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Asymptotic analysis of subwavelength halide perovskite resonators

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 $\mathbf{23}$

Abstract

Halide perovskites are promising materials with many significant applications in photovoltaics and optoelectronics. In this paper, we use integral methods to quantify the resonant properties of halide perovskite nano-particles. We prove that, for arbitrarily small particles, the subwavelength resonant frequencies can be expressed in terms of the eigenvalues of the Newtonian potential associated with its shape. We also characterize the hybridized subwavelength resonant frequencies of a dimer of two halide perovskite particles. Finally, we examine the specific case of spherical resonators and demonstrate that our new results are consistent with previous works.

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1 Introduction

Halide perovskites are set to be at the center of the next generation of electromagnetic devices [11, 14, 15]. They are composed of crystalline lattices which have octohedral shapes and contain atoms of heavier halides, such as chlorine, bromine and iodine [1]. Their excellent optical and electronic properties, combined with being cheap and easy to manufacture, have paved the way for a perovskite revolution. A particular benefit of halide perovskites is that their high absorption coefficient enables microscopic devices (measuring only a few hundred nanometres) to absorb the complete visible spectrum. Thus, we are able to design very small devices that are lightweight and compact while also being low cost and efficient. Research is ongoing to develop perovskites capable of fulfilling their theoretical capabilities for use in applications such as optical sensors [8], solar cells [15] and light-emitting diodes [17].

The dielectric permittivity of a halide perovskite ε is given, in terms of the frequency ω and wavenumber k by [14]

$$\varepsilon(\omega,k) = \varepsilon_0 + \frac{\omega_p^2}{\omega_{exc}^2 - \omega^2 + \hbar\omega_{exc}k^2\mu_{exc}^{-1} - i\gamma\omega},$$

where ω_{exc} is the frequency of the excitonic transition, ω_p is the strength of the dipole oscillator, γ is the damping factor, μ_{exc} is related to the non-local response and ε_0 is the background dielectric constant. We refer to [14] for the values of these constants for different halide perovskites at room temperature. Meanwhile, the dispersion relation for the halide perovskites is observed [10] to take the simplified form

$$n^2 = 1 + \frac{S_0 \lambda_0^2}{1 - \lambda_0^2 k^2},$$

where n is the refractive index, k is the wavenumber and S_0 and λ_0 are positive constants that describe the average oscillator strength, see [10] for the values for some different halide perovskies.

Dielectric nano-particles, and other electromagnetic metamaterials, have been studied using various techniques. In the case of extreme material parameters, such as small particle size or large material contrast, asymptotic methods can be used [3, 2, 7]. Likewise, homogenisation has been used to characterise materials with periodic micro-structures [6, 9]. Multiple scattering formulations are popular, particularly when a convenient choice of geometry (e.g. cylindrical or spherical resonators) facilitates explicit formulas [16]. In this paper, we will use integral methods to study a general class of geometries and will extend the previous theory, e.g. [2], to the case of dispersive materials.

For simplicity, we consider the Helmholtz equation as a model of the propagation of time-harmonic waves, and for the permittivity relation, we consider the form

$$\varepsilon(\omega,k) = \varepsilon_0 + \frac{\alpha}{\beta - \omega^2 + \eta k^2 - i\gamma\omega},\tag{1.1}$$

where $\alpha, \beta, \gamma, \eta$ are positive constants. We will use an approach based on representing the scattered solution using a Lippmann-Schwinger integral formulation and then using asymptotic methods to characterise the resonant frequencies in terms of the eigenvalues of the resulting integral operator (which turns out to be the Newtonian potential). This approach can handle a very general class of resonator shapes and can be adapted to study solutions to the Maxwell's equations [5]. A similar method was used in [2] for a simpler, non-dispersive setting. This paper shows that the asymptotic theory developed in [2] and elsewhere can be developed to model real-world settings and can be used to influence high-impact design problems.

In section 2 of this paper we will introduce the problem setting and retrieve its integral formulation. Then, we will study the one particle case for three and two dimensions, using integral techniques to formulate the subwavelength resonant problem and asymptotic approximations to study the resonant frequencies. In section 3, we will use these methods to describe the hybridization of two halide perovskite resonators. Again, we treat the three- and two-dimensional cases separately. Passing from the integral to a matrix formulation of the problem, we obtain the hybridized subwavelength resonant frequencies. Finally, we examine the case of spherical resonators, making use of the fact that eigenvalues and eigenfunctions of the Newtonian potential can be computed explicitly in this case (see also [12]). We show that our findings are qualitatively consistent with the ones of [2]. Hence, we show that the asymptotic techniques used in [2] can be generalized to less straightforward and more impactful physical settings.

2 Single Resonators

2.1 Problem Setting

Consider a single resonator occupying a bounded domain $\Omega \subset \mathbb{R}^d$, for $d \in \{2,3\}$. We assume that the particle is non-magnetic, so that the magnetic permeability μ_0 is constant on all of \mathbb{R}^d . We will consider a time-harmonic wave with frequency $\omega \in \mathbb{C}$ (which we assume to have positive real part). The wavenumber in the background $\mathbb{R}^d \setminus \overline{\Omega}$ is given by $k_0 := \omega \varepsilon_0 \mu_0$ and we will use k to denote the wavenumber within Ω . We, then, consider the following Helmholtz model for light propagation:

$$\begin{cases} \Delta u + \omega^2 \varepsilon(\omega, k) \mu_0 u = 0 & \text{in } \Omega, \\ \Delta u + k_0^2 u = 0 & \text{in } \mathbb{R}^d \setminus \overline{\Omega}, \\ u|_+ - u|_- = 0 & \text{on } \partial\Omega, \\ \frac{\partial u}{\partial \nu}|_+ - \frac{\partial u}{\partial \nu}|_- = 0 & \text{on } \partial\Omega, \\ u(x) - u_{in}(x) & \text{satisfies the outgoing radiation condition as } |x| \to \infty, \end{cases}$$
(2.1)

where u_{in} is the incident wave, assumed to satisfy

$$(\Delta + k_0^2)u_{in} = 0 \quad \text{in } \mathbb{R}^d,$$

and the appropriate outgoing radiation condition is the Sommerfeld radiation condition, which requires that

$$\lim_{|x|\to\infty} |x|^{\frac{d-1}{2}} \left(\frac{\partial}{\partial|x|} - ik_0\right) (u(x) - u_{in}(x)) = 0.$$

$$(2.2)$$

In particular, we are interested in the case of small resonators. Thus, we will assume that there exists some fixed domain D such that Ω is given by

$$\Omega = \delta D + z, \tag{2.3}$$

for some position $z \in \mathbb{R}^d$ and characteristic size $0 < \delta \ll 1$. Then, making a change of variables, the Helmholtz problem (2.1) becomes

$$\begin{cases} \Delta u + \delta^2 \omega^2 \varepsilon(\omega, k) \mu_0 u = 0 & \text{ in } D, \\ \Delta u + \delta^2 k_0^2 u = 0 & \text{ in } \mathbb{R}^d \setminus \overline{D}, \end{cases}$$
(2.4)

along with the same transmission conditions on ∂D and far-field behaviour. The behaviour of resonators which is of interest is when $\delta \ll k_0^{-1}$, meaning the system can be described as being *subwavelength*. We will study this by performing asymptotics in the regime that the frequency ω is fixed while the size $\delta \to 0$. We will characterise solutions to (2.1) in terms of the system's resonant frequencies. For a given wavenumber k, we define $\omega = \omega(k)$ to be a *resonant frequency* if it is such that there exists a non-trivial solution u to (2.1) in the case that $u_{in} = 0$.

2.2 Integral Formulation

Let G(x,k) be the outgoing Helmholtz Green's function in \mathbb{R}^d , defined as the unique solution to

$$(\Delta + k^2)G(x,k) = \delta_0(x)$$
 in \mathbb{R}^d ,

along with the outgoing radiation condition (2.2). It is well known that G is given by

$$G(x,k) = \begin{cases} -\frac{i}{4}H_0^{(1)}(k|x|), & d = 2, \\ -\frac{e^{ik|x|}}{4\pi|x|}, & d = 3, \end{cases}$$
(2.5)

where $H_0^{(1)}$ is the Hankel function of first kind and order zero.

Theorem 2.1 (Lippmann-Schwinger Integral Representation Formula). The solution to the Helmholtz problem (2.1) is given by

$$u(x) - u_{in}(x) = -\delta^2 \omega^2 \xi(\omega, k) \int_D G(x - y, \delta k_0) u(y) \mathrm{d}y, \quad x \in \mathbb{R}^d,$$
(2.6)

where the function $\xi : \mathbb{C} \to \mathbb{C}$ describes the permittivity contrast between D and the background and is given by

$$\xi(\omega, k) = \mu_0(\varepsilon(\omega, k) - \varepsilon_0).$$

Proof. We see from (2.4) that $\Delta u + \delta^2 \omega^2 \varepsilon(\omega, k) \mu_0 u = 0$ in D, so it holds that

$$\Delta u + \delta^2 k_0^2 u = -\delta^2 \omega^2 \xi(\omega, k) u_k$$

where $\xi(\omega, k) = \mu_0(\varepsilon(\omega, k) - \varepsilon_0)$. Therefore, the Helmholtz problem (2.4) becomes

$$(\Delta + \delta^2 k_0^2)(u(y) - u_{in}(y)) = -\delta^2 \omega^2 \xi(\omega, k) u(y) \chi_D(y), \quad y \in \mathbb{R}^d \setminus \partial D,$$

with χ_D being the indicator function of the set D. Then, we know that for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}^d \setminus \partial D$, the following identity holds:

$$\begin{aligned} \nabla_y \cdot \Big[G(x-y,\delta k_0) \nabla_y \Big(u(y) - u_{in}(y) \Big) - \Big(u(y) - u_{in}(y) \Big) \nabla_y G(x-y,\delta k_0) \Big] \\ &= -\delta^2 \omega^2 \xi(\omega,k) u(y) G(x-y,\delta k_0) \chi_D(y) - \Big(u(y) - u_{in}(y) \Big) \delta_0(x-y). \end{aligned}$$

Let S_R be a large sphere with radius R large enough so that $D \subset S_R$. Integrating the above identity over $y \in S_r \setminus \partial D$ and letting $R \to +\infty$, we can use the radiation condition (2.2) in the far field and the transmission conditions on ∂D to obtain the desired integral representation formula.

We are interested in understanding how the formula from Theorem 2.1 behaves in the case that δ is small. In particular, we wish to understand the operator $K_D^{\delta k_0} : L^2(D) \to L^2(D)$ given by

$$K_D^{\delta k_0}[u](x) = -\int_{\Omega} G(x - y, \delta k_0) u(y) \mathrm{d}y, \quad x \in D.$$
(2.7)

The Helmholtz Green's function has helpful asymptotic expansions which facilitate this. However, the behaviour is quite different in two and three dimensions, so we must now consider these two settings separately. We will first work on the three-dimensional case, and then treat the two-dimensional setting as the asymptotic expansions are more complicated.

2.3 Reformulation as a Subwavelength Resonance Problem

In order to reveal the behaviour of the system of nano-particles, we will characterise the properties of the operator $K_D^{\delta k_0}$. We observe that the Lippmann-Schwinger formulation (2.6) of the problem is equivalent to

$$(u - u_{in})(x) = \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0}[u](x).$$

This is equivalent to

$$(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})[u](x) = u_{in}(x),$$

which gives

$$u(x) = (I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1} [u_{in}](x),$$

for all $x \in D$, where I denotes the identity operator. Then, the subwavelength resonance problem is to find $\omega \in \mathbb{C}$ close to 0, such that the operator $(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1}$ is singular, or equivalently, such that there exists $u \in L^2(D)$, $u \neq 0$ with

$$u(x) - \delta^2 \omega^2 \xi(\omega, k) \int_D G(x - y, \delta k_0) u(y) \mathrm{d}y = 0, \quad \text{for } x \in D.$$
(2.8)

2.4 Three Dimensions

We consider the three-dimensional case, d = 3. Let us define the Newtonian potential on D to be $K_D^{(0)}$: $L^2(D) \to L^2(D)$ such that

$$K_D^{(0)}[u](x) := -\int_D u(y)G(x-y,0)dy = -\frac{1}{4\pi}\int_D \frac{1}{|x-y|}u(y)dy.$$
(2.9)

Similarly, we define the operators $K_D^{(n)}: L^2(D) \to L^2(D)$, for n = 1, 2, ..., as

$$K_D^{(n)}[u](x) = -\frac{i}{4\pi} \int_D \frac{(i|x-y|)^{n-1}}{n!} u(y) \mathrm{d}y.$$
(2.10)

Then, in order to capture the behaviour of $K_D^{\delta k_0}$ for small δ , we can use an asymptotic expansion in terms of small δ .

Lemma 2.2. Suppose that d = 3. The operator $K_D^{\delta k_0}$ can be rewritten as

$$K_D^{\delta k_0} = \sum_{n=0}^{\infty} (\delta k_0)^n K_D^{(n)},$$

where the series converges in the $L^2(D) \to L^2(D)$ operator norm if δk_0 is small enough.

Proof. This follows from an application of the Taylor expansion on the operator $K_D^{\delta k_0}$. Indeed, using Taylor expansion on the second variable of G, we can see that

$$G(x-y,\delta k_0) = \sum_{n=0}^{\infty} (\delta k_0)^n \frac{\partial^n G}{\partial k^n} (x-y,k) \Big|_{k=0}.$$

Since we are working in three dimensions,

$$G(x,k) = -\frac{e^{ik|x|}}{4\pi|x|}$$

and, thus,

$$G(x - y, 0) = -\frac{1}{4\pi |x - y|} \quad \text{and} \quad \frac{\partial^n G}{\partial k^n}(x - y, k) = -\frac{i}{4\pi} \frac{(i|x - y|)^{n-1}}{n!} \quad \text{for } n > 0.$$

Hence,

$$G(x-y,\delta k_0) = \sum_{n=0}^{\infty} (\delta k_0)^n \frac{\partial^n G}{\partial k^n} (x-y,k) \Big|_{k=0} = \sum_{n=0}^{\infty} (\delta k_0)^n \left(-\frac{i}{4\pi}\right) \frac{(i|x-y|)^{n-1}}{n!},$$

and then, multiplying by u and integrating over D, gives

$$K_D^{\delta k_0}[u](y) = \sum_{n=0}^{\infty} (\delta k_0)^n K_D^{(n)}[u](y),$$

which is the desired result.

2.4.1 Eigenvalue Calculation

In order to study the operator $K_D^{\delta k_0}$, we need to find its eigenvalues. From Lemma 2.2, if k_0 is fixed then we can write our operator as

$$K_D^{\delta k_0} = K_D^{(0)} + \delta k_0 K_D^{(1)} + O(\delta^2) \quad \text{as } \delta \to 0.$$
(2.11)

Since we know that $K_D^{(0)}$ is self-adjoint, we know that it admits eigenvalues. Let us denote such an eigenvalue by λ_0 , and by u_0 the associated eigenvector. Let us now consider the problem

$$K_D^{\delta k_0} u_\delta = \lambda_\delta u_\delta, \tag{2.12}$$

where λ_{δ} denotes an eigenvalue of the operator $K_D^{\delta k_0}$ and u_{δ} denotes the associated eigenvector. Using this eigenvalue problem, we will find the resonant frequency ω_s and the associated wavenumber k_s of the halide perovskite nano-particle.

Proposition 2.3. Let λ_{δ} denote an eigenvalue of the operator $K_D^{\delta k_0}$ in dimension three. Then, if δ is small, it is approximately given by

$$\lambda_{\delta} \approx \lambda_0 + \delta k_0 \langle K_D^{(1)} u_0, u_0 \rangle. \tag{2.13}$$

Proof. We start by truncating the $O(\delta^2)$ term in the expansion (2.11). Then, we have that

$$K_D^{\delta k_0} u_{\delta} = \lambda_{\delta} u_{\delta} \iff (K_D^{(0)} + \delta k_0 K_D^{(1)}) u_{\delta} = \lambda_{\delta} u_{\delta} \iff \langle (K_D^{(0)} + \delta k_0 K_D^{(1)}) u_{\delta}, u_0 \rangle = \langle \lambda_{\delta} u_{\delta}, u_0 \rangle$$

Since $K_D^{(0)}$ is self-adjoint, we have that

$$\lambda_0 \langle u_\delta, u_0 \rangle + \delta k_0 \langle K_D^{(1)} u_\delta, u_0 \rangle = \lambda_\delta \langle u_\delta, u_0 \rangle.$$

Finally, since $u_{\delta} \approx u_0$ we find that

$$\lambda_{\delta} = \lambda_0 + \delta k_0 \frac{\langle K_D^{(1)} u_{\delta}, u_0 \rangle}{\langle u_{\delta}, u_0 \rangle} \approx \lambda_0 + \delta k_0 \langle K_D^{(1)} u_0, u_0 \rangle,$$

which is the desired result.

The following corollary is a direct consequence of Proposition 2.13:

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Corollary 2.3.1. Let λ_{δ} denote an eigenvalue of the operator $K_D^{\delta k_0}$ in three dimensions. Then, if δ is small, it is approximately given by

$$\lambda_{\delta} \approx \lambda_0 - \frac{i}{4\pi} \delta k_0 \mathbb{B}, \qquad (2.14)$$

where $\mathbb{B} := (\int_D u_0(y) \mathrm{d}y)^2$ is a constant.

Proof. From (2.10), we get that

$$K_D^{(1)}[u](x) = -\frac{i}{4\pi} \int_D \frac{(i|x-y|)^{1-1}}{1!} u(y) \mathrm{d}y = -\frac{i}{4\pi} \int_D u(y) \mathrm{d}y.$$

Let us define the constant $\mathbb{B} := (\int_D u_0(y) dy)^2$. Then, we observe that

$$\langle K_D^{(1)}u_0, u_0 \rangle = \int_D \left(-\frac{i}{4\pi}\right) u_0(y) \int_D \overline{u_0}(x) \mathrm{d}x \mathrm{d}y = -\frac{i}{4\pi} \left(\int_D u_0(y) \mathrm{d}y\right)^2 = -\frac{i}{4\pi} \mathbb{B}.$$

Substituting into (2.13) gives the desired result.

2.4.2 Frequency and Wavenumber

Let us now find the resonant frequency ω_{δ} and wavenumber k_{δ} associated to this eigenvalue, which will also constitute the basis of our analysis of the operator $K_D^{\delta k_0}$. From (2.8), we see that if $u = u_{\varepsilon}$, then $1 = \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta}$ so, using Corollary 2.14 we have that

$$\varepsilon(\omega,k) = \frac{1}{\mu_0 \delta^2 \omega^2 \left(\lambda_0 - \frac{i}{4\pi} \delta k_0 \mathbb{B}\right)} + \varepsilon_0.$$
(2.15)

In order to study halide perovskite particles, we want the permittivity $\varepsilon(\omega, k)$ to be given by (1.1), that is,

$$\varepsilon(\omega,k) = \varepsilon_0 + \frac{\alpha}{\beta - \omega^2 + \eta k^2 - i\gamma\omega},\tag{2.16}$$

where $\alpha, \beta, \gamma, \eta$ are positive constants. Comparing the two expressions (2.15) and (2.16) we see that

$$\begin{cases} \alpha \mu_0 \delta^2 \omega^2 \lambda_0 - \beta + \omega^2 - \eta k^2 = 0, \\ \gamma \omega - \mu_0 \frac{1}{4\pi} \alpha \delta^3 \omega^2 k_0 \mathbb{B} = 0. \end{cases}$$
(2.17)

We study these two equations separately. First, we look at the second equation of (2.17). We have that

$$\omega\left(\gamma - \mu_0 \frac{1}{4\pi} \alpha \delta^3 \omega k_0 \mathbb{B}\right) = 0.$$

meaning that

$$\omega = 0$$
 or $\omega = \frac{4\pi\gamma}{\alpha\mu_0\delta^3k_0\mathbb{B}}$

For $\omega = \frac{4\pi\gamma}{\alpha\mu_0\delta^3 k_0\mathbb{B}}$, we obtain that

$$\eta k^2 = (1 + \alpha \mu_0 \delta^2 \lambda_0) \omega^2 - \beta_2$$

which has solutions

$$k = \pm \sqrt{\frac{16\pi^2 \gamma^2 (1 + \alpha \mu_0 \delta^2 \lambda_0)}{\alpha^2 \mu_0^2 \delta^6 k_0^2 \mathbb{B}^2 \eta} - \frac{\beta}{\eta}}.$$
 (2.18)

The case of $\omega = 0$ is not of physical interest here. Thus, denoting this specific frequency by ω_{δ} and the associated wavenumber by k_{δ} , we will work with

$$\omega_{\delta} = \frac{4\pi\gamma}{\alpha\mu_0\delta^3 k_0 \mathbb{B}} \quad \text{and} \quad k_{\delta} = \sqrt{\frac{16\pi^2\gamma^2(1+\alpha\mu_0\delta^2\lambda_0)}{\alpha^2\mu_0^2\delta^6 k_0^2 \mathbb{B}^2\eta} - \frac{\beta}{\eta}},\tag{2.19}$$

where we have chosen the wavenumber k_{δ} to be positive.

2.4.3 Asymptotic Analysis

Let us now return to the problem of studying the singularities of the operator $(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1}$. We have the following equivalence:

$$(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1} = 0 \iff \left(I - \delta^2 \omega^2 \xi(\omega, k) \sum_{n=0}^{\infty} (\delta k_0)^n K_D^{(n)} \right)^{-1} = 0.$$

We define

$$A_n := \delta^2 \omega^2 \xi(\omega, k) K_D^{(n)} = -\delta^2 \omega^2 \xi(\omega, k) \frac{i}{4\pi} \int_D \frac{(i|x-y|)^{n-1}}{n!} u(y) \mathrm{d}y$$

Then, it holds that

$$\left(I - \delta^2 \omega^2 \xi(\omega, k) \sum_{n=0}^{\infty} (\delta k_0)^n K_D^{(n)}\right)^{-1} = \left(I - \sum_{n=0}^{\infty} (\delta k_0)^n A_n\right)^{-1}$$
$$= \sum_{i=0}^{\infty} \left((I - A_0 - \delta k_0 A_1)^{-1} \sum_{n=2}^{\infty} (\delta k_0)^n A_n\right)^i (I - A_0 - \delta k_0 A_1)^{-1}$$
$$= (I - A_0 - \delta k_0 A_1)^{-1}$$
$$+ (I - A_0 - \delta k_0 A_1)^{-1} (\delta k_0)^2 A_2 (I - A_0 - \delta k_0 A_1)^{-1} + O(\delta^4).$$

Thus, the above equivalence yields

$$(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1} = 0 \iff \left(I - \delta^2 \omega^2 \xi(\omega, k) \sum_{n=0}^{\infty} (\delta k_0)^n K_D^{(n)} \right)^{-1} = 0 \iff (I - A_0 - \delta k_0 A_1)^{-1} + (I - A_0 - \delta k_0 A_1)^{-1} (\delta k_0)^2 A_2 (I - A_0 - \delta k_0 A_1)^{-1} + O(\delta^4) = 0.$$

Using this expression, we obtain the following proposition.

Proposition 2.4. Let d = 3 and let ω_{δ} be defined by (2.19). Then, as $\delta \to 0$, the $O(\delta^4)$ approximation of the subwavelength resonant frequencies ω_s and the associated wavenumbers k_s of the single halide perovskite resonator $\Omega = \delta D + z$ satisfy

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\delta^4 k_0^2 \omega_s^2 \xi(\omega_s, k_s) \langle K_D^{(2)}[u_\delta], u_\delta \rangle.$$
(2.20)

Proof. For $\psi \in L^2(D)$, and dropping the $O(\delta^4)$ term, we have

$$\left[(I - A_0 - \delta k_0 A_1)^{-1} + (I - A_0 - \delta k_0 A_1)^{-1} (\delta k_0)^2 A_2 (I - A_0 - \delta k_0 A_1)^{-1} \right] [\psi] = 0.$$
(2.21)

We apply a pole-pencil decomposition, as it is defined in [4], to the term $(I - A_0 - \delta k_0 A_1)^{-1}[\psi]$ and obtain

$$(I - A_0 - \delta k_0 A_1)^{-1}[\psi] = \frac{\langle u_\delta, \psi \rangle u_\delta}{1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta} + R(\delta)[\psi]$$

where the remainder term $R(\delta)[\psi]$ can be dropped. Hence, (2.21) is, at leading order, equivalent to

$$\frac{\langle u_{\delta},\psi\rangle u_{\delta}}{1-\delta^{2}\omega^{2}\xi(\omega_{s},k_{s})\lambda_{\delta}}+\frac{\langle u_{\delta},\psi\rangle u_{\delta}}{1-\delta^{2}\omega_{s}^{2}\xi(\omega_{s},k_{s})\lambda_{\delta}}(\delta k_{0})^{2}A_{2}\frac{\langle u_{\delta},\psi\rangle u_{\delta}}{1-\delta^{2}\omega_{s}^{2}\xi(\omega_{s},k_{s})\lambda_{\delta}}=0,$$

which reduces to

$$\frac{u_{\delta}}{1-\delta^2\omega_s^2\xi(\omega_s,k_s)\lambda_{\delta}} + \frac{u_{\delta}\langle K_D^{(2)}[u_{\delta}],u_{\delta}\rangle}{(1-\delta^2\omega_s^2\xi(\omega_s,k_s)\lambda_{\delta})^2}\delta^4k_0^2\omega_s^2\xi(\omega_s,k_s) = 0,$$

which can be rearranged to give the desired result.

Remark. In the appendix, we will recover a formula for $\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle$.

Before we move on to the consequences of this proposition, we recall that

$$K_D^{(2)}[u](x) = -\frac{i}{4\pi} \int_D \frac{i|x-y|}{2} u(y) \mathrm{d}y = \frac{1}{8\pi} \int_D |x-y|u(y) \mathrm{d}y.$$

Thus, we can define the constant $\mathbb F$ to be such that

$$\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle = \int K_D^{(2)}[u_{\delta}](x)\overline{u_{\delta}}(x) \mathrm{d}x = \frac{1}{8\pi} \int_D \int_D |x - y| u_{\delta}(y)\overline{u_{\delta}}(x) \mathrm{d}y \mathrm{d}x =: \frac{1}{8\pi} \mathbb{F}$$

So, from (2.20), we see that

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\frac{\delta^4 k_0^2 \omega_s^2 \xi(\omega_s, k_s)}{8\pi} \mathbb{F}.$$
(2.22)

Then the following two corollaries are immediate consequences of the Proposition 2.4.

Corollary 2.4.1. Let d = 3. Then, as $\delta \to 0$, the $O(\delta^8)$ approximation of the subwavelength resonant frequencies of the halide perovskite resonator $\Omega = \delta D + z$ are given by

$$1 - \frac{\omega_s^2}{\omega_\delta^2} \lambda_\delta(\varepsilon(\omega_s, k_s) - \varepsilon_0) \frac{64\pi^2 \gamma^2}{\alpha^2 \mu_0 \delta^4 k_0^2 \mathbb{B}^2} = -\frac{\delta^4 \omega_s^2 k_0^2 \xi(\omega_s, k_s)}{8\pi} \mathbb{F}.$$
(2.23)

Proof. By a direct calculation and using (2.19), we have

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = 1 - \delta^2 \omega_s^2 \mu_0(\varepsilon(\omega_s, k_s) - \varepsilon_0) \lambda_\delta$$

$$\stackrel{(2.19)}{=} 1 - \delta^2 \frac{\omega_s^2}{\omega_\delta^2} \mu_0(\varepsilon(\omega_s, k_s) - \varepsilon_0) \lambda_\delta \frac{64\pi^2 \gamma^2}{\alpha^2 \mu_0^2 \delta^4 k_0^2 \mathbb{B}^2}$$

$$= 1 - \frac{\omega_s^2}{\omega_\delta^2} \lambda_\delta(\varepsilon(\omega_s, k_s) - \varepsilon_0) \frac{64\pi^2 \gamma^2}{\alpha^2 \mu_0 \delta^4 k_0^2 \mathbb{B}^2}.$$

Then, using (2.22), the result follows.

Corollary 2.4.2. Let d = 3. Then, as $\delta \to 0$, the $O(\delta^4)$ approximation of the subwavelength resonant frequencies of the halide perovskite resonator $\Omega = \delta D + z$ can be computed as

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\frac{\omega_s^2}{\omega_\delta^2} (\varepsilon(\omega_s, k_s) - \varepsilon_0) \frac{8\pi \gamma^2 \mathbb{F}}{\alpha^2 \mu_0 \delta^2 \mathbb{B}^2}.$$
 (2.24)

Proof. Again, we can calculate this directly:

$$\frac{\delta^4 k_0^2 \omega_s^2 \xi(\omega_s, k_s)}{8\pi} \mathbb{F} = \frac{1}{8\pi} \delta^4 \frac{\omega_s^2}{\omega_\delta^2} k_0^2 \mu_0(\varepsilon(\omega_s, k_s) - \varepsilon_0) \omega_\delta^2$$
$$\stackrel{(2.19)}{=} \frac{1}{8\pi} \frac{\omega_s^2}{\omega_\delta^2} \delta^4 k_0^2 \mu_0(\varepsilon(\omega_s, k_s) - \varepsilon_0) \frac{64\pi^2 \gamma^2}{\alpha^2 \mu_0^2 \delta^4 k_0^2 \mathbb{B}^2}$$
$$= \frac{\omega_s^2}{\omega_\delta^2} (\varepsilon(\omega_s, k_s) - \varepsilon_0) \frac{8\pi \gamma^2}{\alpha^2 \mu_0 \delta^2 \mathbb{B}^2}.$$

Then, using (2.22), the result follows.

We finish our analysis of the three-dimensional case with the following proposition.

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Proposition 2.5. Let d = 3. For ω close to the resonant frequency ω_s , the field scattered by the halide perovskite nano-particle $\Omega = \delta D + z$ can be approximated by

$$u(x) - u_{in}(x) \approx \frac{1 + \delta^2 \omega^2 G(x - y, \delta k_0) \xi(\omega, k)}{\delta^2 \omega^2 \left(\lambda_\delta - \lambda_0 + \frac{i}{4\pi} \delta k_0 \mathbb{B}\right) \xi(\omega, k)} \langle u_{in}, u_\delta \rangle \int_D u_\delta.$$

Proof. Our goal is to find $u \in L^2(D)$, $u \neq 0$ such that (2.8) is satisfied. Using the pole-pencil decomposition, we can rewrite

$$u(x) - u_{in}(x) \approx -\delta^2 \omega^2 \xi(\omega, k) G(x - y, \delta k_0) \frac{\langle u_{in}, u_\delta \rangle \int_D u_\delta}{1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta} + \delta^4 k_0^2 \omega^2 \xi(\omega, k) \frac{\langle K_D^{(2)}[u_\delta], u_\delta \rangle \langle u_{in}, u_\delta \rangle \int_D u_\delta}{(1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta)^2}$$

Using (2.20) and plugging it in the above expression, we obtain

$$\begin{split} u(x) - u_{in}(x) &\approx -\delta^2 \omega^2 \xi(\omega, k) G(x - y, \delta k_0) \frac{\langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{-\delta^4 k_0^2 \omega^2 \xi(\omega, k) \langle K_D^{(2)}[u_{\delta}], v_{\delta} \rangle} \\ &+ \delta^4 k_0^2 \omega^2 \xi(\omega, k) \frac{\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle \langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{\delta^8 k_0^4 \omega^4 \xi(\omega, k)^2 \langle K_D^{(2)}[u_{\delta}], v_{\delta} \rangle^2} \\ &= \frac{G(x - y, \delta k_0) \langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{\delta^2 k_0^2 \langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle} + \frac{\langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{\delta^4 k_0^2 \omega^2 \xi(\omega, k) \langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle}. \end{split}$$

Thus, defining the constant $\mathbb{F} := 8\pi \langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle$, we obtain

$$u(x) - u_{in}(x) \approx \frac{8\pi \left(1 + \delta^2 \omega^2 G(x - y, \delta k_0) \xi(\omega, k)\right)}{\delta^4 k_0^2 \omega^2 \xi(\omega, k) \mathbb{F}} \langle u_{in}, u_\delta \rangle \int_D u_\delta.$$
(2.25)

From the Appendix A.1, we have that

$$\mathbb{F} = \frac{8\pi}{\delta^2 k_0^2} \left(\lambda_\delta - \lambda_0 + \frac{i}{4\pi} \delta k_0 \mathbb{B} \right).$$

Plugging it into (2.25), we obtain

$$u(x) - u_{in}(x) \approx \frac{8\pi \left(1 + \delta^2 \omega^2 G(x - y, \delta k_0) \xi(\omega, k)\right)}{\delta^4 k_0^2 \omega^2 \xi(\omega, k) \mathbb{F}} \frac{\delta^2 k_0^2}{8\pi} \frac{1}{\lambda_{\delta} - \lambda_0 + \frac{i}{4\pi} \delta k_0 \mathbb{B}} \langle u_{in}, u_{\delta} \rangle \int_D u_{\delta},$$

from which the result follows.

2.5 Two Dimensions

We now turn our attention to the two-dimensional setting. We define the Newtonian potential on D, $K_D^{(0)}: L^2(D) \to L^2(D)$, by

$$K_D^{(0)}[u](x) := -\int_D u(y)G(x-y,0)dy = -\frac{1}{2\pi}\int_D \log|x-y|u(y)dy.$$

We also define the operators $K_D^{(-1)}: L^2(D) \to L^2(D)$ and $K_D^{(1)}: L^2(D) \to L^2(D)$ by

$$K_D^{(-1)}[u](x) := -\frac{1}{2\pi} \int_D u(y) dy \quad \text{and} \quad K_D^{(n)}[u](x) := \int_D \frac{\partial^n}{\partial k^n} G(x - y, k) \Big|_{k=0} u(y) dy.$$

Then, from the asymptotic expansion of the Hankel function, we have the following result.

Lemma 2.6. Suppose that d = 2. Then, for fixed $k_0 \in \mathbb{C}$, the operator $K_D^{\delta k_0}$ satisfies

$$K_D^{\delta k_0} = \log(\delta k_0 \hat{\gamma}) K_D^{(-1)} + K_D^{(0)} + (\delta k_0)^2 \log(\hat{\gamma} \delta k_0) K_D^{(1)} + O(\delta^4 \log \delta),$$
(2.26)

as $\delta \to 0$, with convergence in the $L^2(D) \to L^2(D)$ operator norm and the constant $\hat{\gamma}$ being given by $\hat{\gamma} := \frac{1}{2}k_0 \exp(\gamma - \frac{i\pi}{2}), \text{ where } \gamma \text{ is the Euler constant.}$

Eigenvalue Calculation 2.5.1

We use the same notation for u_{δ} as in section 2.4.1. Let us consider the eigenvalue problem

$$K_D^{\delta k_0} u_\delta = \lambda_\delta u_\delta, \tag{2.27}$$

where λ_{δ} denotes an eigenvalue of the operator $K_D^{\delta k_0}$, and u_{δ} denotes an associated eigenvector.

Proposition 2.7. Let λ_{δ} denote an eigenvalue of the operator $K_D^{\delta k_0}$ in dimension 2. Then, for small δ , it is approximately given by:

$$\lambda_{\delta} \approx \log(\delta k_0 \hat{\gamma}) \lambda_{-1} + \langle K_D^{(0)} u_{-1}, u_{-1} \rangle + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \langle K_D^{(1)} u_{-1}, u_{-1} \rangle, \qquad (2.28)$$

where λ_{-1} and u_{-1} are an eigenvalue and the associated eigenvector of the potential $K_D^{(-1)}$.

Proof. We start by dropping the $O(\delta^4 \log(\delta))$ term on the expansion (2.26). Then, we have that

$$\begin{split} K_D^{\delta k_0} u_{\delta} &= \lambda_{\delta} u_{\delta} \iff (\log(\delta k_0 \hat{\gamma}) K_D^{(-1)} + K_D^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) K_D^{(1)}) u_{\delta} = \lambda_{\delta} u_{\delta} \\ \Leftrightarrow \log(\delta k_0 \hat{\gamma}) \lambda_{-1} \langle u_{\delta}, u_0 \rangle + \langle K_D^{(0)} u_{\delta}, u_{-1} \rangle + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \langle K_D^{(1)} u_{\delta}, u_{-1} \rangle = \lambda_{\delta} \langle u_{\delta}, u_{-1} \rangle. \end{split}$$

Therefore, assuming that $u_{\delta} \approx u_{-1}$, we can see that

$$\lambda_{\delta} \approx \log(\delta k_0 \hat{\gamma}) \lambda_{-1} + \langle K_D^{(0)} u_{-1}, u_{-1} \rangle + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \langle K_D^{(1)} u_{-1}, u_{-1} \rangle,$$

which is the desired result.

The following corollary is a direct consequence of the above proposition.

Corollary 2.7.1. Let λ_{δ} denote an eigenvalue of the operator $K_D^{\delta k_0}$ in dimension 2. Then, for small δ , it is approximately given by

$$\lambda_{\delta} \approx \log(\delta k_0 \hat{\gamma}) \lambda_{-1} - \frac{\mathbb{P}}{2\pi} - \frac{i(\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \mathbb{G}}{4\pi}, \qquad (2.29)$$

where \mathbb{P} and \mathbb{G} are constants that depend on u_{-1} .

Proof. We observe that

$$\langle K_D^{(0)} u_{-1}, u_{-1} \rangle = \int_D \left(-\frac{1}{2\pi} \int_D \log |x - y| u_{-1}(y) \mathrm{d}y \right) \overline{u_{-1}}(x) \mathrm{d}x$$

= $-\frac{1}{2\pi} \int_D \int_D \log |x - y| u_{-1}(y) \overline{u_{-1}}(x) \mathrm{d}y \mathrm{d}x =: -\frac{1}{2\pi} \mathbb{P}$

Then, for $u \in L^2(D)$,

$$K_D^{(1)}[u](x) = \int_D \frac{\partial}{\partial k} G(x-y,k) \Big|_{k=0} u(y) \mathrm{d}y = \int_D \frac{\partial}{\partial k} \left(-\frac{i}{4} H_0^{(1)}(k|x-y|) \right) \Big|_{k=0} u(y) \mathrm{d}y = -\frac{i}{4\pi} \int_D \frac{u(y)}{|x-y|} \mathrm{d}y,$$

and so, we have

$$\langle K_D^{(1)}u_{-1}, u_{-1} \rangle = \int_D \left(-\frac{i}{4\pi} \int_D \frac{u_{-1}(y)}{|x-y|} \mathrm{d}y \right) \overline{u_{-1}}(x) \mathrm{d}x = -\frac{i}{4\pi} \int_D \int_D \frac{u_{-1}(y)\overline{u_{-1}}(x)}{|x-y|} \mathrm{d}y \mathrm{d}x =: -\frac{i}{4\pi} \mathbb{G}.$$

e. from (2.28), we obtain the desired result.

Hence, from (2.28), we obtain the desired result.

2.5.2 Frequency and Wavenumber

Let us now find the frequency ω_{δ} and the wavenumber k_{δ} associated to this eigenvalue, which will also constitute the basis of our analysis of the operator $K_D^{\delta k_0}$. We see that (2.8) gives us that

$$1 = \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta} \iff 1 = \delta^2 \omega^2 \mu_0(\varepsilon(\omega, k) - \varepsilon_0) \lambda_{\delta}$$

Using the expression (2.28) for λ_{δ} , we see that

$$\varepsilon(\omega,k) = \frac{1}{\mu_0 \delta^2 \omega^2 \left(\log(\delta k_0 \hat{\gamma}) \lambda_{-1} - \frac{\mathbb{P}}{2\pi} - \frac{i(\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \mathbb{G}}{4\pi} \right)} + \varepsilon_0.$$

Arguing in the same way as in section 2.4.4 and comparing the two permittivity expressions, we obtain the following system:

$$\begin{cases} 4\pi\alpha\delta^2\omega^2\mu_0\log(\delta k_0\hat{\gamma})\lambda_{-1} - 2\mathbb{P}\alpha\delta^2\omega^2\mu_0 - 4\pi\beta + 4\pi\omega^2 - 4\pi\eta k^2 = 0, \\ -\alpha\delta^4\omega^2\mu_0k_0^2\log(\delta k_0\hat{\gamma})\mathbb{G} + 4\pi\gamma\omega = 0. \end{cases}$$
(2.30)

From the second equation in (2.30), we see that

$$\omega(-\alpha\delta^4\omega\mu_0k_0^2\log(\delta k_0\hat{\gamma})\mathbb{G}+4\pi\gamma)=0,$$

which shows us that

$$\omega = 0$$
 or $\omega = \frac{4\pi\gamma}{\alpha\delta^4\mu_0k_0^2\log(\delta k_0\hat{\gamma})\mathbb{G}}$

For $\omega = \frac{4\pi\gamma}{\alpha\delta^4\mu_0k_0^2\log(\delta k_0\hat{\gamma})\mathbb{G}}$, we obtain the equation

$$4\pi\alpha\delta^{2}\mu_{0}\lambda_{-1}\log(\delta k_{0}\hat{\gamma})\frac{16\pi^{2}\gamma^{2}}{\alpha^{2}\delta^{8}\mu_{0}^{2}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})^{2}\mathbb{G}^{2}} - 2\mathbb{P}\alpha\delta^{2}\mu_{0}\frac{16\pi^{2}\gamma^{2}}{\alpha^{2}\delta^{8}\mu_{0}^{2}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})^{2}\mathbb{G}^{2}} - 4\pi\beta + 4\pi\frac{16\pi^{2}\gamma^{2}}{\alpha^{2}\delta^{8}\mu_{0}^{2}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})^{2}\mathbb{G}^{2}} - 4\pi\eta k^{2} = 0,$$

which has solutions

$$k = \pm \sqrt{-\frac{\beta}{\eta} + \left(2\pi\alpha\delta^2\mu_0\lambda_{-1}\log(\delta k_0\hat{\gamma}) - \alpha\delta^2\mu_0\mathbb{P} + 2\pi\right)\frac{8\pi\gamma^2}{\eta\alpha^2\delta^8\mu_0^2k_0^4\log(\delta k_0\hat{\gamma})^2\mathbb{G}^2}}$$

Yet again, we discard the case of $\omega = 0$, as there is no physical interest. Denoting the frequency by ω_{δ} and the wavenumber by λ_{δ} , we will work with

$$\omega_{\delta} = \frac{4\pi\gamma}{\alpha\delta^{4}\mu_{0}k_{0}^{2}\log(\delta k_{0}\hat{\gamma})\mathbb{G}},$$

$$k_{\delta} = \sqrt{-\frac{\beta}{\eta} + \left(2\pi\alpha\delta^{2}\mu_{0}\lambda_{-1}\log(\delta k_{0}\hat{\gamma}) - \alpha\delta^{2}\mu_{0}\mathbb{P} + 2\pi\right)\frac{8\pi\gamma^{2}}{\eta\alpha^{2}\delta^{8}\mu_{0}^{2}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})^{2}\mathbb{G}^{2}},$$
(2.31)

where we have chosen the wavenumber to be positive.

2.5.3 Asymptotic Analysis

Let us consider ω near ω_{δ} , and define the coefficients

$$c_n = \begin{cases} \log(\delta k_0 \hat{\gamma}), & n = -1\\ 1, & n = 0,\\ (\delta k_0)^{2n} \log(\delta k_0 \hat{\gamma}), & n \ge 1. \end{cases}$$

Then, we can write

$$K_D^{\delta k_0} = \sum_{n=-1}^{+\infty} c_n K_D^{(n)}$$

We are interested in studying the singularities of the operator $(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1}$. Setting $B_n := \delta^2 \omega^2 \xi(\omega, k) K_D^{(n)}$, we find that $(I - \delta^2 \omega^2 \xi(\omega, k) K_D^{\delta k_0})^{-1} = 0$ can be written as

$$\left(I - \sum_{n=-1}^{+\infty} c_n B_n\right)^{-1} = 0.$$

which can be expanded to give

$$\left(I - \log(\delta k_0 \hat{\gamma}) B_{-1} - B_0 - (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) B_1 - \sum_{n \ge 2}^{+\infty} c_n B_n\right)^{-1} = 0,$$

which gives

$$\mathfrak{L} + \mathfrak{L}(\delta k_0)^4 \log(\delta k_0 \hat{\gamma}) B_2 \mathfrak{L} + O(\delta^6) = 0,$$

where we have defined,

$$\mathfrak{L} := \left(I - \log(\delta k_0 \hat{\gamma}) B_{-1} - B_0 - (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) B_1 \right)^{-1}.$$
(2.32)

Using this expression, we have the following proposition.

Proposition 2.8. Let d = 2 and let ω_{δ} be defined by (2.31). Then, as $\delta \to 0$, the $O(\delta^4)$ approximations of the subwavelength resonant frequencies ω_s and the associated wavenumbers k_s of the single halide perovskite resonator $\Omega = \delta D + z$ satisfy

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\delta^6 k_0^4 \log(\delta k_0 \hat{\gamma}) \omega_s^2 \xi(\omega_s, k_s) \langle K_D^{(2)}[u_\delta], u_\delta \rangle.$$
(2.33)

Proof. Applying a pole-pencil decomposition, we obtain

$$\left(I - \log(\delta k_0 \hat{\gamma}) B_{-1} - B_0 - (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) B_1\right)^{-1} [\cdot] = \frac{\langle \cdot, u_\delta \rangle u_\delta}{1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta} + R(\omega_s) [\cdot],$$

where the remainder $R(\omega_s)$ is analytic in a neighborhood of ω_{δ} and can be dropped. Thus, dropping the $O(\delta^6)$ term, we find for $\psi \in L^2(D)$ that

$$\left[\mathfrak{L} + \mathfrak{L}(\delta k_0)^4 \log(\delta k_0 \hat{\gamma}) B_2 \mathfrak{L}\right](\psi) = 0$$

Applying a pole-pencil decomposition on (2.32), we get

$$\frac{\langle \psi, u_{\delta} \rangle u_{\delta}}{1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_{\delta}} + \frac{\langle \psi, u_{\delta} \rangle u_{\delta}}{1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_{\delta}} (\delta k_0)^4 \log(\delta k_0 \hat{\gamma}) B_2 \frac{\langle \psi, u_{\delta} \rangle u_{\delta}}{1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_{\delta}} = 0.$$

This implies that

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\delta^6 k_0^4 \log(\delta k_0 \hat{\gamma}) \omega_s^2 \xi(\omega_s, k_s) \langle K_D^{(2)}[u_\delta], u_\delta \rangle,$$

which is the desired result.

In order to obtain the associated consequences of this proposition, we observe that, since d = 2, we have that

$$K_D^{(2)}[u_{\delta}](x) = \int_D \frac{\partial^2}{\partial k^2} G(x - y, k) \Big|_{k=0} u_{\delta}(y) dy = \int_D \frac{\partial^2}{\partial k^2} \left(-\frac{i}{4} H_0^{(1)}(k|x|) \right) \Big|_{k=0} u_{\delta}(y) dy = -\frac{i}{4} \int_D -\frac{1}{\pi |x - y|^2} u_{\delta}(y) dy = \frac{i}{4\pi} \int_D \frac{u_{\delta}(y)}{|x - y|^2} dy.$$

Hence,

$$\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle = \int_D \left(\frac{i}{4\pi} \int_D \frac{u_{\delta}(y)}{|x-y|^2} \mathrm{d}y \right) \overline{u_{\delta}}(x) \mathrm{d}x = \frac{i}{4\pi} \int_D \int_D \frac{u_{\delta}(y)\overline{u_{\delta}}(x)}{|x-y|^2} \mathrm{d}y \mathrm{d}x =: \frac{i}{4\pi} \mathbb{S}.$$
(2.34)

So, we get that (2.33) is equivalent to

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = \frac{-i\delta^6 k_0^4 \log(\delta k_0 \hat{\gamma}) \omega_s^2 \xi(\omega_s, k_s) \mathbb{S}}{4\pi}.$$
(2.35)

Remark. In the Appendix A.2 of this paper, we recover a formula for S.

Then, the next two corollaries follow as immediate results.

Corollary 2.8.1. Let d = 2. Then, as $\delta \to 0$, the $O(\delta^{10} \log(\delta)^3)$ approximation of the subwavelength resonant frequencies of the halide perovskite resonator $\Omega = \delta D + z$ can be computed as

$$1 - \frac{\omega_s^2}{\omega_\delta^2} \cdot \frac{16\pi^2 \gamma^2 \lambda_\delta \left(\varepsilon(\omega_s, k_s) - \varepsilon_0\right)}{\alpha^2 \delta^6 \mu_0 k_0^4 \log(\delta k_0 \hat{\gamma})^2 \mathbb{G}^2} = -\frac{i\delta^6 k_0^4 \log(\delta k_0 \hat{\gamma}) \omega_s^2 \xi(\omega_s, k_s) \mathbb{S}}{4\pi}.$$
(2.36)

0

Proof. By a direct computation, we observe that

$$1 - \delta^{2} \omega_{s}^{2} \xi(\omega_{s}, k_{s}) \lambda_{\delta} = 1 - \delta^{2} \omega_{s}^{2} \mu_{0} \Big(\varepsilon(\omega_{s}, k_{s}) - \varepsilon_{0} \Big) \lambda_{\delta} \frac{\omega_{\delta}^{2}}{\omega_{\delta}^{2}}$$

$$\stackrel{(2.31)}{=} 1 - \delta^{2} \frac{\omega_{s}^{2}}{\omega_{\delta}^{2}} \mu_{0} \Big(\varepsilon(\omega_{s}, k_{s}) - \varepsilon_{0} \Big) \lambda_{\delta} \frac{16\pi^{2} \gamma^{2}}{\alpha^{2} \delta^{8} \mu_{0}^{2} k_{0}^{4} \log(\delta k_{0} \hat{\gamma})^{2} \mathbb{G}^{2}}$$

$$= 1 - \frac{\omega_{s}^{2}}{\omega_{\delta}^{2}} \cdot \frac{16\pi^{2} \gamma^{2} \lambda_{\delta} \Big(\varepsilon(\omega_{s}, k_{s}) - \varepsilon_{0} \Big)}{\alpha^{2} \delta^{6} \mu_{0} k_{0}^{4} \log(\delta k_{0} \hat{\gamma})^{2} \mathbb{G}^{2}},$$

and thus, (2.35) gives the desired result.

Corollary 2.8.2. Let d = 2. Then, as $\delta \to 0$, the $O(\delta^4 \log(\delta))$ approximation of the subwavelength resonant frequencies of the halide perovskite resonator $\Omega = \delta D + z$ can be computed as

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \lambda_\delta = -\frac{\omega_s^2}{\omega_\varepsilon^2} \cdot \frac{4\pi i \mathbb{S}\gamma^2 \Big(\varepsilon(\omega_s, k_s) - \varepsilon_0\Big)}{\alpha^2 \delta^2 \log(\delta k_0 \hat{\gamma}) \mu_0 \mathbb{G}^2}.$$
(2.37)

Proof. Again, to show this, we need to make a straightforward calculation:

$$\frac{i\delta^{6}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})\omega_{s}^{2}\xi(\omega_{s},k_{s})\mathbb{S}}{4\pi} = \frac{i}{4\pi} \,\delta^{6} \,k_{0}^{4} \,\log(\delta k_{0}\hat{\gamma}) \,\frac{\omega_{s}^{2}}{\omega_{\delta}^{2}} \,\mathbb{S} \,\mu_{0} \left(\varepsilon(\omega_{s},k_{s})-\varepsilon_{0}\right) \,\omega_{\delta}^{2}$$

$$\stackrel{(2.31)}{=} \frac{i}{4\pi} \,\delta^{6} \,k_{0}^{4} \,\log(\delta k_{0}\hat{\gamma}) \,\frac{\omega_{s}^{2}}{\omega_{\delta}^{2}} \,\mathbb{S} \,\mu_{0} \left(\varepsilon(\omega_{s},k_{s})-\varepsilon_{0}\right) \,\frac{16\pi^{2}\gamma^{2}}{\alpha^{2}\delta^{8}\mu_{0}^{2}k_{0}^{4}\log(\delta k_{0}\hat{\gamma})^{2}\mathbb{G}^{2}}$$

$$= \frac{\omega_{s}^{2}}{\omega_{\varepsilon}^{2}} \cdot \frac{4\pi i\mathbb{S}\gamma^{2} \left(\varepsilon(\omega_{s},k_{s})-\varepsilon_{0}\right)}{\alpha^{2}\delta^{2}\log(\delta k_{0}\hat{\gamma})\mu_{0}\mathbb{G}^{2}}.$$

Hence, (2.35) gives the desired result.

We continue our analysis in the same way as in the previous case.

Proposition 2.9. Let d = 2. For ω real close to the resonant frequency ω_s , the following approximation for the field scattered by the halide perovskite nano-particle $\Omega = \delta D + z$ holds:

$$u(x) - u_{in}(x) \approx \frac{4\pi \left(1 + \delta^2 \omega^2 \xi(\omega, k) G(x - y, \delta k_0)\right)}{i \delta^6 k_0^4 \omega^2 \log(\delta k_0 \hat{\gamma}) \omega^2 \xi(\omega, k) \mathbb{S}} \langle u_{in}, u_\delta \rangle \int_D u_\delta.$$
(2.38)

Proof. As we mentioned at the beginning or our analysis, our goal is to find $u \in L^2(D)$, $u \neq 0$, such that (2.8) is satisfied. Using the pole-pencil decomposition on this Lippmann-Schwinger formulation of the problem, we can rewrite, as in Corollary 2.3 in [2],

$$\begin{aligned} u(x) - u_{in}(x) &\approx -\delta^2 \omega^2 \xi(\omega, k) G(x - y, \delta k_0) \frac{\langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta}} \\ &+ \delta^6 k_0^4 \log(\delta k_0 \hat{\gamma}) \omega^2 \xi(\omega, k) \frac{\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle \langle u_{in}, u_{\delta} \rangle \int_D u_{\delta}}{\left(1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta}\right)^2}, \end{aligned}$$

which, using (2.35), becomes:

$$u(x) - u_{in}(x) \approx \frac{G(x - y, \delta k_0) \langle u_{in}, u_\delta \rangle \int_D u_\delta}{\delta^4 k_0^4 \log(\delta k_0 \hat{\gamma}) \langle K_D^{(2)}[u_\delta], u_\delta \rangle} + \frac{\langle u_{in}, u_\delta \rangle \int_D u_\delta}{\delta^6 k_0^4 \omega^2 \log(\delta k_0 \hat{\gamma}) \omega^2 \xi(\omega, k) \langle K_D^{(2)}[u_\delta], u_\delta \rangle}.$$

From (2.34), this gives

$$u(x) - u_{in}(x) \approx \frac{4\pi \left(1 + \delta^2 \omega^2 \xi(\omega, k) G(x - y, \delta k_0)\right)}{i \delta^6 k_0^4 \omega^2 \log(\delta k_0 \hat{\gamma}) \omega^2 \xi(\omega, k) \mathbb{S}} \langle u_{in}, u_\delta \rangle \int_D u_\delta,$$

which is the desired result.

We finish our analysis with the following result.

Proposition 2.10. Let d = 2 and δ be small enough. Then, the $o(\delta^4)$ approximation of the subwavelength resonant frequencies ω_s of the halide perovskite nano-particle $\Omega = \delta D + z$ satisfies

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \left(-\frac{|D|}{2\pi} \log(\delta k_0 \hat{\gamma}) + \langle K_D^{(0)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + \delta^2 k_0^2 \log(\delta) \langle K_D^{(1)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle \right) \right) = O(\delta^4), \qquad (2.39)$$

where |D| is the volume of D and $\hat{\mathbb{I}}_D = \mathbb{I}_D / \sqrt{|D|}$.

Proof. We want to find $\omega_s \in \mathbb{C}$ such that

$$\left(I - \delta^2 \omega_s^2 \xi(\omega_s, k_s) K_D^{\delta k_0}\right)[u](x) = 0,$$

which, for small δ , can be written as

$$\left(I - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \left(\log(\delta k_0 \hat{\gamma}) K_D^{(-1)} + K_D^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) K_D^{(1)}\right)\right) [u](x) = O\left(\delta^6 \log(\delta)\right).$$

Let us denote

$$M_D^{\delta k_0} := \log(\delta k_0 \hat{\gamma}) K_D^{(-1)} + K_D^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) K_D^{(1)}.$$

We take $\nu(\delta) \in \sigma(M_D^{\delta k_0})$ and consider the eigenvalue problem for $M_D^{\delta k_0}$:

$$M_D^{\delta k_0}[\Psi] = \nu(\delta)\Psi. \tag{2.40}$$

We employ the ansatz

$$\Psi(\delta) = \Psi_0 + O\left(\frac{1}{\log(\delta)}\right),$$

$$\nu(\delta) = \log(\delta)\nu_0 + \nu_1 + \delta^2 \log(\delta)\nu_2 + O\left(\delta^2\right).$$

From (2.40) and the fact that $\delta^2 \log(\delta k_0 \hat{\gamma}) = \delta^2 \log(\delta) + O(\delta^2)$ we have that

$$\left(\log(\delta) K_D^{(-1)} + \log(k_0 \hat{\gamma}) K_D^{(-1)} + K_D^{(0)} + (\delta k_0)^2 \log(\delta) K_D^{(1)} \right) [\Psi_0] = \\ \left(\log(\delta) \nu_0 + \nu_1 + \delta^2 \log(\delta) \nu_2 \right) [\Psi_0] + O\left(\delta^2\right)$$

Equating the $O(\log \delta)$ terms gives

$$K_D^{(-1)}[\Psi_0] = \nu_0 \Psi_0 \Rightarrow \nu_0 \hat{\mathbb{I}}_D = K_D^{(-1)}[\hat{\mathbb{I}}_D] \Rightarrow \nu_0 \hat{\mathbb{I}}_D = -\frac{|D|}{2\pi} \hat{\mathbb{I}}_D \Rightarrow \nu_0 = -\frac{|D|}{2\pi}.$$

Then, equating the O(1) terms gives

$$\log(k_0\hat{\gamma})K_D^{(-1)}[\hat{\mathbb{I}}_D] + K_D^{(0)}[\hat{\mathbb{I}}_D] = \nu_1\hat{\mathbb{I}}_D \Rightarrow \nu_1\hat{\mathbb{I}}_D = -\frac{|D|}{2\pi}\log(k_0\hat{\gamma})\hat{\mathbb{I}}_D + K_D^{(0)}[\hat{\mathbb{I}}_D] \\ \Rightarrow \nu_1 = -\frac{|D|}{2\pi}\log(k_0\hat{\gamma}) + \langle K_D^{(0)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle.$$

Using the same reasoning for the $O(\delta^2 \log(\delta))$ terms, we get

$$\nu_2 \hat{\mathbb{I}}_D = k_0^2 K_D^{(1)}[\hat{\mathbb{I}}_D] \Rightarrow \nu_2 = k_0^2 \langle K_D^{(1)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle$$

Thus,

$$\nu(\delta) = \log(\delta)\nu_0 + \nu_1 + \delta^2 \log(\delta)\nu_2 + O\left(\delta^2\right) \\
= -\frac{|D|}{2\pi}\log(\delta) - \frac{|D|}{2\pi}\log(k_0\hat{\gamma}) + \langle K_D^{(0)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + \delta^2 k_0^2 \log(\delta) \langle K_D^{(1)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + O\left(\delta^2\right) \\
= -\frac{|D|}{2\pi}\log(\delta k_0\hat{\gamma}) + \langle K_D^{(0)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + \delta^2 k_0^2 \log(\delta) \langle K_D^{(1)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + O\left(\delta^2\right).$$

Using these expressions, $1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) M_D^{\delta k_0} = O(\delta^6 \log(\delta))$ can be rewritten as

$$1 - \delta^2 \omega_s^2 \xi(\omega_s, k_s) \Big(-\frac{|D|}{2\pi} \log(\delta k_0 \hat{\gamma}) + \langle K_D^{(0)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + \delta^2 k_0^2 \log(\delta) \langle K_D^{(1)}[\hat{\mathbb{I}}_D], \hat{\mathbb{I}}_D \rangle + O\Big(\delta^2\Big) \Big) = O\Big(\delta^6 \log(\delta)\Big),$$

from which the result follows.

3 Hybridization of Two Resonators

3.1 Three Dimensions

Let us consider two identical halide perovskite resonators D_1 and D_2 (e.g. the speres in Figure 1), made from the same material. From now on, we will denote the permittivity by $\xi(\omega, k)$, where ω is the frequency and k the associated wavenumber. In order to generalize our results, we will define it by

$$\xi(\omega,k) := \frac{\mu_0 \alpha}{\beta - \omega^2 + \eta k^2 - i\gamma\omega},\tag{3.1}$$

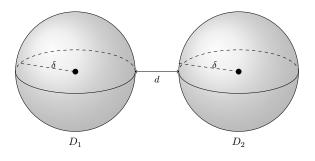


Figure 1: Two identical spherical halide perovskite resonators D_1 and D_2 of radius δ , made from the same material, placed at a distance d from each other.

where the positive constants α, β, γ and η characterise the material.

Then, since there is an interaction between the two resonators, the field $u - u_{in}$ scattered by the two particles will be given by the following representation formula:

$$(u - u_{in})(x) = -\delta^2 \omega^2 \xi(\omega, k) \left[\int_{D_1} G(x - y, \delta k_0) u(y) \mathrm{d}y + \int_{D_2} G(x - y, \delta k_0) u(y) \mathrm{d}y \right] \quad \text{for } x \in \mathbb{R}^d.$$
(3.2)

Definition 3.1. We define the integral operators $K_{D_i}^{\delta k_0}$ and $R_{D_i D_j}^{\delta k_0}$, for i, j = 1, 2, by

$$K_{D_i}^{\delta k_0} : u \big|_{D_i} \in L^2(D_i) \longmapsto -\int_{D_i} G(x - y, \delta k_0) u(y) \mathrm{d}y \big|_{D_i} \in L^2(D_i)$$

and

$$R_{D_iD_j}^{\delta k_0} : u\big|_{D_i} \in L^2(D_i) \longmapsto -\int_{D_i} G(x-y,\delta k_0)u(y)\mathrm{d}y\Big|_{D_j} \in L^2(D_j).$$

Then, the following lemma is a direct consequence of these definitions.

Lemma 3.2. The scattering problem (3.2) can be restated, using the Definition 3.1, as

$$\begin{pmatrix} 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_1}^{\delta k_0} & -\delta^2 \omega^2 \xi(\omega, k) R_{D_2 D_1}^{\delta k_0} \\ -\delta^2 \omega^2 \xi(\omega, k) R_{D_1 D_2}^{\delta k_0} & 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0} \end{pmatrix} \begin{pmatrix} u|_{D_1} \\ u|_{D_2} \end{pmatrix} = \begin{pmatrix} u_{in}|_{D_1} \\ u_{in}|_{D_2} \end{pmatrix}.$$
(3.3)

Thus, the scattering resonance problem is to find ω such that the operator in (3.3) is singular, or equivalently, such that there exists $(u_1, u_2) \in L^2(D_1) \times L^2(D_2)$, $(u_1, u_2) \neq 0$, such that

$$\begin{pmatrix} 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_1}^{\delta k_0} & -\delta^2 \omega^2 \xi(\omega, k) R_{D_2 D_1}^{\delta k_0} \\ -\delta^2 \omega^2 \xi(\omega, k) R_{D_1 D_2}^{\delta k_0} & 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$
(3.4)

Theorem 3.3. Let d = 3. Then, the hybridized subwavelength resonant frequencies ω satisfy

$$\left(1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta\right)^2 - \delta^4 \omega^4 \xi(\omega, k)^2 \langle R_{D_1 D_2}^{\delta k_0} \phi_1^{(\delta)}, \phi_2^{(\delta)} \rangle \langle R_{D_2 D_1}^{\delta k_0} \phi_2^{(\delta)}, \phi_1^{(\delta)} \rangle = 0, \tag{3.5}$$

where $\phi_i^{(\delta)}$, for i = 1, 2, is the eigenfunction associated to the eigenvalue λ_{δ} of the potential $K_{D_i}^{\delta k_0}$. Proof. We observe that (3.4) is equivalent to

$$\begin{pmatrix} 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_1}^{\delta k_0} & 0\\ 0 & 1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0} \end{pmatrix} \begin{pmatrix} u_1\\ u_2 \end{pmatrix} - \delta^2 \omega^2 \xi(\omega, k) \begin{pmatrix} 0 & R_{D_2 D_1}^{\delta k_0}\\ R_{D_1 D_2}^{\delta k_0} & 0 \end{pmatrix} \begin{pmatrix} u_1\\ u_2 \end{pmatrix} = 0,$$

which gives

$$\binom{u_1}{u_2} - \delta^2 \omega^2 \xi(\omega, k) \begin{pmatrix} \left(1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_1}^{\delta k_0}\right)^{-1} & 0\\ 0 & \left(1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0}\right)^{-1} \end{pmatrix} \begin{pmatrix} R_{D_2 D_1}^{\delta k_0} u_2\\ R_{D_1 D_2}^{\delta k_0} u_1 \end{pmatrix} = 0.$$
(3.6)

Let us now apply a pole-pencil decomposition on the operators $\left(1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_i}^{\delta k_0}\right)^{-1}$, for i = 1, 2. We see that

$$\left(1-\delta^2\omega^2\xi(\omega,k)K_{D_1}^{\delta k_0}\right)^{-1}(\cdot) = \frac{\langle\cdot,\phi_1^{(\delta)}\rangle\phi_1^{(\delta)}}{1-\delta^2\omega^2\xi(\omega,k)\lambda_\delta} + R_1[\omega](\cdot)$$

and

$$\left(1 - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0}\right)^{-1}(\cdot) = \frac{\langle \cdot, \phi_2^{(\delta)} \rangle \phi_2^{(\delta)}}{1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta} + R_2[\omega](\cdot),$$

where the remainder terms $R_1[\omega](\cdot)$ and $R_2[\omega](\cdot)$ are holomorphic for ω in a neighborhood of ω_{δ} , so can be neglected. Then, (3.6), is equivalent to

$$\begin{pmatrix} u_1\\ u_2 \end{pmatrix} - \delta^2 \omega^2 \xi(\omega, k) \begin{pmatrix} \frac{\langle \cdot, \phi_1^{(\delta)} \rangle \phi_1^{(\delta)}}{1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta}} & 0\\ 0 & \frac{\langle \cdot, \phi_2^{(\delta)} \rangle \phi_2^{(\delta)}}{1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_{\delta}} \end{pmatrix} \begin{pmatrix} R_{D_2 D_1}^{\delta k_0} u_2\\ R_{D_1 D_2}^{\delta k_0} u_1 \end{pmatrix} = 0.$$

This gives us the system

$$\begin{cases} u_1 - \frac{\delta^2 \omega^2 \xi(\omega,k)}{1 - \delta^2 \omega^2 \xi(\omega,k) \lambda_{\delta}} \langle R_{D_2 D_1}^{\delta k_0} u_2, \phi_1^{(\delta)} \rangle \phi_1^{(\delta)} = 0, \\ u_2 - \frac{\delta^2 \omega^2 \xi(\omega,k)}{1 - \delta^2 \omega^2 \xi(\omega,k) \lambda_{\delta}} \langle R_{D_1 D_2}^{\delta k_0} u_1, \phi_2^{(\delta)} \rangle \phi_2^{(\delta)} = 0. \end{cases}$$

Applying the operator $R_{D_1D_2}^{\delta k_0}$ (resp. $R_{D_2D_1}^{\delta k_0}$) to the first (resp. second) equation, and then applying $\langle \cdot, \phi_2^{(\varepsilon)} \rangle$ (resp. $\langle \cdot, \phi_1^{(\varepsilon)} \rangle$), we find that

$$\begin{cases} \langle R_{D_1D_2}^{\delta k_0}u_1, \phi_2^{(\delta)} \rangle - \frac{\delta^2 \omega^2 \xi(\omega,k)}{1 - \delta^2 \omega^2 \xi(\omega,k) \lambda_{\delta}} \langle R_{D_1D_2}^{\delta k_0} \phi_1^{(\delta)}, \phi_2^{(\delta)} \rangle \langle R_{D_2D_1}^{\delta k_0}u_2, \phi_1^{(\delta)} \rangle = 0, \\ \langle R_{D_2D_1}^{\delta k_0}u_2, \phi_1^{(\delta)} \rangle - \frac{\delta^2 \omega^2 \xi(\omega,k)}{1 - \delta^2 \omega^2 \xi(\omega,k) \lambda_{\delta}} \langle R_{D_2D_1}^{\delta k_0} \phi_2^{(\delta)}, \phi_1^{(\delta)} \rangle \langle R_{D_1D_2}^{\delta k_0}u_1, \phi_2^{(\delta)} \rangle = 0. \end{cases}$$

This system has a solution only if its determinant is zero. That is, if

$$1 - \frac{\delta^4 \omega^4 \xi(\omega, k)^2}{\left(1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta\right)^2} \langle R_{D_1 D_2}^{\delta k_0} \phi_1^{(\delta)}, \phi_2^{(\delta)} \rangle \langle R_{D_2 D_1}^{\delta k_0} \phi_2^{(\delta)}, \phi_1^{(\delta)} \rangle = 0,$$

which gives the desired result.

The following corollary is a direct result of Theorem 3.3.

Corollary 3.3.1. Let d = 3. Then, the hybridized subwavelength resonant frequencies are given by

$$\omega = \frac{i\gamma \pm \sqrt{-\gamma^2 - 4\Gamma(\beta + \eta k^2)}}{2\Gamma},$$
(3.7)
where
$$\Gamma = -1 - \delta^2 \alpha \lambda_{\delta} \pm \alpha \delta^2 \sqrt{\langle R_{D_1 D_2}^{\delta k_0} \phi_1^{(\delta)}, \phi_2^{(\delta)} \rangle \langle R_{D_2 D_1}^{\delta k_0} \phi_2^{(\delta)}, \phi_1^{(\delta)} \rangle}.$$

where ϕ_i^{δ} , for i = 1, 2, is the eigenfunction associated to the eigenvalue λ_{δ} of the potential $K_{D_i}^{\delta k_0}$ and the \pm in the two expressions do not have to agree.

Proof. We introduce the notation $\mathbb{K} := \langle R_{D_1 D_2}^{\delta k_0} \phi_1^{(\delta)}, \phi_2^{(\delta)} \rangle$ and $\mathbb{M} := \langle R_{D_2 D_1}^{\delta k_0} \phi_2^{(\delta)}, \phi_1^{(\delta)} \rangle$. Then, (3.5) becomes

$$\left(1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta\right)^2 - \delta^4 \omega^4 \xi(\omega, k)^2 \mathbb{KM} = 0 \iff 1 - \delta^2 \omega^2 \xi(\omega, k) \lambda_\delta \pm \delta^2 \omega^2 \xi(\omega, k) \sqrt{\mathbb{KM}} = 0 \iff \left(-1 - \delta^2 \alpha \lambda_\delta \pm \alpha \delta^2 \sqrt{\mathbb{KM}}\right) \omega^2 - i\gamma \omega + \beta + \eta k^2 = 0,$$

and the roots to this second degree polynomial are given by

$$\omega = \frac{i\gamma \pm \sqrt{-\gamma^2 - 4\Gamma(\beta + \eta k^2)}}{2\Gamma} \quad \text{where} \quad \Gamma = -1 - \delta^2 \alpha \lambda_\delta \pm \alpha \delta^2 \sqrt{\mathbb{KM}},$$

with the two \pm not necessarily agreeing. Finally, substituting the expressions for \mathbb{K} and \mathbb{M} , we obtain the result.

3.2 Two Dimensions

Let us move on to the case of dimension d = 2. For simplicity, we again consider two identical halide perovskite resontators D_1 and D_2 , made from the same material with permittivity given by the formula (3.1). We define the operators $K_{D_i}^{\delta k_0}$ and $R_{D_iD_j}^{\delta k_0}$, for i, j = 1, 2, as in Definition 3.1 and we continue by defining the following integral operators.

Definition 3.4. We define the integral operators $M_{D_i}^{\delta k_0}$ and $N_{D_iD_j}^{\delta k_0}$ for i, j = 1, 2 as

$$M_{D_i}^{\delta k_0} := \hat{K}_{D_i}^{\delta k_0} + K_{D_i}^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) K_{D_i}^{(1)},$$

and

$$N_{D_i D_j}^{\delta k_0} := \hat{K}_{D_i D_j}^{\delta k_0} + R_{D_i D_j}^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) R_{D_i D_j}^{(1)}$$

where

$$\begin{split} K_{D_i}^{(0)} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \int_{D_i} G(x-y,0) u(y) \mathrm{d}y \Big|_{D_i} \in L^2(D_i), \\ \hat{K}_{D_i}^{\delta k_0} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \log(\hat{\gamma} \delta k_0) \hat{K}_{D_i}[u] \Big|_{D_i} \in L^2(D_i), \\ \hat{K}_{D_i} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto -\frac{1}{2\pi} \int_{D_i} u(y) \mathrm{d}y \Big|_{D_i} \in L^2(D_i), \\ K_{D_i}^{(1)} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \int_{D_i} \frac{\partial}{\partial k} G(x-y,k) \Big|_{k=0} u(y) \mathrm{d}y \Big|_{D_i} \in L^2(D_i) \end{split}$$

,

and

$$\begin{split} R_{D_iD_j}^{(0)} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \int_{D_i} G(x-y,0)u(y) \mathrm{d}y \Big|_{D_j} \in L^2(D_j), \\ \hat{K}_{D_iD_j}^{\delta k_0} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \log(\hat{\gamma}\delta k_0)\hat{K}_{D_iD_j}[u] \Big|_{D_j} \in L^2(D_j), \\ \hat{K}_{D_iD_j} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto -\frac{1}{2\pi} \int_{D_i} u(y) \mathrm{d}y \Big|_{D_j} \in L^2(D_j), \\ R_{D_iD_j}^{(1)} &: u \Big|_{D_i} \in L^2(D_i) \longmapsto \int_{D_i} \frac{\partial}{\partial k} G(x-y,k) \Big|_{k=0} u(y) \mathrm{d}y \Big|_{D_j} \in L^2(D_j) \end{split}$$

We observe the following result.

Proposition 3.5. For the integral operators $K_{D_i}^{\delta k_0}$ and $R_{D_i D_j}^{\delta k_0}$, we can write

$$K_{D_{i}}^{\delta k_{0}} = M_{D_{i}}^{\delta k_{0}} + O\left(\delta^{4}\log(\delta)\right), \quad and \quad R_{D_{i}D_{j}}^{\delta k_{0}} = N_{D_{i}D_{j}}^{\delta k_{0}} + O\left(\delta^{4}\log(\delta)\right), \tag{3.8}$$

as $\delta \to 0$ and with k_0 fixed.

Proof. The proof is a direct result of the expansion of the Green's function in dimension d = 2. Indeed, for $u|_{D_i} \in L^2(D_i)$, we observe that

$$\begin{split} K_{D_{i}}^{\delta k_{0}}[u](x) &= -\int_{D_{i}} G(x-y,\delta k_{0})u(y)\mathrm{d}y\Big|_{D_{i}} \\ &= -\int_{D_{i}} \left(\log(\hat{\gamma}\delta k_{0})\frac{1}{2\pi} + G(x-y,0) + (\delta k_{0})^{2}\log(\delta k_{0}\hat{\gamma})\frac{\partial}{\partial k}G(x-y,k)\Big|_{k=0} \right. \\ &+ O\left(\delta^{4}\log(\delta)\right) u(y)\mathrm{d}y\Big|_{D_{i}} \\ &= \left(\hat{K}_{D_{i}}^{\delta k_{0}} + K_{D_{i}}^{(0)} + (\delta k_{0})^{2}\log(\delta k_{0}\hat{\gamma})K_{D_{i}}^{(1)}\right) [u](x) + O\left(\delta^{4}\log(\delta)\right) \\ &= M_{D_{i}}^{\delta k_{0}}[u](x) + O\left(\delta^{4}\log(\delta)\right). \end{split}$$

Similarly, for $u|_{D_i} \in L^2(D_i)$,

$$\begin{split} R_{D_i D_j}^{\delta k_0}[u](x) &= -\int_{D_i} G(x - y, \delta k_0) u(y) \mathrm{d}y \Big|_{D_j} \in L^2(D_j) \\ &= -\int_{D_i} \left(\log(\hat{\gamma} \delta k_0) \frac{1}{2\pi} + G(x - y, 0) + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \frac{\partial}{\partial k} G(x - y, k) \Big|_{k=0} \right. \\ &\quad + O\left(\delta^4 \log(\delta)\right) \Big) u(y) \mathrm{d}y \Big|_{D_j} \\ &= \left(\hat{K}_{D_i D_j}^{\delta k_0} + R_{D_i D_j}^{(0)} + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) R_{D_i D_j}^{(1)} \right) [u](x) + O\left(\delta^4 \log(\delta)\right) \\ &= N_{D_i D_j}^{\delta k_0} [u](x) + O(\delta^4 \log(\delta)). \end{split}$$

Therefore, our problem is to determine the frequencies ω and the associated wavenumber k, for which the following holds:

$$\begin{pmatrix} I - \delta^2 \omega^2 \xi(\omega, k) K_{D_1}^{\delta k_0} & -\delta^2 \omega^2 \xi(\omega, k) R_{D_2 D_1}^{\delta k_0} \\ -\delta^2 \omega^2 \xi(\omega, k) R_{D_1 D_2}^{\delta k_0} & I - \delta^2 \omega^2 \xi(\omega, k) K_{D_2}^{\delta k_0} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
(3.9)

for nontrivial $u := (u_1, u_2)$, such that $u|_{D_i} \in L^2(D_i)$, for i = 1, 2.

Proposition 3.6. Let d = 2. Then, the hybridized subwavelength resonant frequencies ω satisfy

$$1 - \delta^{2} \omega^{2} \xi(\omega, k) \Big(-\frac{|D_{1}|}{2\pi} \log(\hat{\gamma} \delta k_{0})(1 \pm 1) + \langle K_{D_{1}}^{(0)}[\hat{\mathbb{I}}_{D_{1}}], \hat{\mathbb{I}}_{D_{1}} \rangle + (\delta k_{0})^{2} \log(\delta k_{0} \hat{\gamma}) \langle K_{D_{1}}^{(1)}[\hat{\mathbb{I}}_{D_{1}}], \hat{\mathbb{I}}_{D_{1}} \rangle \\ \pm \langle R_{D_{2}D_{1}}^{(0)}[\hat{\mathbb{I}}_{D_{2}}], \hat{\mathbb{I}}_{D_{1}} \rangle \pm (\delta k_{0})^{2} \log(\delta k_{0} \hat{\gamma}) \langle R_{D_{2}D_{1}}^{(1)}[\hat{\mathbb{I}}_{D_{2}}], \hat{\mathbb{I}}_{D_{1}} \rangle \Big) = 0,$$
(3.10)

where the \pm symbols coincide.

Proof. The first thing that we do is to observe that, by applying the expansion (3.8) to (3.9), we reach the problem

$$\begin{pmatrix} I - \delta^2 \omega^2 \xi(\omega, k) M_{D_1}^{\delta k_0} & -\delta^2 \omega^2 \xi(\omega, k) N_{D_2 D_1}^{\delta k_0} \\ -\delta^2 \omega^2 \xi(\omega, k) N_{D_1 D_2}^{\delta k_0} & I - \delta^2 \omega^2 \xi(\omega, k) M_{D_2}^{\delta k_0} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} O\left(\delta^4 \log(\delta)\right) \\ O\left(\delta^4 \log(\delta)\right) \end{pmatrix} .$$

We note that $|D_1| = |D_2|$. Then, using the symmetries of the dimer, let us denote

$$\hat{\nu}(\delta) := -\frac{|D_1|}{2\pi} \log(\delta k_0 \hat{\gamma}) + \langle K_{D_1}^{(0)}[\hat{\mathbb{I}}_{D_1}], \hat{\mathbb{I}}_{D_1} \rangle + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \langle K_{D_1}^{(1)}[\hat{\mathbb{I}}_{D_1}], \hat{\mathbb{I}}_{D_1} \rangle$$
$$= -\frac{|D_2|}{2\pi} \log(\delta k_0 \hat{\gamma}) + \langle K_{D_2}^{(0)}[\hat{\mathbb{I}}_{D_2}], \hat{\mathbb{I}}_{D_2} \rangle + (\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \langle K_{D_2}^{(1)}[\hat{\mathbb{I}}_{D_2}], \hat{\mathbb{I}}_{D_2} \rangle,$$

and

$$\hat{\eta} := \langle N_{D_1 D_2}^{\delta k_0} [\hat{\mathbb{I}}_{D_1}], \hat{\mathbb{I}}_{D_2} \rangle = \langle N_{D_2 D_1}^{\delta k_0} [\hat{\mathbb{I}}_{D_2}], \hat{\mathbb{I}}_{D_1} \rangle.$$

In addition, we have that

$$\hat{K}_{D_i D_j}^{\delta k_0}[\hat{\mathbb{I}}_{D_i}] = \hat{K}_{D_j}^{\delta k_0}[\hat{\mathbb{I}}_{D_j}].$$

Now, we define the quantity $\nu(\delta)$ to be the eigenvalues of the operator $M_{D_i}^{\delta k_0}$, that is,

$$\nu(\delta) = \langle M_{D_1}^{\delta k_0}[\Psi_{D_1}], \Psi_{D_1} \rangle = \langle M_{D_2}^{\delta k_0}[\Psi_{D_2}], \Psi_{D_2} \rangle,$$

for the eigenfunctions $\Psi_{D_i}(\delta) \in L^2(D_i)$, $\Psi_{D_i}(\delta) = \hat{\mathbb{I}}_{D_i} + O\left(\frac{1}{\log(d)}\right)$. Thus, we have that (3.9) is equivalent to

$$\binom{u_1}{u_2} - \delta^2 \omega^2 \xi(\omega, k) \begin{pmatrix} \left(I - \delta^2 \omega^2 \xi(\omega, k) M_{D_1}^{\delta k_0}\right)^{-1} & 0\\ 0 & \left(I - \delta^2 \omega^2 \xi(\omega, k) M_{D_2}^{\delta k_0}\right)^{-1} \end{pmatrix} \begin{pmatrix} N_{D_2 D_1}^{\delta k_0} u_2\\ N_{D_1 D_2}^{\delta k_0} u_1 \end{pmatrix} = 0.$$
(3.11)

Applying a pole-pencil decomposition, we observe that

$$\left(I - \delta^2 \omega^2 \xi(\omega, k) M_{D_i}^{\delta k_0}\right)^{-1} [\cdot] = \frac{\langle \cdot, \hat{\mathbb{I}}_{D_i} \rangle \hat{\mathbb{I}}_{D_i}}{1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta)} + R[\omega](\cdot),$$

where the remainder terms $R[\omega](\cdot)$ can be neglected. Hence, (3.11) is equivalent to

$$\begin{cases} u_1 - \delta^2 \omega^2 \xi(\omega, k) \frac{\langle N_{D_2D_1}^{\delta k_{D_1}} u_2, \hat{\mathbb{I}}_{D_1} \rangle \hat{\mathbb{I}}_{D_1}}{1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta)} = 0, \\ u_2 - \delta^2 \omega^2 \xi(\omega, k) \frac{\langle N_{D_1D_2}^{\delta k_{D_1}} u_1, \hat{\mathbb{I}}_{D_2} \rangle \hat{\mathbb{I}}_{D_2}}{1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta)} = 0, \end{cases}$$

which is equivalent to

$$\begin{cases} \langle N_{D_1D_2}^{\delta k_0} u_1, \hat{\mathbb{I}}_{D_2} \rangle - \frac{\delta^2 \omega^2 \xi(\omega, k)}{1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta)} \langle N_{D_1D_2}^{\delta k_0} \hat{\mathbb{I}}_{D_1}, \hat{\mathbb{I}}_{D_2} \rangle \langle N_{D_2D_1}^{\delta k_0} u_2, \hat{\mathbb{I}}_{D_1} \rangle = 0, \\ \langle N_{D_2D_1}^{\delta k_0} u_2, \hat{\mathbb{I}}_{D_1} \rangle - \frac{\delta^2 \omega^2 \xi(\omega, k)}{1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta)} \langle N_{D_2D_1}^{\delta k_0} \hat{\mathbb{I}}_{D_2}, \hat{\mathbb{I}}_{D_1} \rangle \langle N_{D_1D_2}^{\delta k_0} u_1, \hat{\mathbb{I}}_{D_2} \rangle = 0. \end{cases}$$

For this to have a solution, we need the determinant of the matrix induced by this system to be zero. This gives

$$1 - \frac{\delta^4 \omega^4 \xi(\omega, k)^2}{(1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta))^2} \langle N_{D_1 D_2}^{\delta k_0} \hat{\mathbb{I}}_{D_1}, \hat{\mathbb{I}}_{D_2} \rangle \langle N_{D_2 D_1}^{\delta k_0} \hat{\mathbb{I}}_{D_2}, \hat{\mathbb{I}}_{D_1} \rangle = 0.$$

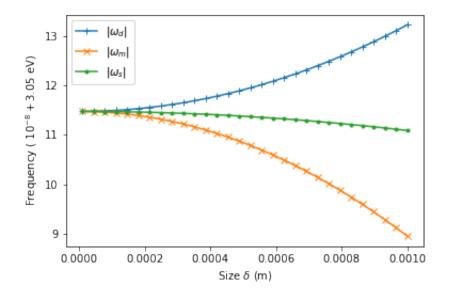


Figure 2: Behaviour of the subwavelength resonances for small circular nano-particles of radius δ . The resonant frequency ω_s of a single circular methylammonium lead chloride nano-particle is shown. For two circular nano-particles, made from the same material, we see how the hybridization causes the frequencies ω_d (dipole) and ω_m (monopole) to shift either side of ω_s .

Given the symmetry of our setting, we have that

$$\langle N_{D_1D_2}^{\delta k_0} \hat{\mathbb{I}}_{D_1}, \hat{\mathbb{I}}_{D_2} \rangle = \langle N_{D_2D_1}^{\delta k_0} \hat{\mathbb{I}}_{D_2}, \hat{\mathbb{I}}_{D_1} \rangle$$

and hence, we get

$$1 - \delta^2 \omega^2 \xi(\omega, k) \nu(\delta) \pm \delta^2 \omega^2 \xi(\omega, k) \langle N_{D_1 D_2}^{\delta k_0} \hat{\mathbb{I}}_{D_1}, \hat{\mathbb{I}}_{D_2} \rangle = 0.$$

This is equivalent to

$$1 - \delta^{2} \omega^{2} \xi(\omega, k) \Big(-\frac{|D_{1}|}{2\pi} \log(\delta k_{0} \hat{\gamma})(1 \pm 1) + \langle K_{D_{1}}^{(0)}[\hat{\mathbb{I}}_{D_{1}}], \hat{\mathbb{I}}_{D_{1}} \rangle + (\delta k_{0})^{2} \log(\delta k_{0} \hat{\gamma}) \langle K_{D_{1}}^{(1)}[\hat{\mathbb{I}}_{D_{1}}], \hat{\mathbb{I}}_{D_{1}} \rangle \\ \pm \langle R_{D_{2}D_{1}}^{(0)}[\hat{\mathbb{I}}_{D_{2}}], \hat{\mathbb{I}}_{D_{1}} \rangle \pm (\delta k_{0})^{2} \log(\delta k_{0} \hat{\gamma}) \langle R_{D_{2}D_{1}}^{(1)}[\hat{\mathbb{I}}_{D_{2}}], \hat{\mathbb{I}}_{D_{1}} \rangle \Big) = 0,$$

which is the desired result.

4 Example: Circular Resonators

In this section, we illustrate our results for the case of two-dimensional circular halide perovskite resonators. We can find the resonant frequencies of a single particle ω_s by solving (2.35). Similarly, the hybridized resonant frequencies of a pair of circular resonators can be found by solving (3.10). The two solutions of (3.10) are denoted by ω_m and ω_d , to describe their monopolar and dipolar characteristics. As is expected from other hybridized systems, it holds that $\omega_m < \omega_d$. We plot these three frequencies as a function of the particle size δ in Figure 2. We use the parameter values from [14] to model resonators made from methylammonium lead chloride (MAPbCl₃), which is a popular halide perovskite.

The first thing we observe from Figure 2 is that in the $\delta \to 0$ limit, the frequencies coincide. This is because the nano-particles behave as isolated, identical resonators when δ is very small. Then, as δ increases the single-particle resonance ω_s always stays between the monopole and dipole frequencies of the hybridized case. The phenomenon of the dipole frequency ω_d being shifted above ω_s and the monopole frequency ω_m being shifted below ω_s is a typical behaviour of hybridized resonator systems, see e.g. [3].

5 Conclusion

We have established a new mathematical model for halide perovskite resonators. This is a significant development of the existing theory of subwavelength resonators [2, 3], as it generalizes the techniques to dispersive settings where the permittivity of the material depends on both the frequency and the wavenumber. Given the rapidly growing use of halide perovskites in engineering applications, this theory will have a significant impact on the design of advanced devices [11, 13]. The integral methods used here are able to describe a very broad class of resonator shapes, so are an ideal approach for studying complex geometries, such as the biomimetic eye developed by [8].

Data Availability

There are no associated data, arising from this work. The only data used in this work are the material parameter values for methylammonium lead chloride, which are stated in [14].

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A Appendix

A.1 Calculation of Three-dimensional Constants

We derive a formula for \mathbb{F} , which was a crucial quantity in section 2.4.3, in the case of a single threedimensional halide perovskite resonator. We have that

$$\langle K_D^{(2)}[u_\delta], u_\delta \rangle = \frac{1}{8\pi} \mathbb{F}.$$

From (2.22), we observe that

$$\delta^2 \omega^2 \xi(\omega,k) = \frac{8\pi}{8\pi\lambda_\delta - \delta^2 k_0^2 \mathbb{F}}$$

Also, we know that $\xi(\omega, k) = \mu_0(\varepsilon(\omega, k) - \varepsilon_0)$, and we have shown that

$$\varepsilon(\omega,k) = \varepsilon_0 + \frac{1}{\mu_0 \delta^2 \omega^2 \left(\lambda_0 - \frac{i}{4\pi} \delta k_0 \mathbb{B}\right)}$$

Substituting this into the above equation, we get

$$\mathbb{F} = \frac{8\pi}{\delta^2 k_0^2} \Big(\lambda_\delta - \lambda_0 + \frac{i}{4\pi} \delta k_0 \mathbb{B} \Big).$$

Therefore, we obtain that

$$\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle = \frac{1}{\delta^2 k_0^2} \Big(\lambda_{\delta} - \lambda_0 + \frac{i}{4\pi} \delta k_0 \mathbb{B} \Big).$$

A.2 Calculation of Two-dimensional Constants

We derive a formula for S, which was a crucial quantity in section 2.5.3, in the case of a single twodimensional halide perovskite resonator. We have that

$$\langle K_D^{(2)}[u_\delta], u_\delta \rangle = \frac{i}{4\pi} \mathbb{S}$$

From (2.35), we can obtain an expression for S. Indeed, (2.35) is equivalent to

$$4\pi = \delta^2 \omega^2 \xi(\omega, k) \Big(4\pi \lambda_\delta - i \delta^4 k_0^4 \log(\delta k_0 \hat{\gamma}) \mathbb{S} \Big).$$

We know that $\xi(\omega, k) = \mu_0 \Big(\varepsilon(\omega, k) - \varepsilon_0 \Big)$ and we have shown that

$$\varepsilon(\omega,k) = \frac{1}{\mu_0 \delta^2 \omega^2 \left(\log(\delta k_0 \hat{\gamma}) \lambda_{-1} - \frac{\mathbb{P}}{2\pi} - \frac{i(\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \mathbb{G}}{4\pi} \right)} + \varepsilon_0.$$

Substituting this into the above equality, we get

$$\mathbb{S} = \frac{-i}{\delta^4 k_0^4 \log(\delta k_0 \hat{\gamma})} \Big(4\pi (\lambda_\delta - \log(\delta k_0 \hat{\gamma}) \lambda_{-1}) + 2\mathbb{P} + i(\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \mathbb{G} \Big)$$

Therefore, we obtain that

$$\langle K_D^{(2)}[u_{\delta}], u_{\delta} \rangle = \frac{1}{4\pi \delta^4 k_0^4 \log(\delta k_0 \hat{\gamma})} \Big(4\pi (\lambda_{\delta} - \log(\delta k_0 \hat{\gamma}) \lambda_{-1}) + 2\mathbb{P} + i(\delta k_0)^2 \log(\delta k_0 \hat{\gamma}) \mathbb{G} \Big).$$

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