x)$ is to give a formulation in L^2, while the operator multiplier, $\langle D \rangle$, enables us to view a perturbation as small provided it is sufficiently oscillatory, but not pointwise small. In particular,

PROPOSITION 4.1. *Let δV be an $L^2(\mathbb{R}^2)$ function. Let (r, θ) denote standard polar coordinates in $\mathbb{R}^2$ and consider the $N-$ fold symmetric function $\delta V_N = \delta V(r, N\theta)$. Then,*

$$||| \ \delta V_N \ ||| \ \equiv \ \| T_{\delta V_N} \|_{\mathcal{B}(L^2)} \ \le \ \frac{C}{N}, \tag{4.8}$$

where $\|A\|_{\mathcal{B}(L^2)}$ denotes the L^2 operator norm of A.

As N increases, the structure described by the potential δV_N becomes progressively more "microstructured," yet remains of fixed contrast. We have the following

THEOREM 4.1. *(a) Let V_0 denote a potential for which $|||V_0|||$ is finite. Let (E_0, ψ_0) denote a solution of the corresponding scattering resonance problem. Assume*

$$\text{dimension} \ \{ \ f \in L^2 : \ (\ I \ + \ T_+(E_0) T_{V_0} \ ) \ \Psi \ = \ 0 \ \} \ = \ 1 \tag{4.9}$$

and this subspace is spanned by the function

$$\Psi_0 = \langle D \rangle \chi \psi_0 .$$

Then, there exists $\varepsilon_0 > 0$ such that for any potential V satisfying $|||V - V_0||| \ < \varepsilon_0$ ($\delta V \ = \ V - V_0$), there corresponds a unique solution $(E(V), \psi(V))$ of the scattering resonance problem which lies near (E_0, ψ_0).
(b) The mapping

$$V \ \mapsto \ (E, \psi) \ \in \ \mathbb{C} \times H^1(\chi(x) dx),$$

which associates to a potential V a solution $(E(V), \psi(V))$ of the scattering resonance problem, is analytic in a neighborhood $|||V - V_0||| < \varepsilon_0$ of V_0.

Theorem 4.1 enables us to expand $E(V_0 + \delta V) - E(V_0)$ in δV:

$$E(V_0 + \delta V) - E(V_0) \ = \ \delta E^{(1)} \ + \ \delta E^{(2)} \ + \ \cdots , \tag{4.10}$$

where $\delta E^{(j)}$ is of order j in δV. For the case, $\delta V = \delta V(r, N\theta)$, where δV has angular average zero, we have $\delta E^{(1)} = 0$ and

PROPOSITION 4.2. *Then,*

$$\delta E_N^{(2)} \;=\; \frac{\left\langle\; \delta V_N\overline{\psi_0}\;,\; (-\Delta - E_0 + V_0)_+^{-1}\; \delta V_N \psi_0 \;\right\rangle}{\left\langle\; V_0\overline{\psi_0}\;,\; (-\Delta - E_0)_+^{-2}\; V_0\psi_0 \;\right\rangle} \tag{4.11}$$

In the following section, we derive by multiple scale perturbation theory an asymptotic expansion of solutions of the scattering resonance problem in powers of N^{-1}. For the above $N-$ fold symmetric structure, this gives the *homogenization expansion*:

$$E \;-\; E_0 \;=\; \frac{1}{N^2} E_2^{\text{homog}} \;+\; \mathcal{O}(\frac{1}{N^4});$$

see section 5. For large N, we have shown that the resonance perturbation theory of this section agrees with higher order homogenization through second order:

PROPOSITION 4.3. *Let $V \in C^2$. Then,*

$$\delta E_N^{(2)} \;=\; \frac{1}{N^2}\left(\; E_2^{\text{homog}} \;+ \mathcal{O}\left(\frac{1}{N^2}\right)\;\right),\quad N\to\infty. \tag{4.12}$$

The case where V is less regular is under study. We remark that the the condition (4.9) may not be satisfied due to degeneracies arising from symmetries of the potential. Theorem 4.1 can still be seen to apply, however, as we describe in [**6**].

5. Multiple scales and homogenization expansion

In this section we derive a multiple scale expansion of solutions to the resonance problem for microstructures, giving a homogenized (averaged) theory at leading order plus systematically computable corrections. We carry out the analysis for a class of potentials V with the dependence:

$$V \;=\; V(r,\theta,N\theta) \;=\; V(r,\theta,\Theta), \tag{5.1}$$

where V is $2\pi-$periodic in θ and Θ. Thus (5.1) allows both a slow and a fast angular modulation of the index profile. In the special case where V does not depend on θ and we have $V = V(r,N\theta)$, the potential corresponds to an index profile with an N- fold symmetry. Assume $V \geq 0$ and that for $r \geq r_L$, $V \equiv 0$. We will show the following:

Homogenization Expansion: *The resonance mode problem (3.1-3.5) has, for large N, solutions with the formal expansion:*

$$\varphi(r,\theta;N) \;=\; \Phi^{(N)}(r,\theta,\Theta),\;\; \Theta = N\theta$$

given by

$$\begin{aligned} \Phi^{(N)} \;&=\; \Phi_0 \;+\; \frac{1}{N^2}\Phi_2 \;+\; \mathcal{O}(\frac{1}{N^3}) \\ E^{(N)} \;&=\; E_0 \;+\; \frac{1}{N^2}E_2 \;+ \mathcal{O}(\frac{1}{N^3}). \end{aligned} \tag{5.2}$$

(The coefficient E_2 is referred to as E_2^{homog} in section 4.)

- $(\Phi_0(r,\theta), E_0)$ *is a non-trivial solution of the resonance problem:*

$$H_{\text{av}}\Phi_0 \;=\; E_0\Phi_0 \tag{5.3}$$

where Φ_0 is subject to the outward going radiation condition (3.5), and the averaged operator is given by

$$H_{\rm av} \equiv \frac{1}{2\pi}\int_0^{2\pi} H\ d\Theta\ \equiv -\Delta_\perp\ +\ V_{\rm av}(r,\theta). \tag{5.4}$$

• $\Phi_2 = \Phi_2^{(p)} + \Phi_2^{(h)}$, *where $\Phi_2^{(p)}$ is the mean zero solution (easily derived from the Fourier series of $V(\cdot,\cdot,\Theta)$) of:*

$$\frac{1}{r^2}\partial_\Theta^2\Phi_2^{(p)}\ =\ [\ V(r,\theta,\Theta) - V_{\rm av}(r,\theta)\ ]\,\Phi_0(r,\theta). \tag{5.5}$$

and $(\Phi_2^{(h)}, E_2)$ solves:

$$(\ H_{\rm av}\ -\ E_0)\,\Phi_2^{(h)} = \left(\ E_2\ +\ \frac{r^2}{2\pi}\int_0^{2\pi}\ \left|\partial_\Theta^{-1}[V(r,\theta,\Theta) - V_{\rm av}(r,\theta)]\right|^2\ d\Theta\ \right)\Phi_0(r,\theta) \tag{5.6}$$

Finally, E_2 is uniquely determined by the condition that (5.6) has a solution which satisfies an outgoing radiation condition at $r = \infty$; see (3.5).

• *This yields an approximate solution of the scalar wave equation and an approximation (neglecting vector effects) of the transverse electric field, $\mathcal{E}_\perp = (\mathcal{E}_{\perp 1}, \mathcal{E}_{\perp 2})$, of Maxwell's equations:*

$$\mathcal{E}_{\perp,q}(\mathbf{x};\beta)\ \sim e^{i(\beta x_3 - \omega t)}\ \left[\ \Phi_0(|\mathbf{x}_\perp|,\theta;\omega)\ +\ \frac{1}{N^2}\Phi_2(|\mathbf{x}_\perp|,\theta,N\theta;\omega)\ +\ \mathcal{O}\left(\frac{1}{N^3}\right)\ \right]$$

Here, $\omega = ck$ and $\beta = \sqrt{k^2 n_g^2 - E} = \Re\beta + i\Im\beta$, with $\Im\beta > 0$. $\mathcal{E}_{\perp,q}(\mathbf{x}_\perp, x_3)$ decays with increasing x_3 and is therefore a "leaky mode." These modes are not square integrable.

In section 6, we present the results of numerical simulations performed using a two-term truncation of our homogenization expansion, compare them with published computations of solutions to the full problem, and discuss the question of convergence of our expansion.

5.1. Multiple scale expansion. Due to the rapidly varying coefficient in (2.12) we expect rapid variations in its solutions. We therefore explicitly introduce the fast angular variable:

$$\Theta\ =\ N\theta, \tag{5.7}$$

and view φ as a function of the three independent variables: r, θ and Θ:

$$\varphi(r,\theta)\ =\ \Phi(r,\theta,\Theta). \tag{5.8}$$

Here, we use polar coordinates $x = (r,\theta)$ and note that

$$\Delta_\perp\ =\ \Delta_r\ +\ \frac{1}{r^2}\partial_\theta^2, \tag{5.9}$$

where Δ_r denotes the radial part of the transverse Laplacian:

$$\Delta_r\ \equiv \partial_r^2\ +\frac{1}{r}\partial_r.$$

Thus, the operator ∂_θ is replaced by $\partial_\theta + N\partial_\Theta$ and equation (2.12) becomes:

$$(-\Delta_r - \frac{1}{r^2}(\partial_\theta + N\partial_\Theta)^2 + V(r,\theta,\Theta)\ )\Phi\ =\ E\ \Phi, \tag{5.10}$$

Equivalently

$$\left(H - \frac{2N}{r^2}\partial_\theta\partial_\Theta - \frac{N^2}{r^2}\partial_\Theta^2 \right) \Phi \ = \ E\Phi \tag{5.11}$$

We seek an expansion of Φ and E in the small parameter $1/N$

$$\begin{aligned} \Phi^{(N)} &= \Phi_0 + \frac{1}{N}\Phi_1 + \frac{1}{N^2}\Phi_2 + \frac{1}{N^3}\Phi_3 + \frac{1}{N^4}\Phi_4 + \Phi_5^{(N)} \\ E^{(N)} &= E_0 + \frac{1}{N}E_1 + \frac{1}{N^2}E_2 + E_3^{(N)} \end{aligned} \tag{5.12}$$

Here, $\Phi_j \ = \ \Phi(r,\theta,\Theta)$.

Substitution of (5.12) into (5.11) and equating like powers of $1/N$ we obtain a hierarchy of equations arising at each order in $1/N$. We display the first five equations of this hierarchy.

$$\mathcal{O}(N^2): \quad \frac{1}{r^2}\partial_\Theta^2\Phi_0 = 0 \tag{5.13}$$

$$\mathcal{O}(N): \quad \frac{1}{r^2}\partial_\Theta^2\Phi_1 = -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_0 \tag{5.14}$$

$$\mathcal{O}(1): \quad \frac{1}{r^2}\partial_\Theta^2\Phi_2 = -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_1 + (H - E_0)\,\Phi_0 \tag{5.15}$$

$$\mathcal{O}(N^{-1}): \quad \frac{1}{r^2}\partial_\Theta^2\Phi_3 = -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_2 + (H - E_0)\,\Phi_1 - E_1\Phi_0 \tag{5.16}$$

$$\mathcal{O}(N^{-2}): \quad \frac{1}{r^2}\partial_\Theta^2\Phi_4 = -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_3 + (H - E_0)\,\Phi_2 - E_1\Phi_1 - E_2\Phi_0 \tag{5.17}$$

5.2. Construction of the multiple scale expansion. As is typical in perturbation expansions, we must solve a hierarchy of inhomogeneous linear equations, which have a *fixed* linear operator to invert and varying inhomogeneous term. Each member of the hierarchy is of the form:

$$\frac{1}{r^2}\partial_\Theta^2 F = G(r,\theta,\Theta). \tag{5.18}$$

A necessary and sufficient condition for solvability in the space of 2π periodic in Θ functions is:

$$\int_0^{2\pi} G(r,\theta,p)\,dp = 0. \tag{5.19}$$

We now proceed with a term by term construction of the perturbation expansion.

$\mathcal{O}(N^2)$ *Terms:*

$$\frac{1}{r^2}\partial_\Theta^2\Phi_0 = 0 \tag{5.20}$$

From this it follows that Φ_0 is independent of the fast phase, Θ:

$$\Phi_0(r,\theta,\Theta) = \Phi_0(r,\theta) \tag{5.21}$$

$\mathcal{O}(N)$ *Terms:*

$$-\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_0 - \frac{1}{r^2}\partial_\Theta^2\Phi_1 = 0 \tag{5.22}$$

Using (5.21) in (5.22) we have that

$$\frac{1}{r^2}\partial_\Theta^2\Phi_1 = 0 \tag{5.23}$$

and therefore:

$$\Phi_1(r,\theta,\Theta) = \Phi_1(r,\theta) \tag{5.24}$$

Using (5.24) we find:

$\mathcal{O}(1)$ *Terms:*

$$\frac{1}{r^2}\partial_\Theta^2\Phi_2 = (H - E_0)\,\Phi_0 \tag{5.25}$$

Equation (5.25) has a solution in the space of 2π-periodic in Θ functions if and only if the following solvability condition holds:

$$(H_{\rm av} - E_0)\,\Phi_0 = 0. \tag{5.26}$$

Here, $H_{\rm av}$ and $V_{\rm av}$ denote, respectively, the average operator and potential with respect to the fast angular dependence. They are given by:

$$\begin{aligned} H_{\rm av} &= -\Delta_\perp + V_{\rm av} = -\Delta_r - \frac{1}{r^2}\partial_\theta^2 + V_{\rm av}(r,\theta) \\ V_{\rm av}(r,\theta) &= \frac{1}{2\pi}\int_0^{2\pi} V(r,\theta,p)\,dp. \end{aligned} \tag{5.27}$$

Note that

$$H - H_{\rm av} = V - V_{\rm av}.$$

We fix $(\Phi_0(r,\theta), E_0)$ to be a scattering resonance pair of an outgoing solution and its associated *complex* eigenvalue.

Since Φ_0 satisfies (5.26), the inhomogeneous equation (5.25) can be put in the simpler form:

$$\frac{1}{r^2}\partial_\Theta^2\Phi_2 \;=\; [\; V(r,\theta,\Theta) - V_{\rm av}(r,\theta)\;]\,\Phi_0(r,\theta). \tag{5.28}$$

We express the solution of (5.28) in the form

$$\Phi_2 \;=\; \Phi_2^{(p)}(r,\theta,\Theta) \;+ \Phi_2^{(h)}(r,\theta), \tag{5.29}$$

where $\Phi_2^{(p)}(r,\theta,\Theta)$ and $\Phi_2^{(h)}(r,\theta)$ are, respectively, a particular solution of mean zero and a homogeneous solution of (5.28), which is to be determined at higher order in N^{-1}. That $\Phi_2^{(p)}(r,\theta,\Theta)$ can be chosen to be 2π-periodic in Θ follows from the mean zero property of $V(r,\theta,\Theta) - V_{\rm av}(r,\theta)$. Also, $\Phi_2^{(p)}$ is mean zero in Θ because the constant term in its Fourier expansion is included in $\Phi_2^{(h)}$. To compute $\Phi_2^{(p)}$, we expand $V(r,\theta,\Theta) - V_{\rm av}(r,\theta)$ in a Fourier series in Θ:

$$V(r,\theta,\Theta) - V_{\rm av}(r,\theta) \;=\; \sum_{|j|\geq 1} \eta_j(r,\theta)\; e^{ij\Theta} \tag{5.30}$$

We have

$$\begin{aligned} \Phi_2^{(p)}(r,\theta,\Theta) &= \partial_\Theta^{-2}\;[V(r,\theta,\Theta) - V_{\rm av}(r,\theta)]\cdot r^2\Phi_0(r,\theta) \\ &= \sum_{|j|\geq 1} (ij)^{-2}\eta_j(r,\theta)e^{ij\Theta}\cdot r^2\Phi_0(r,\theta) \end{aligned} \tag{5.31}$$

$\mathcal{O}(N^{-1})$ *Terms:*

$$\begin{aligned} \frac{1}{r^2}\partial_\Theta^2\Phi_3 &= -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_2 + (\ H - E_0\ )\,\Phi_1 - E_1\Phi_0 \\ &= -\frac{2}{r^2}\partial_\theta\partial_\Theta\Phi_2^{(p)} + (\ H - E_0\ )\,\Phi_1 - E_1\Phi_0 \end{aligned} \tag{5.32}$$

The solvability condition becomes

$$(\ H_{\rm av} - E_0\ )\,\Phi_1 \ = \ E_1\Phi_0, \tag{5.33}$$

which we satisfy by taking $E_1 = 0$ and $\Phi_1 \equiv 0$.

Using the mean zero property of $\Phi_2^{(p)}$, we see that equation (5.32) becomes

$$\partial_\Theta\Phi_3(r,\theta,\Theta) \ = \ -2\partial_\theta\Phi_2^{(p)}(r,\theta,\Theta) \tag{5.34}$$

$\mathcal{O}(N^{-2})$ *Terms:* Using that $E_1 = 0$, $\Phi_1 \equiv 0$ and (5.34) to solve for Φ_3 in terms of $\Phi_2^{(p)}$ we find at this order that:

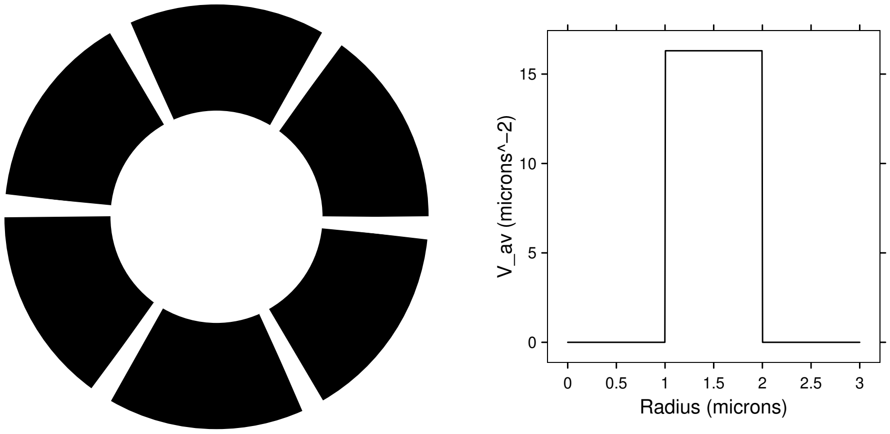
$$\begin{aligned} \frac{1}{r^2}\partial_\Theta^2\Phi_4 &= \frac{4}{r^2}\partial_\theta^2\Phi_2^{(p)} \ + \ (H \ - E_0)\,\Phi_2 \ - \ E_2\Phi_0 \\ &= \left(H \ - E_0 + \frac{4}{r^2}\partial_\theta^2\right)\Phi_2^{(p)} + \ (H \ - E_0)\,\Phi_2^{(h)} \ - \ E_2\Phi_0 \\ &= \left(H_{\rm av} - E_0 + \frac{4}{r^2}\partial_\theta^2\right)\Phi_2^{(p)} + (H \ - H_{\rm av})\,\Phi_2^{(h)} \\ &\qquad + (H_{\rm av} \ - E_0)\,\Phi_2^{(h)} \ - \ E_2\Phi_0 + (H - H_{\rm av})\,\Phi_2^{(p)}. \end{aligned} \tag{5.35}$$

The first two terms on the right hand side of (5.35) have zero average in Θ. Therefore, the solvability condition for Φ_4 becomes:

$$\begin{aligned} &(\ H_{\rm av} \ - \ E_0)\,\Phi_2^{(h)} \\ &\quad = E_2\Phi_0 - \frac{1}{2\pi}\int_0^{2\pi} (H - H_{\rm av})\,\Phi_2^{(p)}dp \\ &\quad = E_2\Phi_0 - \frac{1}{2\pi}\int_0^{2\pi} [V(r,\theta,p) - V_{\rm av}(r,\theta)]\Phi_2^{(p)}(r,\theta,p)dp \\ &\quad = \left(E_2 + \frac{r^2}{2\pi}\int_0^{2\pi}\left|\partial_p^{-1}[V(r,\theta,p) - V_{\rm av}(r,\theta)]\right|^2 dp\right)\Phi_0(r,\theta), \end{aligned} \tag{5.36}$$

where we have used (5.31), and where ∂_p^{-1} denotes the mean-zero antiderivative. We seek an *outgoing* solution of (5.36). This determines E_2 and therewith the expansion for the scattering resonance (effective index) through order N^{-2}.

In the following section we use this truncated expansion to numerically obtain the complex effective indexes (scattering resonances) for various structures. The details of the implementation are set out in section 7. In particular, in section 7 we derive an explicit expression for E_2 (see equations (7.17,7.18,7.8)) for the class of N-fold symmetric waveguides.



(a) (b)

FIGURE 2. (a) A ring of "air wedges" supported by $N = 6$ webs of glass. The inner and outer radii of the annulus are 1 and 2μm, respectively, while the air fill fraction within the annulus is $f = 0.9$. (b) The averaged potential $V_{\rm av}$.

6. Numerical simulations for selected structures

We now illustrate the theory of the preceding section with numerical calculations performed for a class of structures. These structures consist of an annulus of air supported with glass "webs;" see figure 2. More general structures are considered in [**7**], *e.g.* rings of circular holes, truncated hexagonal lattices of circular holes. General structures can be approximated by such "simple layered structures," of the type in figure 2. The details of the implementation are set out in section 7.

We will identify individual leaky modes, or scattering resonances, of these structures using the LP_{lm} (linearly polarized) notation [**11**] appropriate for solutions of the scalar wave equation. Usually this notation applies to guided modes, but no ambiguity will result as none of the structures we consider supports guided modes. The subscript $l \in \{0, 1, 2, ...\}$ refers to the angular dependence $e^{il\theta}$ of solutions to the averaged equation, while $m \in \{1, 2, 3, ...\}$ indexes the collection of leaky modes with fixed l. This collection is ordered by $\Re n_{\rm eff}$, with $m = 1$ corresponding to the largest such value. In the figures, we will use distinct plotting symbols to represent different values of l; the various values of m for fixed l are not explicitly displayed, but can be inferred from the monotonic relationship between m and $\Re n_{\rm eff}$.

In all of the examples, the refractive index of glass was taken to be 1.45 and the holes were assumed empty. The calculations were all performed at $\lambda_{\rm fs} = 1.55\mu$m. All of these structures support only continuous spectrum, so we report on the complex eigenvalues associated with resonances of the structures.

We computed the following sets of resonances for the webbed structures depicted in 2. We restricted attention to leaky mode solutions of the averaged structure with effective indexes $\Re n_{\rm eff} \in [1.41, 1.45]$, attenuation coefficients less than about 2 dB/mm, and angular index $l \in \{0, 1, 2, 3\}$. To express these quantities in our notation, recall from (2.11) that

$$\beta = \sqrt{k^2 n_g^2 - E} \tag{6.1}$$

and that the effective index is given by

$$n_{\text{eff}} \;=\; k^{-1}\,\beta \tag{6.2}$$

Also, the attenuation γ (in dB/cm, if β has units of $1/\mu$m) of a leaky mode is given by

$$\gamma \;\equiv 10\log_{10}\frac{\text{Power Input}}{\text{Power Output}} \;=\; \frac{2\times 10^5}{\ln(10)}\Im\beta. \tag{6.3}$$

The factor of 2 in (6.3) is due to the definition of γ as the attenuation coefficient for intensity, rather than field amplitude. Once this set of leaky modes of the averaged potential was found, the leading order corrections E_2 to the leading order energies E_0 were computed.

The results for three scalings and two air-fill fractions, along with various values of the periodicity N, of the ring of "air wedges" are presented in figure 3.

We also computed resonances of a structure of the type shown in figure 2 with $R_{\text{in}} = 1\mu$m, $R_{\text{out}} = 2\mu$m for the fill fractions $f = 0.8$, 0.9, and 1, with $N = 3$ and $N = 6$ holes. The calculations were performed for a range of free-space wavelengths λ_{fs} ranging from 1μm to 2μm. The structure with $f = 1$ is an idealized ring of air with no supporting structure. In figure 4 we compare the results of our theory to parallel calculations performed in [**15**] by a Fourier decomposition algorithm. We observe that the two methods agree exactly for the $f = 1$ case, as they should. Additionally, in all cases our method agrees with the Fourier calculation as $\lambda_{\text{fs}} \to 2\mu$m. Even for smaller λ_{fs} the agreement is quite good except for the $f = 0.8$, $N = 3$ case, which is not surprising given the small value of N and the fact that the width of the ring is equal to the smallest free space wavelength considered. The plots displayed in figure 4 are consistent with the expectation that approximation by the homogenization expansion improves (a) for fixed λ_{fs} and increasing N, as well as (b) for fixed N and λ_{fs} increasing.

The dashed lines in figure 4 display the attenuations of the averaged structures, without the $\mathcal{O}(N^{-2})$ correction. The necessity of including these corrections is evident, though the effect in these structures is not as dramatic as in some of the other structures we consider in [**7**].

Another result reported in [**15**] is the effective index of the first excited state above the fundamental (the LP_{11} state) for the $f = 0.9$, $N = 3$ structure at $\lambda_{\text{fs}} = 1.55\mu$m. In table 1 we compare the results of the Fourier method with truncations of our homogenization expansion to one and two terms, for both the fundamental and first excited leaky modes. We note that the one-term (averaged theory) truncation predicts the real part of the effective index well, as reported in [**2**], but again, the $\mathcal{O}(N^{-2})$ corrections are necessary to obtain good agreement of the attenuation rates.

6.1. Convergence as $N \to \infty$. In this section we describe a consistency check on our implementation of the scheme described in section 7.2 for simple layered potentials. We compute the first non-trivial corrections $N^{-2}\Phi_2$ and $N^{-2}E_2$ to the field and energy, respectively, in (5.12) and express the field and energy as our

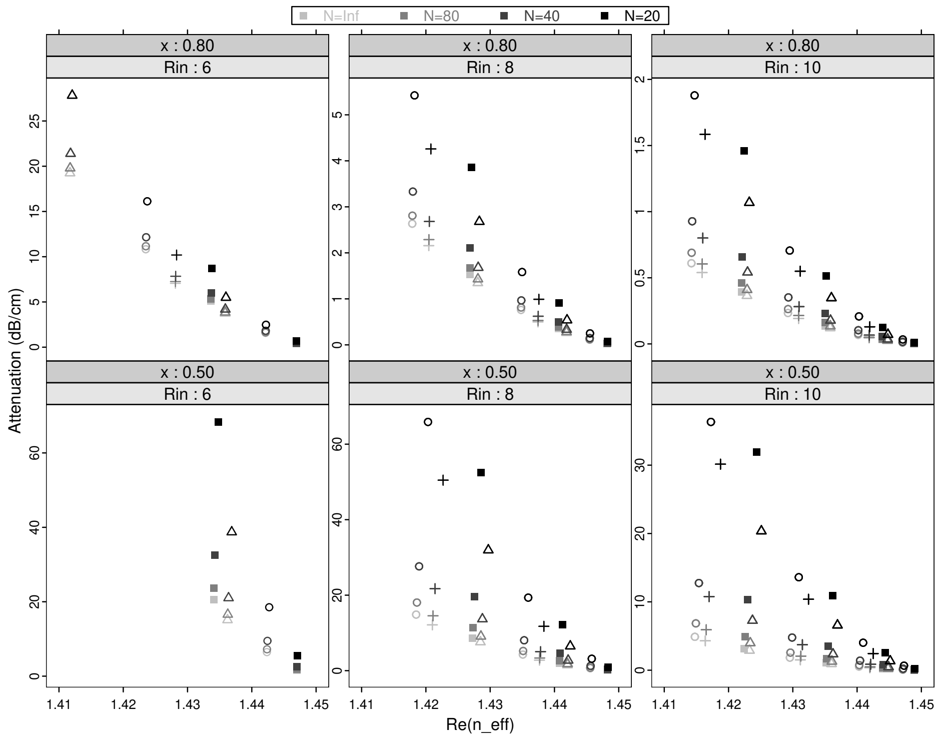


FIGURE 3. The effective indexes and attenuation coefficients of a set of the least-lossy resonances with $l \in \{0, 1, 2, 3\}$ of the structure depicted in figure 2, for two choices of fill fraction x and three different radii. The plotting symbol encodes the angular index l: $\blacksquare$, $\circ$, $\triangle$, $+$ correspond to $l = 0, 1, 2, 3$; the shade of grey encodes the periodicity N. The results of the averaged structure are labelled $N = \infty$.

approximation plus error terms:

$$\begin{aligned} \Phi &= \Phi_0 + \frac{1}{N^2}\Phi_2 + \Phi_3^{(N)} \\ E &= E_0 + \frac{1}{N^2}E_2 + E_3^{(N)}. \end{aligned} \tag{6.4}$$

We consider by how much the mode equation (3.1) is *not* satisfied by the first two terms of the expansion (6.4). Therefore, we define the residual:

$$F_{\text{res}} \equiv \left(-\Delta + V - \left(E_0 + \frac{1}{N^2}E_2\right)\right)\left(\Phi_0 + \frac{1}{N^2}\Phi_2\right). \tag{6.5}$$

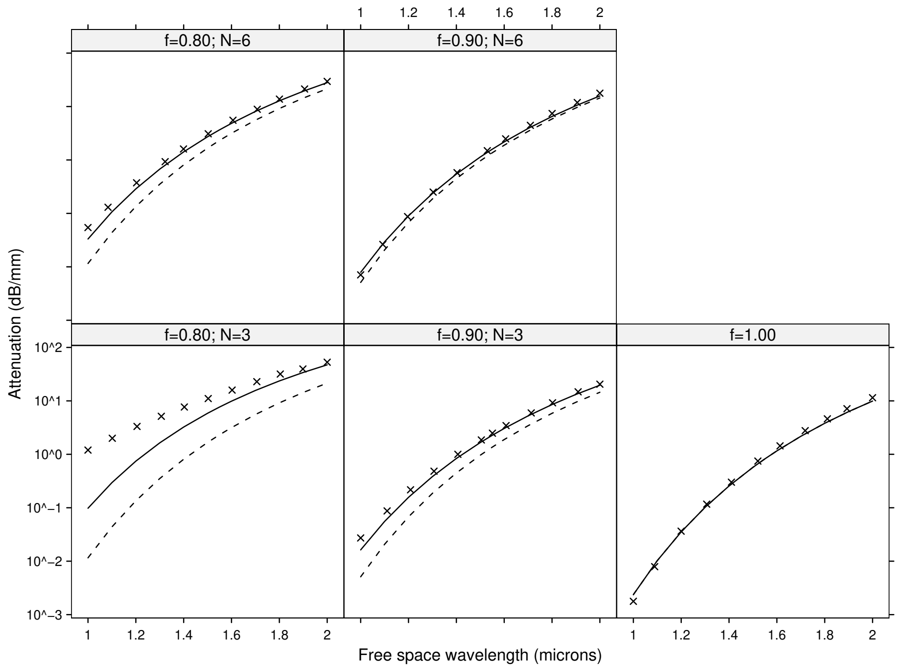


FIGURE 4. Attenuation of the lowest order (fundamental, or LP_{01}) resonance for a structure of the type shown in figure 2, with $R_{\rm in} = 1\mu$m, $R_{\rm out} = 2\mu$m for the fill fractions $f = 0.8$, 0.9, and 1, with $N = 3$ and $N = 6$ holes. The calculations were performed for a range of free-space wavelengths $\lambda_{\rm fs}$ ranging from 1μm to 2μm. The solid lines are the attenuations computed according to the methods of this paper, including the $\mathcal{O}(N^{-2})$ corrections; the dashed lines are the attenuations of the averaged structure; and the crosses correspond to the results presented in figure 3a of [**15**].

Substituting (6.4) into the (3.1) (3.1), we find that the residual is given by

$$F_{\rm res} = E_3^{(N)} \left(\Phi_0 + \frac{1}{N^2}\Phi_2 + \Phi_3^{(N)} \right) - \left(\Delta + V - \left(E_0 + \frac{1}{N^2} E_2 \right) \right) \Phi_3^{(N)}. \tag{6.6}$$

We expect $F_{\rm res}$ to be of order N^{-1} because $\Phi_3^{(N)}$ and $E_3^{(N)}$ are formally of order N^{-3} and the Laplacian in (6.6), when acting on the fast angular dependence, gives a factor of N^2. Expanding $F_{\rm res}$ in powers of $1/N$, we find that when $l > 0$ the

	Averaged		*2nd Order Homog.*		*Fourier*	
mode	n_{eff}	*atten.*	n_{eff}	*atten.*	n_{eff}	*atten.*
LP_{01}	1.3712+ $0.0000387i$	1.36	1.3727+ $0.0000644i$	2.27	1.365+ $0.000071i$	2.48
LP_{11}	1.2468+ $0.000436i$	15.3	1.2515+ $0.000832i$	29.3	1.255+ 0.00075i	27

TABLE 1. Comparison of results for the first two leaky modes of a ring of "air wedges" with $R_{\mathrm{in}} = 1\mu$m, $R_{\mathrm{out}} = 2\mu$m, fill fraction $f = 0.9$, and $N = 3$ holes. The effective indexes and attenuations (in dB/mm) of the leading term (averaged), and of the two-term truncation, of the homogenization expansion are compared with that of the Fourier expansion [**15**] (the values for the LP_{01} mode calculated by the Fourier expansion were read off of figure 3 of [**15**]).

leading term, $F_{\mathrm{res}}^{(1)}$, is the $\mathcal{O}(1/N)$ term

$$F_{\mathrm{res}}^{(1)} = \frac{1}{N}\frac{1}{r^2}\partial_\Theta^2\Phi_3. \tag{6.7}$$

This may be simplified using (5.34) and (5.31) to

$$F_{\mathrm{res}}^{(1)} = -\frac{2}{N}\left(\partial_\theta\Phi_0\right)\left(\partial_\Theta^{-1}\left(V - V_{\mathrm{av}}\right)\right). \tag{6.8}$$

Therefore, when $l > 0$, we expect that as $N \to \infty$

$$F_{\mathrm{res}} \to F_{\mathrm{res}}^{(1)} \sim \mathcal{O}\left(\frac{1}{N}\right) \quad \text{and} \quad F_{\mathrm{res}} - F_{\mathrm{res}}^{(1)} \sim \mathcal{O}\left(\frac{1}{N^2}\right). \tag{6.9}$$

When $l = 0$ ($\Phi_0 = \Phi_0(r)$), $\partial_\theta\Phi_0$ vanishes and the leading behavior of the residual is higher order in $1/N$.

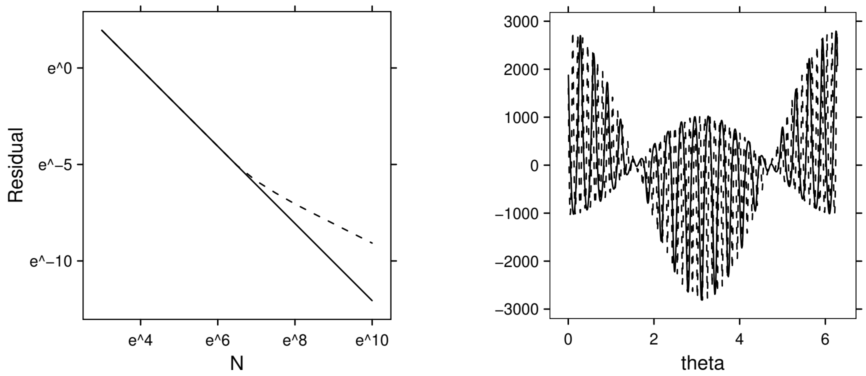
Since the potential V or its derivatives may have discontinuities, we encounter a problem when attempting to compute F_{res} using (6.6); it is possible that $\Phi_2^{(p)}$ is discontinuous as a function of r. We therefore interpret (6.6) as holding in the "weak sense" or sense of distributions, and integrate both sides against a radial test function $\phi_R(r)$ of compact support. This allows us to move the radial part of the Laplacian over to act on ϕ_R, and to define the "weak residual"

$$\begin{aligned} F_{\mathrm{res}}^{(\mathrm{weak})}(\theta) &= \int_0^\infty r\,dr\left(-\phi_R'' - \frac{1}{r}\phi_R' - \phi_R\frac{1}{r^2}\partial_\theta^2 + \phi_R\left(V - E_0 - \frac{1}{N^2}E_2\right)\right) \\ &\qquad \times\left(\Phi_0 + \frac{1}{N^2}\Phi_2\right) \end{aligned} \tag{6.10}$$

and its leading behavior in $1/N$

$$F_{\mathrm{res}}^{(\mathrm{weak},1)}(\theta) = -\frac{2}{N}\int_0^\infty r\,dr\,\phi_R\left(\partial_\theta\Phi_0\right)\left(\partial_\Theta^{-1}\left(V - V_{\mathrm{av}}\right)\right). \tag{6.11}$$

We computed (6.10) and (6.11) for the structure of example 2 (figure 2), with $R_{\mathrm{in}} = 10\mu$m, $R_{\mathrm{out}} = 11\mu$m, for the LP_{11} leaky mode. We allowed N to vary from 20 to 22,000. The results are presented in figure 5. The solid line in (a) represents $\|F_{\mathrm{res}}^{(\mathrm{weak})}(\theta) - F_{\mathrm{res}}^{(\mathrm{weak},1)}(\theta)\|_\infty$ as a function of N. The scales are logarithmic on both



(a) (b)

FIGURE 5. Results of the weak residual calculation. (a) $\|F_{\text{res}}^{(\text{weak})}(\theta) - F_{\text{res}}^{(\text{weak},1)}(\theta)\|_\infty$ (solid); $\|F_{\text{res}}^{(\text{weak})}(\theta)\|_\infty$ (dashed) (b) $N^2\,\Re(F_{\text{res}}^{(\text{weak})}(\theta) - F_{\text{res}}^{(\text{weak},1)}(\theta))$ for $N = 20$ (solid) and $N = 54$ (dashed).

axes, so the slope of -2 verifies that (6.9) holds over the entire range considered. The dashed line in (a) represents $\|F_{\text{res}}^{(\text{weak})}(\theta)\|_\infty$; we see that the slope changes from -2 to -1 at around $N = 1000$, which again verifies (6.9).

Figure 5 (b) shows the pointwise behavior of the weak residuals by plotting $N^2\,\Re(F_{\text{res}}^{(\text{weak})}(\theta) - F_{\text{res}}^{(\text{weak},1)}(\theta))$ vs. θ for $N = 20$ and $N = 54$. We observe that the envelope of the residuals is invariant after scaling by N^2, suggesting that the N^{-2} term dominates the residual after the leading term is subtracted, even for these moderate values of N. This behavior persists for all N we considered, up to $N = 22,000$.

7. Implementation of homogenization expansion

In this section, we give a detailed description of the procedure used to obtain the simulation results of the previous section.

We specialize to the case of a potential with no slow angular dependence, so $V(r,\theta,\Theta) = V(r,\Theta)$. In this case, the potential has an N-fold symmetry. We first, in section 7.1, sketch the expansion of solutions to the resonance problem summarized in the homogenization expansion of section 5 with no additional assumptions. This discussion pertains to N-fold symmetric microstructure, whose individual microfeatures have arbitrary geometry. Our strategy is to then approximate a general microstucture potential V by a *simple layered potential* in section 7.2. For the case of simple layered potentials, analytic expressions can be obtained which facilitate the numerical computations.

7.1. General Structures. The angularly averaged potential is a radial function, $V_{\text{av}} = V_{\text{av}}(r)$. We take

$$\Phi_0(r,\theta) = f(r)e^{il\theta},\ l \text{ an integer}$$

Then, $f(r)$ satisfies

$$\left(-\Delta_r + \frac{l^2}{r^2} + V_{\rm av}(r) - E_0\right)\ f(r)\ =\ 0 \tag{7.1}$$

A solution of the resonance problem is a pair $(f(r), E_0)$, such that $f(r)$ is a nonsingular solutions of (7.1) satisfying an *outgoing radiation condition at* $r = \infty$, (3.5). As noted in section 3, E_0 is complex with $\Im E_0 < 0$. In general, the existence of solutions to the resonance problem is a subtle technical problem. In the next subsection, we analyze it in detail for the particular class of *simple* layered structures, which we define there. In this section, we posit the existence of a solution, $(f(r), E_0)$. Note that since $V_{\rm av}(r) = 0$ for $r \ge r_*$,

$$f(r)\ =\ k_*\ H_l^{(1)}(\sqrt{E_0}r),\ r \ge r_*, \tag{7.2}$$

for some constant k_*.

We next calculate the leading order correction, $N^{-2}\Phi_2$, by our perturbation scheme. In the separable case, the equation for $\Phi_2^{(h)}$ is of the form:

$$(\ H_{\rm av} - E_0\ )\Phi_2^{(h)} = (\ E_2 + Q(r)\ )\ \Phi_0, \tag{7.3}$$

where $Q(r)$ has compact support. Since $\Phi_0(r,\theta) = f(r)e^{il\theta}$, all of the Fourier modes of $\Phi_2^{(h)}(r,\theta)$ except the $l^{\rm th}$ vanish and so we define $\Phi_2^{(h)}(r,\theta) = U(r)e^{il\theta}$ and consider the equation

$$\left(\ -\Delta_r + \frac{l^2}{r^2} + V_{\rm av}(r) - E_0\ \right)U(r)\ =\ (\ E_2 + Q(r)\ )\,f(r) \tag{7.4}$$

Recall that by (2.13), both Q and $V_{\rm av}$ are zero for $r \ge r_*$ and we have

$$\left(\ -\Delta_r + \frac{l^2}{r^2} - E_0\ \right)U(r)\ =\ E_2\ f(r),\quad r \ge r_*. \tag{7.5}$$

We proceed with the solution of the inhomogeneous problem (7.4) for $r \ge 0$ and then obtain an expression for E_2 by imposing the outward going radiation condition.

We have assumed that V is regular at the origin. We let $\tilde y_1(r)$ denote the solution to the homogeneous equation associated with (7.4) that is regular at $r = 0$, and $\tilde y_2(r)$ denote an independent solution, which together with $\tilde y_1$ spans the solution set. Then $\tilde y_1(r) \propto r^l$, and $\tilde y_2(r) \propto r^{-l}$ if $l > 0$, or $\tilde y_1(r) \propto \ln(r)$ if $l = 0$. For $r > r_*$, an appropriate set of homogeneous solutions of (7.5) is in terms Hankel functions, $H_l^{(j)}(\sqrt{E_0}\ r)$, $j = 1,2$. $H_l^{(1)}$ satisfies the outward going radiation condition and infinity and $H_l^{(2)}$ the inward going radiation condition at infinity.

A particular solution of (7.4) can be constructed by variation of parameters using these homogeneous solutions in the intervals:

$$R_{\rm in} = [0, r_*],\quad \text{and}\quad R_{\rm out} = (r_*, \infty).$$

Specifically, we have

$$\text{in } R_{\rm in}:\quad U(r)\ =\ E_2\ \mathcal{G}_{\rm in}[f](r)\ +\ \mathcal{G}_{\rm in}[Qf](r) \tag{7.6}$$

$$\text{in } R_{\rm out}:\quad U(r)\ =\ \xi_* H_l^{(1)}(\sqrt{E_0}\ r)\ +\ \eta_* H_l^{(2)}(\sqrt{E_0}\ r)\ +\ E_2\ \mathcal{G}_{\rm out}[f](r). \tag{7.7}$$

Imposing continuity of U and $\partial_r U$ at $r = r_*$ yields the system:

$$\begin{aligned}\begin{pmatrix} \xi_*(E_2) \\ \eta_*(E_2) \end{pmatrix} &= E_2\ \mathcal{Y}^{-1}(r_*) \begin{pmatrix} \mathcal{G}_{\rm in}[f](r_*) - \mathcal{G}_{\rm out}[f](r_*) \\ E_0^{-\frac{1}{2}} \left(\partial\mathcal{G}_{\rm in}[f](r_*) - \partial\mathcal{G}_{\rm out}[f](r_*)\right) \end{pmatrix} \\ &+ \ \mathcal{Y}^{-1}(r_*) \begin{pmatrix} \mathcal{G}_{\rm in}[Qf](r_*) \\ E_0^{-\frac{1}{2}}\ \partial\mathcal{G}_{\rm in}[Qf](r_*) \end{pmatrix}. \end{aligned} \tag{7.8}$$

Here, $\mathcal{G}_{\rm in}[F]$ denotes a choice of particular solution of

$$\left(-\Delta_r + \frac{l^2}{r^2} + V_{\rm av}(r) - E_0 \right) \mathcal{G}_{\rm in}[F] \ = \ F(r),\ 0 \le r < r_*\ (r \in R_{\rm in}), \tag{7.9}$$

$\mathcal{G}_{\rm out}[F]$ denotes a choice of particular solution of

$$\left(-\Delta_r + \frac{l^2}{r^2} - E_0 \right) \mathcal{G}_{\rm out}[F] \ = \ F(r),\ r_* \ge r\ (r \in R_{\rm out}), \tag{7.10}$$

and

$$\mathcal{Y}(r) \ = \ \begin{pmatrix} H_l^{(1)}(\sqrt{E_0}r) & H_l^{(2)}(\sqrt{E_0}r) \\ \partial_s H_l^{(1)}(\sqrt{E_0}r) & \partial_s H_l^{(2)}(\sqrt{E_0}r) \end{pmatrix}.$$

Since

$$W\{H_l^{(1)}(s), H_l^{(2)}(s)\} = -\frac{4i}{\pi s},$$

it follows that

$$\mathcal{Y}^{-1}(r) \ = \ \frac{i\pi r}{4} \begin{pmatrix} \partial_s H_l^{(2)}(\sqrt{E_0}r) & -H_l^{(2)}(\sqrt{E_0}r) \\ -\partial_s H_l^{(1)}(\sqrt{E_0}r) & H_l^{(1)}(\sqrt{E_0}r) \end{pmatrix}.$$

With ξ_* and η_* given by (7.8), (7.6-7.7) defines a nonsingular solution of (7.4). It remains to impose radiation condition at $r = \infty$. Consider $U(r)$ for $r \ge r_*$. Let

$$z = \sqrt{E_0}r,\ z_* = \sqrt{E_0}r_*,\ G(z) = U(r(z)).$$

Then, (7.5) becomes:

$$z^2 G'' + z G' + (z^2 - l^2) G \ = \ \frac{E_2}{E_0} k_*\ z^2 H_l^{(1)}(z),\ r(z) \ge r_*. \tag{7.11}$$

By (7.7) and (7.2)

$$G(z) = U(r(z)) \ = \ \xi_*(E_2)\ H_l^{(1)}(z) + \eta_*(E_2)\ H_l^{(2)}(z) + \frac{E_2}{E_0} k_*\ \mathcal{G}_{\rm out}[H_l^{(1)}](z), \tag{7.12}$$

$\mathcal{G}_{\rm out}$ can be constructed by variation of parameters. A particular solution is

$$\xi_*^{(p)}(z) H_l^{(1)}(z) \ + \ \eta_*^{(p)}(z) H_l^{(2)}(z),$$

where [1]

$$\xi_*^{(p)}[h](z) \ = \ -\int_{z_*}^{z} \frac{H_l^{(2)}(\zeta) h(\zeta)}{\zeta^2 W\{H_l^{(1)}, H_l^{(2)}\}}\ d\zeta \tag{7.13}$$

$$\eta_*^{(p)}[h](z) \ = \ +\int_{z_*}^{z} \frac{H_l^{(1)}(\zeta) h(\zeta)}{\zeta^2 W\{H_l^{(1)}, H_l^{(2)}\}}.\ d\zeta \tag{7.14}$$

[1] Note that z can be complex-valued. The complex integral $\int_{z_*}^{z}$ is computed by parameterizing the line from z_* to z as: $t \mapsto z_* + t(z - z_*)$. Then, $\int_{z_*}^{z} F(\zeta) d\zeta = (z - z_*) \int_0^1 F(z_* + t(z - z_*)) dt$.

Therefore,

$$\mathcal{G}_{\rm out}[F](z) \;=\; \Big(\; \xi_*^{(p)}[\zeta^2 F](z) H_l^{(1)}(z) + \eta_*^{(p)}[\zeta^2 F](z) H_l^{(2)}(z) \;\Big)\,, \tag{7.15}$$

Using (7.15) in (7.12) we have:

$$\begin{aligned} G(z) = U(r(z)) \;&=\; \xi_*(E_2)\; H_l^{(1)}(z) \;+\; \eta_*(E_2)\; H_l^{(2)}(z) \\ &-\; \frac{i\pi}{4}\frac{E_2}{E_0} k_* \cdot \int_{z_*}^{z} H_l^{(2)}(\zeta) H_l^{(1)}(\zeta)\zeta\; d\zeta\; H_l^{(1)}(z) \\ &+\; \frac{i\pi}{4}\frac{E_2}{E_0} k_* \cdot \int_{z_*}^{z} [H_l^{(1)}(\zeta)]^2 \zeta\; d\zeta\; H_l^{(2)}(z). \end{aligned} \tag{7.16}$$

Recall that $\xi_*(E_2)$ and $\eta_*(E_2)$ are determined by the continuity conditions at $r = r_*$ and are given by (7.8). The condition determining E_2 is that the *incoming* part of $G(z)$ be identically zero. Derivation of this condition on E_2 requires the use of certain integral identities involving Hankel functions.

Note that both terms in (7.16) that are proportional to $H_l^{(1)}$ are outgoing, as can be seen by referring to the asymptotic forms (3.4). From [**8**] (page 634, equation 5.54) we have

$$\int \;\zeta [H_l^{(j)}(\zeta)]^2 d\zeta \;=\; \frac{\zeta^2}{2}\,\Big(\; [H_l^{(j)}(\zeta)]^2 - H_{l-1}^{(j)}(\zeta) H_{l+1}^{(j)}(\zeta) \;\Big)\,.$$

Therefore, the terms in (7.16) that are proportional to $H_l^{(2)}$ can be written as:

$$\begin{aligned} &\eta_*(E_2) H_l^{(2)}(z) \;+\; \frac{ik_*\pi}{4}\frac{E_2}{E_0}\cdot\frac{\zeta^2}{2}\,\Big(\; [H_l^{(1)}(\zeta)]^2 - H_{l-1}^{(1)}(\zeta) H_{l+1}^{(1)}(\zeta) \;\Big)\Big|_{z_*}^{z}\; H_l^{(2)}(z) \\ &= \Big[\; \eta_*(E_2) - \frac{ik_*\pi}{4}\frac{E_2}{E_0}\cdot\frac{z_*^2}{2}\,\Big(\; [H_l^{(1)}(z_*)]^2 - H_{l-1}^{(1)}(z_*) H_{l+1}^{(1)}(z_*) \;\Big) \;\Big]\; H_l^{(2)}(z) \\ &+\; \frac{ik_*\pi}{4}\frac{E_2}{E_0}\cdot\frac{z^2}{2}\,\Big(\; [H_l^{(1)}(z)]^2 - H_{l-1}^{(1)}(z) H_{l+1}^{(1)}(z) \;\Big)\; H_l^{(2)}(z). \end{aligned}$$

Again from (3.4) the latter term is seen to be outgoing at infinity so the condition on E_2 is:

$$\eta_*(E_2) - \frac{ik_*\pi}{4}\frac{E_2}{E_0}\cdot\frac{z_*^2}{2}\,\Big(\; [H_l^{(1)}(z_*)]^2 - H_{l-1}^{(1)}(z_*) H_{l+1}^{(1)}(z_*) \;\Big) = 0. \tag{7.17}$$

We can write $\eta_*(E_2)$ as

$$\eta_*(E_2) \;= \eta_{*0} + E_2 \eta_{*1}, \tag{7.18}$$

where η_{*j} can be read off from the second component of (7.8). Equations (7.17) and (7.18) give a linear relation for E_2 which can be solved.

7.2. Simple layered structures: Leading order resonances. We now give the details of the above scheme for case of a *simple layered* structure, which we define to be one with potential $V(r,\theta,\Theta)$ that is both independent of the slow angular variable θ and is a simple function of the form

$$V(r,\Theta) = \sum_{i=1}^{L}\sum_{j=1}^{M_i} \mathbf{1}_{[r_i,r_{i+1}]}(r)\, \mathbf{1}_{[\Theta_j,\Theta_{j+1}]}(\Theta)\, V_{i,j}, \tag{7.19}$$

where L is the number of radial layers and M_i is the number of angular sectors in one period of the $i^{\rm th}$ layer. $\mathbf{1}_A(\zeta)$ denotes the indicator function of the set A,

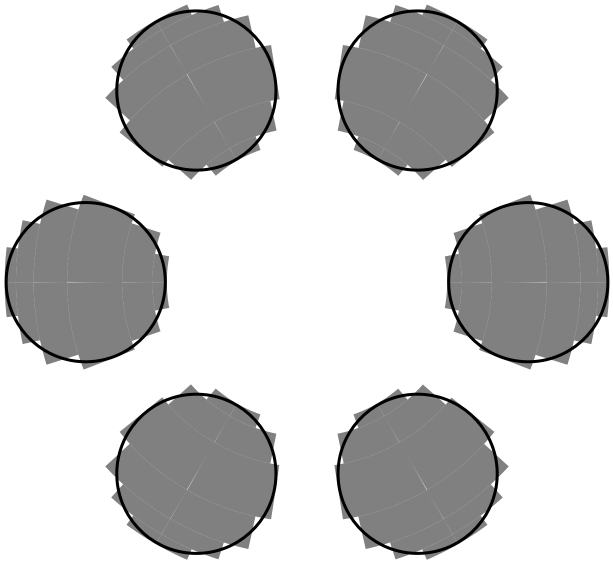


FIGURE 6. An example of an approximation by "simple layered structures" (see (7.19)) of a structure consisting of six circular air holes.

taking the value one for $\zeta \in A$ and zero for $\zeta \notin A$. By definition, $r_1 = 0$, $\Theta_1 = 0$ and $\Theta_{M_i+1} = 2\pi$. The potential in (7.19) has, as a function of Θ, M_i jumps in layer R_i and, as a function of θ NM_i jumps in layer R_i. An example of a simple layered approximation to a structure containing six circular air holes is presented in figure 6.

In the remainder of this section, we describe the calculation of the leading order resonances, those associated with the averaged potential $V_{\rm av}$. In the next section, we will compute the leading corrections due to microstructure.

With the definition (7.19) of $V(r,\Theta)$, $V_{\rm av}(r)$ is constant on each region $R_i = [r_i, r_{i+1}]$; equivalently,

$$V_{\rm av}(r) = V_{{\rm av},i} \qquad r \in R_i. \tag{7.20}$$

In the special case where the index profile, $n(r,\theta)$, takes on two values n_g and n_h and $2\pi f_i$ denotes the total angle of the annulus R_i occupied by "material h," we have by averaging V in (2.11):

$$V_{\rm av}(r) \;=\; k^2 f_i [n_g^2 - n_h^2], \quad r \in R_i. \tag{7.21}$$

In each interval, R_i, the solution will be oscillatory or nonoscillatory depending on whether (i) $\Re E_0 > V_{{\rm av},i}$ or (ii) $\Re E_0 < V_{{\rm av},i}$. Accordingly, we transform equation (7.1) to Bessel's equation in case (i) and the modified Bessel equation in case (ii).

(i) $\Re E_0 > V_{{\rm av},i}$*:* In this case, we set

$$z = \sqrt{E_0 - V_{{\rm av},i}}\; r \quad \text{and } f(r) = g(z). \tag{7.22}$$

Then, $g(z)$ satisfies Bessel's equation [**1**]:

$$z^2 g'' + zg' + (z^2 - l^2)g \;=\; 0. \tag{7.23}$$

For $i < L$, we write

$$g(z) \;=\; \alpha_i J_l(z) \;+\; \beta_i Y_l(z), \tag{7.24}$$

where J_l and Y_l are standard Bessel functions of order l that satisfy the Wronksian relation

$$W\{J_l, Y_l\} \;=\; \frac{2}{\pi z}. \tag{7.25}$$

In the outermost region R_L, we choose to express g as a linear combination of $H_l^{(1)}$, $H_l^{(2)}$ instead of J_l, Y_l in (7.24).
(ii) $\Re E_0 < V_{\mathrm{av},i}$*:* In this case, we set

$$z = \sqrt{V_{\mathrm{av},i} - E_0}\; r \quad \text{and } f(r) = g(z). \tag{7.26}$$

Then, $g(z)$ satisfies the modified Bessel equation [**1**]:

$$z^2 g'' + zg' - (z^2 + l^2)g \;=\; 0. \tag{7.27}$$

In this case we write

$$g(z) \;=\; \alpha_i I_l(z) \;+\; \beta_i K_l(z), \tag{7.28}$$

where I_l and K_l are standard modified Bessel functions of order l that satisfy the Wronksian relation

$$W\{I_l, K_l\} \;=\; \frac{1}{z}. \tag{7.29}$$

Solutions of (7.1) are pieced together subject to the conditions of regularity at $r = 0$, continuity of f and f' at $r = r_i$ and the radiation (boundary) condition at $r = \infty$. We now discuss these in detail.

Boundary condition at $r = 0$*:* Since Y_l and K_l have singularities at $r = 0$, for the solution to be non-singular at $r = 0$ we require $\beta = 0$ in both cases (i) and (ii).

Radiation condition at $r = \infty$*:* This concerns the region $\{r > r_L\}$. Here, $\Re E_0 > V_{\mathrm{av},L}$ and therefore, the solution is oscillatory. Note that the outgoing radiation condition is satisfied by the first Hankel function, $H_l^{(1)}(z)$, and therefore we require

$$\beta_L = 0. \tag{7.30}$$

In particular, for $r > r_L$,

$$g(z) = \alpha_L H_l^{(1)}(z). \tag{7.31}$$

Continuity of f *and* f' *across interfaces:* The interfaces are defined by the values of the radius $r = r_i$, which correspond to $z = z_i$ given by (7.22) in case (i) and (7.26) in case (ii). Continuity of f at interfaces means $f(r_i^-) = f(r_i^+)$, which corresponds to:

$$g(z_i^-) \;=\; g(z_i^+). \tag{7.32}$$

Continuity of f' at the interfaces means $f'(r_i^-) = f'(r_i^+)$. Since

$$\frac{dz}{dr} = \sqrt{V_{\rm av} - E_0}, \text{ where } \Re E_0 < V_{\rm av}$$
$$\frac{dz}{dr} = \sqrt{E_0 - V_{\rm av}}, \text{ where } \Re E_0 > V_{\rm av},$$

in terms of $g(z)$, continuity of derivatives is given by:

$$\left.\frac{dg}{dz}\frac{dz}{dr}\right|_{z=z_i^+} = \left.\frac{dg}{dz}\frac{dz}{dr}\right|_{z=z_i^-}. \tag{7.33}$$

We now implement the matching across interfaces. Let (y_1, y_2) denote either (J_l, Y_l) or (I_l, K_l) our fundamental sets of solutions corresponding to cases (i) and (ii), respectively, and let $\mathcal{Y}$ denote the fundamental matrix:

$$\mathcal{Y} = \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix}. \tag{7.34}$$

Note that $W\{y_1, y_2\} = \det \mathcal{Y}$.

For $r \in R_i$,

$$\begin{pmatrix} g \\ g' \end{pmatrix} = \mathcal{Y}(z) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

The pair of interface matching conditions at $z = z_i$ is then

$$\left.\begin{pmatrix} 1 & 0 \\ 0 & \frac{dz}{dr} \end{pmatrix}\right|_{r=r_i^+} \left.\begin{pmatrix} g \\ g' \end{pmatrix}\right|_{z=z(r_i^+)} = \left.\begin{pmatrix} 1 & 0 \\ 0 & \frac{dz}{dr} \end{pmatrix}\right|_{r=r_i^-} \left.\begin{pmatrix} g \\ g' \end{pmatrix}\right|_{z=z(r_i^-)}.$$

Equivalently,

$$\begin{aligned} &\left.\begin{pmatrix} 1 & 0 \\ 0 & \frac{dz}{dr} \end{pmatrix}\right|_{r=r_i^+} \mathcal{Y}(z(r_i^+)) \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} \\ &= \left.\begin{pmatrix} 1 & 0 \\ 0 & \frac{dz}{dr} \end{pmatrix}\right|_{r=r_i^-} \mathcal{Y}(z(r_i^-)) \begin{pmatrix} \alpha_{q-1} \\ \beta_{q-1} \end{pmatrix} \end{aligned} \tag{7.35}$$

or

$$\begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = \mathbf{T}_l(E_0) \begin{pmatrix} \alpha_{q-1} \\ \beta_{q-1} \end{pmatrix}, \tag{7.36}$$

where $\mathbf{T}_i$ denotes the transfer matrix from R_{i-1} to R_i:

$$\mathbf{T}_i = \mathcal{Y}(z(r_i^+))^{-1}\, \mathbf{J}_i\, \mathcal{Y}(z(r_i^-)), \tag{7.37}$$

where $\mathbf{J}_i$ is the "jump matrix":

$$\mathbf{J}_i = \begin{pmatrix} 1 & 0 \\ 0 & \left(\frac{dz}{dr}(r_i^+)\right)^{-1} \frac{dz}{dr}(r_i^-) \end{pmatrix}. \tag{7.38}$$

Therefore, the connection formula relating the coefficients α_1, β_1 in region R_1 with α_L, β_L in region R_L is:

$$\begin{pmatrix} \alpha_L \\ \beta_L \end{pmatrix} = \mathbf{T}(E_0) \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}, \tag{7.39}$$

where

$$\mathbf{T}(E_0) = \mathbf{T}_L(E_0) \cdots \mathbf{T}_3(E_0)\mathbf{T}_2(E_0). \tag{7.40}$$

The condition that the solution be nonsingular at $r = 0$ implies that

$$\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

or a multiple thereof. The radiation condition (7.30) is equivalent to the orthogonality of $(0, 1)$ and (α_L, β_L). Therefore, the resonance or scattering energies are determined by the following scalar transcendental equation:

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \mathbf{T}(E_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \tag{7.41}$$

or equivalently

$$T_{21}(E_0) = 0, \tag{7.42}$$

where T_{kj} denotes the (k, j) entry of the matrix $\mathbf{T}(E_0)$.

7.3. Simple layered structures: Microstructure corrections to Φ_0 and E_0. In this subsection we construct the order N^{-2} correction to Φ_0 ($N^{-2}\Phi_2$) and to E_0 ($N^{-2}E_2$) for the special case of a simple layered structure (7.19). Recall that $\Phi_2 = \Phi_2^{(p)} + \Phi_2^{(h)}$. Here $\Phi_2^{(p)}$ is, in general, given by the Fourier series (5.31). When the potential is of the form (7.19), $\Phi_2^{(p)}$ can be explicitly calculated, which is done in appendix A. $\Phi_2^{(h)}$ solves equation (5.36) and E_2 is chosen so that (5.31) has a solution satisfying the outgoing radiation condition at $r = \infty$. We now focus on the determination of E_2 and $\Phi_2^{(h)}$ in the separable case.

Recall that the equation (5.36) for $u = \Phi_2^{(h)}$ is of the form:

$$(H_{\rm av} - E_0)u = (E_2 + Q(r)) \Phi_0, \tag{7.43}$$

where $Q(r)$ has compact support; its explicit form for simple structures is presented in appendix A. Since $\Phi_0(r, \theta) = f(r)e^{il\theta}$, we define $u(r) = U(r)e^{il\theta}$ and consider the equation

$$\left(-\Delta_r + \frac{l^2}{r^2} + V_{\rm av}(r) - E_0 \right) U(r) = (E_2 + Q(r)) f(r) \tag{7.44}$$

As in the previous subsection, we define

$$\begin{aligned} z &= \sqrt{E_0 - V_{\rm av}}\, r \ , \ \Re E_0 > V_{\rm av} \\ z &= \sqrt{V_{\rm av} - E_0}\, r \ , \ \Re E_0 < V_{\rm av} \end{aligned}$$

and

$$Q_1(z) = Q(r(z)), \quad U_1(z) = U(r(z)), \quad g(z) = f(r(z)).$$

Then,

$$\begin{aligned} z^2U_1'' + zU_1' + (z^2 - l^2)U_1 &= b_+(z) \equiv \frac{-z^2}{E_0 - V_{\rm av}}(Q_1 + E_2)g(z), \quad \Re E_0 > V_{\rm av} \\ z^2U_1'' + zU_1' - (z^2 + l^2)U_1 &= b_-(z) \equiv \frac{-z^2}{V_{\rm av} - E_0}(Q_1 + E_2)g(z), \quad \Re E_0 < V_{\rm av}. \end{aligned} \tag{7.45}$$

We now solve (7.45). Fix any interval R_q where $V_{\rm av}(r(z))$ is constant. The solution in this interval can be written as:

$$U_{1,q}(z) = U_{1,q}^{(p)}(z) + \xi_q y_1(z) + \eta_q y_2(z), \tag{7.46}$$

where $U_1^{(p)}(z)$ denotes a particular solution obtained by variation of parameters:

$$U_{1,q}^{(p)}(z) \;=\; U_{1,q}^{(p)}(z;E_2) \;=\; \xi_q^{(p)}(z)\; y_1(z) + \eta_q^{(p)}(z)\; y_2(z). \tag{7.47}$$

In regions $R_1, ..., R_{L-1}$, y_1 and y_2 are taken to be Bessel or modified Bessel while

$$\text{in region } R_L: \qquad y_1 = H_l^{(1)} \text{ and } y_2 = H_l^{(2)},$$

where $H_l^{(1)}$ and $H_l^{(2)}$ are Hankel functions satisfying, respectively, outgoing and incoming radiation conditions at $r = \infty$. We have

$$\xi_q^{(p)}(z) \;=\; -\int^z \frac{y_2(\zeta) b_\pm(\zeta)}{\zeta^2 W\{y_1,y_2\}}\, d\zeta \tag{7.48}$$

$$\eta_q^{(p)}(z) \;=\; +\int^z \frac{y_1(\zeta) b_\pm(\zeta)}{\zeta^2 W\{y_1,y_2\}}\, d\zeta. \tag{7.49}$$

The Wronskian, $W\{y_1, y_2\} = \det \mathcal{Y}$ is given in (7.25) in the case of Bessel functions, (7.29) in the case of modified Bessel functions and (7.11) in the case of Hankel functions. The lower limits of integration in (7.48) and (7.49) are chosen to be z_q, the left endpoint of the interval R_q.

Boundary condition at $r = 0$: The lower limit of integration of $U_1^{(p)}$ in R_1 is $z = 0$, so we require, due to the singularity at $r = 0$ of Y_l and K_l, that $\eta_1 = 0$. In fact, for simplicity we take the homogeneous part of the solution in this region to be identically zero. Thus,

$$\begin{pmatrix} \xi_1 \\ \eta_1 \end{pmatrix} \;=\; \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{7.50}$$

Continuity across interfaces: We require continuity of $U_1(r)$ and $\partial_r U_1(r)$ at the interfaces $r = r_q$ ($z = z_q = z(r_q)$), for $q = 2, \ldots, L$. This gives (*cf.* (7.35))

$$\left.\begin{pmatrix} U_{1,q}(z) \\ \partial_z U_{1,q}(z) \end{pmatrix}\right|_{z=z_q^+} = \mathbf{J}_q \left.\begin{pmatrix} U_{1,q-1}(z) \\ \partial_z U_{1,q-1}(z) \end{pmatrix}\right|_{z=z_q^-}. \tag{7.51}$$

Equation (7.51) is equivalent to the following set of algebraic relations on the coefficients ξ and η:

$$\begin{aligned} \begin{pmatrix} \xi_q \\ \eta_q \end{pmatrix} \;&=\; \mathcal{Y}(z_q^+)^{-1} \left[-\mathbf{U_1^{(P)}}(z_q^+) + \mathbf{J}_q \mathbf{U_1^{(P)}}(z_q^-) \right] \\ &\quad + \mathcal{Y}(z_q^+)^{-1} \mathbf{J}_q \mathcal{Y}(z_q^-) \begin{pmatrix} \xi_{q-1} \\ \eta_{q-1} \end{pmatrix} \end{aligned} \tag{7.52}$$

Here, $\mathbf{U_1^{(P)}} = \mathbf{U_1^{(P)}}(E_2)$ denotes the column 2-vector with components $U_1^{(p)}$ and $\partial U_1^{(p)}$. Equation (7.52) has the form

$$\begin{pmatrix} \xi_q \\ \eta_q \end{pmatrix} \;=\; \mathbf{F}_q(E_2) \;+\; \mathbf{T}_q \begin{pmatrix} \xi_{q-1} \\ \eta_{q-1} \end{pmatrix}, \tag{7.53}$$

where $\mathbf{F}_q(E_2)$ and $\mathbf{T}_q$ is the transfer matrix from (7.37), as can be read off from (7.52).

Starting with $(\xi_1, \eta_1) = (0, 0)$, given in (7.50), repeated application of (7.53) for $q = 2, \ldots, L$ yields explicit expressions for the coefficients, ξ_q and η_q in each region, ensuring that (7.46) is a non-singular solution of (7.44) for all $r < \infty$.

Radiation boundary condition at $r = \infty$: It remains to impose the condition of outward going radiation, which is where E_2 is determined. To see this, note that iteration of (7.53) and use of (7.50) yields:

$$\begin{pmatrix} \xi_L(E_2) \\ \eta_L(E_2) \end{pmatrix} = \mathbf{F}_L + \mathbf{T}_L\mathbf{F}_{L-1} + \mathbf{T}_L\mathbf{T}_{L-1}\mathbf{F}_{L-2} + \ldots + \mathbf{T}_L\mathbf{T}_{L-1}\cdots\mathbf{T}_3\mathbf{F}_2 \tag{7.54}$$

For $r \in R_L$, $(r > r_L)$ we have:

$$U_1(z) = U_{1,L}(z) = U_{1,L}^{(p)}(z;E_2) + \xi_L(E_2)H_l^{(1)}(z) + \eta_L(E_2)H_L^{(2)}(z).$$

We now construct $U_{1,L}^{(p)}(z;E_2)$ for $r(z) \in R_L$. Noting that in this region $\Re E_0 > V_{\text{av}} = 0$ and $Q_1(z) = 0$, we find from the first equation in (7.45) and (7.31) that $U_{1,L}^{(p)}$ satisfies

$$z^2U_1'' + zU_1' + (z^2 - l^2)U_1 = z^2\left(\frac{E_2}{E_0}\right)\alpha_L H_l^{(1)}(z). \tag{7.55}$$

This is precisely equation (7.11) with $k_* = \alpha_L$. We can therefore use the calculations of this previous subsection to obtain a particular solution. This gives the equation for E_2:

$$\eta_L(E_2) - \frac{i\alpha_L\pi}{4}\frac{E_2}{E_0}\frac{z_L^2}{2}\left([H_l^{(1)}(z_L)]^2 - H_{l-1}^{(1)}(z_L)H_{l+1}^{(1)}(z_L) \right) = 0, \tag{7.56}$$

where

$$\eta_L(E_2) \equiv \eta_{L0} + E_2\,\eta_{L1} \tag{7.57}$$

is read off from (7.54). E_2 is then found by solving the linear relation (7.56–7.57).

8. Summary and discussion

Motivated by the problem of light propagation in a microstructured waveguide, we have considered the scattering resonance problem for the Schrödinger equation with high contrast and "microstructured" potentials. We outline the results of the authors [**6**] in the special case of 2-dimensional N-fold symmetric potentials potentials, which correspond to waveguides whose cross-section has an N-fold symmetry.

We have further derived a systematic homogenization expansion for such microstructured cylindrical waveguides with transverse N-fold symmetry. The method of derivation, multiple scale analysis, facilitates the removal of fast scales due the rapid variations in the microstructure. Therefore, numerical implementation of the expansion does not encounter the intrinsic "stiffness" associated with problems having large separations of scales, and gives an efficient algorithm for calculation of scattering resonances in certain regimes.

We have implemented the expansion for a number of sample structures and have computed the effective indexes (scattering resonance energies) of their leaky modes. Of great importance are the imaginary parts of the effective indexes, which correspond to the radiative leakage rates, resulting from a combination of propagation and tunneling losses. In contrast to the real parts of the effective indexes, these leakage rates are very sensitive to the geometry of the microstructure in the case of low index (air) holes.

Appendix A. Calculations for simple layered structures

In this appendix we present the expressions needed to compute the leading corrections to Φ_0 and E_0 due to microstructure. There are two quantities we require:

$$\Phi_2^{(p)}(r,\theta,\Theta) = r^2\,\Phi_0(r,\theta)\,\partial_\Theta^{-2}\Big[V(r,\Theta) - V_{\text{av}}(r)\Big] \tag{A.1}$$

and

$$Q(r) = \frac{r^2}{2\pi}\int_0^{2\pi}\Big|\partial_p^{-1}\Big[V(r,p) - V_{\text{av}}(r)\Big]\Big|^2\,dp. \tag{A.2}$$

The mean-zero antiderivatives in (A.1) and (A.2) are explicitly calculable due to the form of the potential (7.19). For $r \in R_i$,

$$\partial_\Theta^{-1}\Big[V(r,\Theta) - V_{\text{av}}(r)\Big] = C_1 - V_{\text{av,i}}\,\Theta + \sum_{j=1}^{M_i}\mathbf{1}_{[\Theta_j,\Theta_{j+1}]}(\Theta)\Big(S_j + V_{i,j}\,(\Theta - \Theta_j)\Big), \tag{A.3}$$

where

$$S_j = \sum_{k=1}^{j-1} V_{i,k}\,(\Theta_{k+1} - \Theta_k) \tag{A.4}$$

and the constant C_1 is given below. Integrating again, once more for $r \in R_i$,

$$\begin{aligned}\partial_\Theta^{-2}\Big[V(r,\Theta) - V_{\text{av}}(r)\Big] &= C_2 + C_1\,\Theta - \frac{1}{2}V_{\text{av},i}\,\Theta^2 + \\ &\sum_{j=1}^{M_i}\mathbf{1}_{[\Theta_j,\Theta_{j+1}]}(\Theta)\Big(T_j + S_j\,(\Theta - \Theta_j) + \frac{1}{2}V_{i,j}\,(\Theta - \Theta_j)^2\Big)\end{aligned} \tag{A.5}$$

where

$$T_j = \sum_{k=1}^{j-1}\Big(S_k\,(\Theta_{k+1} - \Theta_k) + \frac{1}{2}V_{i,k}\,(\Theta_{k+1} - \Theta_k)^2\Big) \tag{A.6}$$

and the constants C_1, C_2 are given by

$$\begin{aligned} C_1 &= \pi V_{\text{av},i} - T_{M_i+1} \\ C_2 &= -\pi C_1 + \frac{(2\pi)^2}{6}V_{\text{av},i} - \\ &\frac{1}{2\pi}\sum_{j=1}^{M_i}\Big(T_j\,(\Theta_{j+1} - \Theta_j) + \frac{1}{2}S_j\,(\Theta_{j+1} - \Theta_j)^2 + \frac{1}{6}V_{i,j}\,(\Theta_{j+1} - \Theta j)^3\Big).\end{aligned} \tag{A.7}$$

Finally, for $r \in R_i$, the integral in (A.2) evaluates to

$$\begin{aligned}\frac{1}{2\pi}\int_0^{2\pi}\Big|\partial_p^{-1}\Big[V(r,p) - V_{\text{av}}(r)\Big]\Big|^2\,dp &= C_1^2 + \frac{1}{\pi}C_1 T_{M_i+1} \\ &+\frac{1}{2\pi}\sum_{j=1}^{M_i}\Big(S_j^2\,(\Theta_{j+1} - \Theta_j) + S_j(V_{i,j} - V_{\text{av},i})(\Theta_{j+1} - \Theta_j)^2 \\ &+\frac{1}{3}(V_{i,j} - V_{\text{av},i})^2(\Theta_{j+1} - \Theta_j)^3\Big).\end{aligned} \tag{A.8}$$

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