

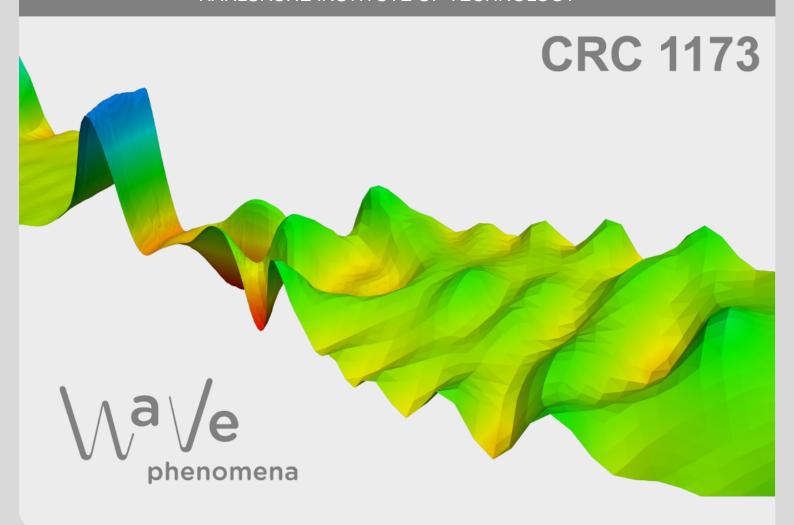


Quadrature by parity asymptotic expansions (QPAX) for scattering by high aspect ratio particles

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CRC Preprint 2021/22, May 2021

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QUADRATURE BY PARITY ASYMPTOTIC EXPANSIONS (QPAX) FOR SCATTERING BY HIGH ASPECT RATIO PARTICLES

CAMILLE CARVALHO, ARNOLD D. KIM, LORI LEWIS, AND ZOÏS MOITIER

ABSTRACT. We study scattering by a high aspect ratio particle using boundary integral equation methods. This problem has important applications in nanophotonics problems, including sensing and plasmonic imaging. Specifically, we consider scattering in two dimensions by a sound-hard, high aspect ratio ellipse. For this problem, we find that the boundary integral operator is nearly singular due to the collapsing geometry from an ellipse to a line segment. We show that this nearly singular behavior leads to qualitatively different asymptotic behaviors for solutions with different parities. Without explicitly taking this nearly singular behavior and this parity into account, computed solutions incur a large error. To address these challenges, we introduce a new method called Quadrature by Parity Asymptotic expansions (QPAX) that effectively and efficiently addresses these issues. We first develop QPAX to solve the Dirichlet problem for Laplace's equation in a high aspect ratio ellipse. Then, we extend QPAX for scattering by a sound-hard, high aspect ratio ellipse. We demonstrate the effectiveness of QPAX through several numerical examples.

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1. Introduction

Metal nanoparticles are being used extensively for chemical and biological sensing applications because they exhibit strong electromagnetic field responses and they are biologically and chemically inert (e.g. see [2] for a review). For these applications, the shape of individual metal nanoparticles can drastically affect the sensitivity of sensors. Consequently, there has been much interest in understanding how nanoparticle shape affects scattering by electromagnetic

Date: May 6, 2021.

²⁰¹⁰ Mathematics Subject Classification. 41A60, 65D30, 65R20.

Key words and phrases. Boundary integral methods; asymptotic analysis; numerical quadrature; scattering. This research was funded by the NSF (DMS-1819052 and DMS-1840265) and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) — Project-ID 258734477 — SFB 1173.

fields. In particular, there has been interest in studying so-called high aspect ratio nanoparticles [5, 24, 3]. Examples of these include nano-rods, nano-wires, nano-tubes, etc. High aspect ratio nanoparticles have anisotropic and tunable chemical, electrical, magnetic, and optical properties that make them attractive for designing sensors. Moreover, the diffusion of high aspect ratio nanoparticles provides enhanced functionality such as delivering DNA in plant cells [10].

It is then fundamental to understand the scattering properties of high aspect ratio nanoparticles to design next-generation sensors. However, these scattering problems are challenging due to the inherently high anisotropy affecting both the near- and far-field behaviors of the scattered field. Indeed, the narrow axis of a high aspect ratio nanoparticle may be much smaller than the wavelength of the incident field, while the long axis may be comparable to or larger than it.

Motivated by these sensing applications, we seek to study the fundamental issues inherent in scattering by high aspect ratio particles. To that end, we study here a simple model of two dimensional scalar wave scattering by a high aspect ratio ellipse. We study this problem using boundary integral equation methods [14, 21, 18]. We are interested in using boundary integral equations to study this problem because they provide high accuracy [19, 16, 20, 11, 9, 15, 27], they provide valuable physical insight over all scales of the problem, and they generalize easily to more complex problems including multiply connected domains, e.g. ensembles of high aspect ratio particles.

The two-dimensional problem we study here is advantageous because we can compute its analytical solution in terms of special functions (see Appendix A). We use this analytical solution to validate our methods. Moreover, Geer has studied scattering by slender bodies using asymptotic analysis and obtained a uniformly valid asymptotic solution [12]. That asymptotic analysis can be applied to this problem and adds further insight. Essentially, Geer's asymptotic solution for this scattering problem is given by a continuous distribution of point sources over a line segment along the semi-major axis of the ellipse. This insightful asymptotic analysis allows us to anticipate the challenges that the boundary integral equation formulation will have with this problem.

In this paper we show that there is an underlying nearly singular behavior within the scattering boundary integral operator, in the limit where the ellipse coalesces to a line segment. Nearly singular behaviors arise when the kernel of the integral operator is sharply peaked (but not singular), leading to a large error in computations. Typically we see nearly singular behaviors in the so-called close evaluation problem, corresponding to evaluating layer potentials near the boundary [14, 15, 25, 6, 7, 8]. In other words, the close evaluation problem happens after one has accurately solved the boundary integral equation. For this present problem, the high aspect ratio ellipse leads to a nearly singular integral operator in the boundary integral equation, itself, thereby adversely affecting the accuracy of the computed solution. Nearly singular boundary integral equations also arise when boundaries in a multiply-connected domain are close to one another. This nearly singular behavior was seen when particles suspended in Stokes flow were situated closely to one another [1, 26, 4]. To our knowledge, there is not a systematic treatment of nearly singular boundary integral equations. Thus, this study provides valuable insight into those problems as well.

By exploring the causes of the emerging nearly singular boundary integral operator, we find that it is due to a factor that is the kernel of the double-layer potential fo Laplace's equation. Thus, we study the related interior Dirichlet problem for Laplace's equation and find that there exists qualitative differences in the asymptotic behaviors of solutions with different parity (with respect to the major axis of the ellipse). By addressing this difference in parity explicitly, we develop a new method which we call Quadrature by Parity Asymptotic eXpansions (QPAX). We show that this method effectively solves the interior Dirichlet problem for Laplace's equation. Then we extend QPAX for the scattering problem and show that it effectively addresses the nearly singular behavior of the associated boundary integral operator.

The remainder of this paper is organized as follows. Section 2 presents the problem of scattering by a high aspect ratio ellipse that we study here and its boundary integral equation formulation. This formulation reveals the cause of the nearly singular behavior. To isolate the nearly singular behavior of the boundary integral operator identified in Section 2, we study the related Dirichlet problem for Laplace's equation in a high aspect ratio ellipse in Section 3. Here we identify that the nearly singular behavior leads to qualitatively different asymptotic behaviors based on parity. We then introduce Quadrature by Parity Asymptotic eXpansions (QPAX) to effectively and efficiently solve that problem. Finally, we extend QPAX for scattering by a sound-hard, high aspect ratio ellipse in Section 4. Section 5 gives our conclusions. Appendix A provides details about the exact solutions used for validation in our numerical results, and Appendix B gives proofs of the considered asymptotic expansions in the paper.

2. Scattering by a high aspect ratio ellipse

We introduce a simple, two-dimensional model for studying scattering of scalar waves by a high aspect ratio particle. Let $D \subset \mathbb{R}^2$ be a bounded simply connected set denoting the support of a particle with smooth boundary ∂D and let $\overline{D} = D \cup \partial D$. We study the sound-hard scattering problem, which can be written as

Find
$$u = u^{\mathsf{in}} + u^{\mathsf{sc}} \in \mathscr{C}^2(E := \mathbb{R}^2 \setminus \overline{D}) \cup \mathscr{C}^1(\mathbb{R}^2 \setminus D)$$
 such that:
$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } E, \\ \partial_n u = 0 & \text{on } \partial D, \\ \lim_{r \to \infty} \int_{|x| = r} |\partial_n u^{\mathsf{sc}} - \mathsf{i} k u^{\mathsf{sc}}|^2 \, \mathrm{d}\sigma = 0, \end{cases}$$

where u denotes the total field, k is the wavenumber, u^{sc} is the scattered field, u^{in} is the incident field, and ∂_n denotes the normal derivative. The last equation in Eq. (1) is the Sommerfeld radiation condition. To study scattering by a high aspect ratio particle, we consider the ellipse defined according to

(2)
$$y(t) = (\varepsilon \cos(t), \sin(t)), \quad t \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z},$$

with $0 < \varepsilon \ll 1$. The aspect ratio for this ellipse is ε^{-1} . Hence, we study the asymptotic limit, $\varepsilon \to 0^+$ for high aspect ratio particles. Given $x \in E$, we denote $x^b \in \partial D$ the closest point on the boundary, and we write $x^b = y(s)$ for $s \in \mathbb{T}$ (see Fig. 1).

We can write the analytical solution of Eq. (1) in terms of angular and radial Mathieu functions (see Appendix A for details), and use that analytical solution to study the behavior of fields scattered by the high aspect ratio ellipse. In particular, we evaluate this analytical solution using the following incident field,

$$u^{\rm in}(x,y) = \sum_{n=0}^{15} \alpha_m^{\rm in} \, \mathrm{Mc}_m^{(1)}(\xi,q) \, \mathrm{ce}_m(\eta,q) + \sum_{n=1}^{15} \beta_m^{\rm in} \, \mathrm{Ms}_m^{(1)}(\xi,q) \, \mathrm{se}_m(\eta,q),$$

with (ce_m, se_m) denoting the angular Mathieu functions of order m, $(Mc_m^{(1)}, Ms_m^{(1)})$ the radial Mathieu function of the first-kind and order m, defined using elliptical coordinates (see Appendix A for more details). The coefficients are $\alpha_m^{\text{in}} = 2i^m ce_m(\frac{\pi}{2}, q)$ and $\beta_m^{\text{in}} = 2i^m se_m(\frac{\pi}{2}, q)$, and Eq. (3) approximates a plane wave propagating in the $+\hat{x}$ direction (see [23, Sec. 28.28(i)]). In Fig. 2a, we plot the real part of u^{in} given by Eq. (3) for k=2. We observe in Fig. 2a that this incident field closely approximates a plane wave propagating in the $+\hat{x}$ direction within the window $[-5,5] \times [-5,5]$, which provides bounds for our computational domain.

Using Eq. (3) as the incident field, we evaluate the analytical solution for the sound-hard scattering problem, and we plot its amplitude in Fig. 2b for k = 2 and $\varepsilon = 0.01$. Note that with this choice of parameters, the semi-major axis of the ellipse is on the order of the wavelength, but the semi-minor axis is much smaller than the wavelength. The black bar in Fig. 2b represents the high aspect ratio ellipse that cannot otherwise be seen.

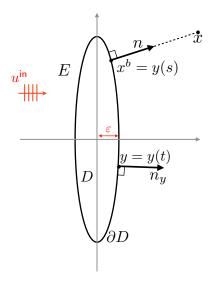


FIGURE 1. Sketch and notations of the scattering by a high aspect ratio ellipse problem.

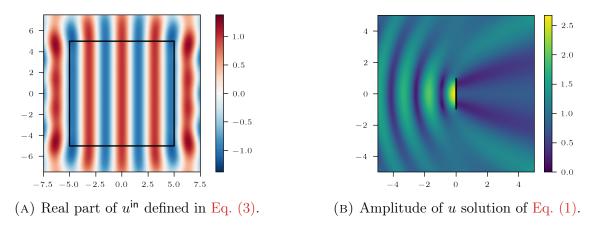


FIGURE 2. Plots of the real part of the incident field u^{in} and the amplitude of the total field u.

We find that scattering by the high aspect ratio ellipse is highly anisotropic. We observe a strong diffraction behavior around the high curvature regions, the solution demonstrates a strong amplitude near the illuminated face of the ellipse and a shadow regions on the other side of the ellipse. It is clear from this result that the scattered field on or near the boundary plays an important role in this scattering problem, with impact on the far-field.

2.1. Boundary integral equation formulation. The solution of Helmholtz's equation in the exterior domain E is given by the representation formula [18]

(4)
$$u(x) = u^{\mathsf{in}}(x) + \int_{\partial D} \partial_{n_y} G(x, y) u(y) \, \mathrm{d}\sigma_y - \int_{\partial D} G(x, y) \partial_{n_y} u(y) \, \mathrm{d}\sigma_y, \quad x \in E,$$

with n_y denoting the outward normal at y (see Fig. 1). The fundamental solution is given by

$$G(x,y) = \frac{\mathrm{i}}{4} \, \mathsf{H}_0^{(1)}(k|x-y|)$$

with $\mathsf{H}_0^{(1)}$ denoting the Hankel function of the first kind of order zero. Since $\partial_n u = 0$ on ∂D , we find that Eq. (4) reduces to

(5)
$$u(x) = u^{\mathsf{in}}(x) + \int_{\partial D} \partial_{n_y} G(x, y) u(y) \, \mathrm{d}\sigma_y, \qquad x \in E.$$

Using classic properties of the double-layer potential [18], the unknown field u on the boundary solves the boundary integral equation

(6)
$$\frac{1}{2}u(x^b) - \int_{\partial D} \partial_{n_y} G(x^b, y) u(y) \, d\sigma_y = u^{\mathsf{in}}(x^b), \qquad x^b \in \partial D.$$

On the high aspect ratio ellipse defined in Eq. (2), we can write the integral in Eq. (6) as

$$\int_{\partial D} \partial_{n_y} G(x^b, y) \ u(y) \, d\sigma_y = \int_{\mathbb{T}} \partial_{n_y} G(y(s), y(t)) \ u(y(t)) \ |y'(t)| \, dt,$$

we then rewrite the kernel

(7)
$$\partial_{n_y} G(y(s), y(t))|y'(t)| = \frac{\mathrm{i}k\pi}{2} r(s, t; \varepsilon) \,\mathsf{H}_1^{(1)}(k\, r(s, t; \varepsilon)) \,K^L(s, t; \varepsilon),$$

with

$$r(s,t;\varepsilon) = 2\left|\sin\left(\frac{s-t}{2}\right)\right|\sqrt{\cos\left(\frac{s+t}{2}\right)^2 + \varepsilon^2\sin\left(\frac{s+t}{2}\right)^2},$$

and

(8)
$$K^{L}(s,t;\varepsilon) = \frac{1}{2\pi} \frac{-\varepsilon}{1 + \varepsilon^{2} + (1 - \varepsilon^{2})\cos(s+t)}.$$

The kernel K^L given in Eq. (8) corresponds to the kernel for the double-layer potential solution of Laplace's equation for this narrow ellipse. In light of Eq. (7), we make the following remarks.

- Due to the factor of $\mathsf{H}_1^{(1)}(k\,r(s,t;\varepsilon))$ appearing in the kernel given in Eq. (7), the derivative of the kernel has a logarithmic singularity on s=t. This singularity is well understood (see [18]).
- For t_s such that $s+t_s \equiv \pi$ [2π] (with the notation k [X] denoting k modulo X), $K^L(s,t;\varepsilon)$ given in Eq. (8) behaves according to

$$K^{L}(s, t_{s}; \varepsilon) = -\frac{1}{4\pi\varepsilon} \xrightarrow[\varepsilon \to 0^{+}]{} -\infty.$$

Since

$$\left|\frac{\mathrm{i}k\pi}{2}\,r(s,t_s;\varepsilon)\,\,\mathrm{H}_1^{(1)}(k\,r(s,t_s;\varepsilon))\right|\underset{\varepsilon\to 0^+}{\longrightarrow}1,$$

it follows that the asymptotic behavior for Eq. (7) on t_s is given by this asymptotic behavior for K^L .

- The kernel K^L is sharply peaked at the *anti-points* $s + t \equiv \pi [2\pi]$, and this peak is enhanced as the ellipse collapses, in other words when the anti-points become closer. This sharp peak leads to a nearly singular integral operator in the boundary integral equation.
- The cases $s = \left\{-\frac{\pi}{2}, \frac{\pi}{2}\right\}$ are degenerate since the derivative of the kernel Eq. (7) admits a singularity for s = t, and we have the nearly singular behavior (the anti-points coincide in this case).

The integral operator in the boundary integral equation Eq. (6) is weakly singular on s = t and nearly singular on $s + t \equiv \pi[2\pi]$. The weak singularity on s = t can be addressed using the product quadrature rule due to Kress [17]. The nearly singular behavior, however, is problematic. In the results that follow, we show that this nearly singular behavior leads to large error unless it is explicitly addressed.

3. Dirichlet problem for Laplace's equation in a high aspect ratio ellipse

In the previous section, we identified that the factor of K^L given in Eq. (8) causes nearly singular behaviors in the boundary integral equation. To isolate this issue, we consider here the following interior Dirichlet problem for Laplace's equation,

(9) Find
$$u \in \mathscr{C}^2(D) \cup \mathscr{C}^1(\overline{D})$$
 such that:
 $\Delta u = 0 \text{ in } D, \quad u = -f \text{ on } \partial D,$

where the prescribed boundary data -f is smooth. The solution of Eq. (9) can be represented as the double-layer potential [14, 18]:

$$u(x) = \frac{1}{2\pi} \int_{\partial D} \frac{n_y \cdot (x - y)}{|x - y|^2} \mu(y) d\sigma_y, \quad x \in D,$$

with μ denoting a continuous (at least) function solution of the following boundary integral equation,

(10)
$$\frac{1}{2}\mu(x^b) - \frac{1}{2\pi} \int_{\partial D} \frac{n_y \cdot (x^b - y)}{|x^b - y|^2} \, \mu(y) \, d\sigma_y = f(x^b), \quad x^b \in \partial D.$$

Note that Eq. (10) is similar to Eq. (6). On the high aspect ratio ellipse Eq. (2), this boundary integral equation becomes

(11)
$$\frac{1}{2}\mu(s) - \int_{\mathbb{T}} K^L(s, t; \varepsilon)\mu(t) \, \mathrm{d}t = f(s), \quad s \in \mathbb{T},$$

with K^L given in Eq. (8).

3.1. Analytical solution of boundary integral equation Eq. (11). We compute the analytical solution of Eq. (11) as follows. By computing the discrete Fourier transform of Eq. (11), we obtain

$$\frac{1}{2}\mu_m - 2\pi \mathsf{K}_m \mu_{-m} = f_m, \quad m \in \mathbb{Z},$$

with $(\mu_m)_{m\in\mathbb{Z}}$, $(\mathsf{K}_m)_{m\in\mathbb{Z}}$, and $(f_m)_{m\in\mathbb{Z}}$ denoting the complex Fourier coefficients of μ , K^L , and f:

$$X(s) \coloneqq \sum_{m \in \mathbb{Z}} X_m e^{ims}, \quad X = \mu, K^L, f.$$

One can check using Eq. (8) that $K^L(s,t;\varepsilon)$ boils down to a function in s+t. We rewrite this system as

$$\left(\frac{1}{2} - 2\pi \mathsf{K}_0\right)\mu_0 = f_0$$

and

$$\begin{pmatrix} \frac{1}{2} & -2\pi \mathsf{K}_m \\ -2\pi \mathsf{K}_{-m} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mu_m \\ \mu_{-m} \end{pmatrix} = \begin{pmatrix} f_m \\ f_{-m} \end{pmatrix}, \quad \text{for } m \neq 0.$$

The solutions of these problems are given by

(12)
$$\mu_0 = \frac{2f_0}{1 - 4\pi \mathsf{K}_0}$$

and

(13)
$$\mu_m = \frac{4}{1 - 16\pi^2 \mathsf{K}_m \mathsf{K}_{-m}} \left(\frac{1}{2} f_m + 2\pi \mathsf{K}_m f_{-m} \right), \quad \text{for } m \neq 0.$$

Since K^L is a rational trigonometric function, one can analytically compute K_m using [13, Eq. (2.5)], for $m \in \mathbb{Z}$ leading to

$$\mathsf{K}_m = -\frac{1}{4\pi} \rho_{\varepsilon}^{|m|}, \quad \text{with } \rho_{\varepsilon} = \frac{\varepsilon - 1}{\varepsilon + 1} \in (-1, 0).$$

Substituting this expression for K_m into Eq. (12) and Eq. (13), we find that

(14)
$$\mu(s) = f_0 + \sum_{m \in \mathbb{Z}^*} \frac{2}{1 - \rho_{\varepsilon}^{2|m|}} \left(f_m - \rho_{\varepsilon}^{|m|} f_{-m} \right) e^{ims}, \quad s \in \mathbb{T}.$$

With the solution given in Eq. (14), we find the following.

- When f = C where C is a constant, $\mu = C$.
- When $f = \cos(ms)$ for $m \in \mathbb{N}$, we have $\mu = 2\cos(ms)/(1 + \rho_{\varepsilon}^m)$.
- When $f = \sin(ms)$ for $m \in \mathbb{N}^*$, we have $\mu = 2\sin(ms)/(1 \rho_{\varepsilon}^m)$.

Note that $\rho_{\varepsilon} < 0$, and $\rho_{\varepsilon} = -1 + 2\varepsilon + \mathcal{O}(\varepsilon^2)$ as $\varepsilon \to 0^+$. As a consequence depending on the parity of m, as $\varepsilon \to 0^+$, we have

$$1 + \rho_{\varepsilon}^m \sim \begin{cases} 2m\varepsilon & \text{when } m \text{ is odd} \\ 1 & \text{when } m \text{ is even} \end{cases}$$

and

$$1 - \rho_{\varepsilon}^{m} \sim \begin{cases} 1 & \text{when } m \text{ is odd} \\ 2m\varepsilon & \text{when } m \text{ is even} \end{cases}.$$

In light of these results, we are motivated to introduce the following definition.

Definition 1. For any function $f: \mathbb{T} \to \mathbb{C}$:

- We say that f is even if it belongs to the space $\mathscr{C}_{ev}(\mathbb{T}) := \{ f \in \mathscr{C}(\mathbb{T}) \mid f(\pi s) = f(s) \};$
- We say that f is odd if it belongs to the space $\mathscr{C}_{od}(\mathbb{T}) := \{ f \in \mathscr{C}(\mathbb{T}) \mid f(\pi s) = -f(s) \}.$

We define the even and odd parts of f as $f_{\text{ev}}(s) = \frac{1}{2}(f(s) + f(\pi - s))$ and $f_{\text{od}}(s) = \frac{1}{2}(f(s) - f(\pi - s))$.

With Definition 1 established, we state the following results.

- When f is even in the sense of Definition 1 (typically $s \mapsto \sin((2p+1)s)$ or $\cos(2ps)$ for $p \in \mathbb{N}$), then the solution μ is bounded as $\varepsilon \to 0^+$.
- When f is odd in the sense of Definition 1 (typically $s \mapsto \sin(2ps)$ or $\cos((2p+1)s)$ for $p \in \mathbb{N}^*$) then the solution μ is unbounded as $\varepsilon \to 0^+$.

The qualitative differences between solutions when the Dirichlet boundary data is even or odd will play an important role in addressing the nearly singular behavior of K^L .

3.2. Modified trapezoid rule (MTR). A method to compute the leading behavior of nearly singular integrals is given in [8]. In what follows we apply that method to Eq. (11). Recall that K^L exhibits nearly singular behavior on $s+t\equiv\pi[2\pi]$. For this reason, we introduce

$$I_{\delta}(\varepsilon) = \int_{\pi - s - \frac{\delta}{2}}^{\pi - s + \frac{\delta}{2}} K^{L}(s, t; \varepsilon) \, \mu(t) \, \mathrm{d}t,$$

where $\delta > 0$ is fixed. To determine the leading behavior of $I_{\delta}(\varepsilon)$ as $\varepsilon \to 0^+$, we perform a series of substitutions. First, we shift by substituting $t = \pi - s + x$, then we rescale using the stretched coordinate $x = \varepsilon X$. These lead to

(15)
$$I_{\delta}(\varepsilon) = \frac{1}{2\pi} \int_{-\frac{\delta}{2\varepsilon}}^{\frac{\delta}{2\varepsilon}} \frac{-\varepsilon^{2}}{1 + \varepsilon^{2} - (1 - \varepsilon^{2})\cos(\varepsilon X)} \,\mu(\pi - s + \varepsilon X) \,\mathrm{d}X.$$

Assuming μ is also differentiable, we expand the integrand in Eq. (15) about $\varepsilon = 0^+$ and find

(16)
$$\frac{-\varepsilon^2 \mu(\pi - s + \varepsilon X)}{1 + \varepsilon^2 - (1 - \varepsilon^2) \cos(\varepsilon X)} = -\frac{2}{4 + X^2} \left[\mu(\pi - s) + \varepsilon X \mu'(\pi - s) \right] + \mathcal{O}(\varepsilon^2).$$

All expansions have been computed via Mathematica and SymPy, and notebooks can be found in the Github repository [22]. Integrating this expansion term-by-term, the $\mathcal{O}(\varepsilon)$ in Eq. (16) vanishes upon integration since it is odd (in the classic sense), and we find

(17)
$$I_{\delta}(\varepsilon) = -\frac{1}{\pi} \arctan\left(\frac{\delta}{4\varepsilon}\right) \mu(\pi - s) + \mathcal{O}(\varepsilon).$$

We refer the reader to [8] for a proper justification of the obtained order after integration. This result gives the asymptotic behavior of the portion of boundary integral operator in Eq. (11) about $s+t \equiv \pi \left[2\pi\right]$ leading to its nearly singular behavior. We now use this leading behavior to modify the periodic trapezoid rule (PTR). Let $s_n = t_n = n\Delta t - \pi/2$ with $\Delta t = \pi/N$. It follows that $s_i + t_{-i[2N]} \equiv \pi \left[2\pi\right]$ (with the notation $t_{k[N]}$ denoting t_k for $k \in \mathbb{Z}$ modulo N). Instead of using the trapezoid rule on those anti-points, we replace it with $I_{\Delta t}(\varepsilon)$ (namely Eq. (17) where we substitute $\delta = \Delta t$). We call this method the modified trapezoid rule (MTR). Applying this MTR to Eq. (10) yields the following linear system,

(18)
$$\frac{1}{2}\mu_i + \frac{1}{\pi}\arctan\left(\frac{\Delta t}{4\varepsilon}\right)\mu_{-i[2N]} - \Delta t \sum_{\substack{j=0\\j\neq -i[2N]}}^{2N-1} K^L(s_i, t_j; \varepsilon)\mu_j = f(s_i)$$

for $i \in [0, 2N - 1]$. Using Eq. (18), we relieve the trapezoid rule from having to approximate the underlying nearly singular behavior coming from K^L . It is in this way that we expect this modification to help in computing solutions of Eq. (11).

Figure 3 shows results for the relative error made by the MTR to solve Eq. (11) using 2N = 64 quadrature points, and two different sources: $f(s) = \cos(4s)$, and $f(s) = \sin(5s)$. For comparison, we include the relative error made by the PTR and by the Quadrature by Parity Asymptotic eXpansions (QPAX) described below, with the same number of quadrature points. Results show that the MTR works well when f is even (in the sense of Definition 1) where the relative error exhibits an $\mathcal{O}(\varepsilon)$ behavior as $\varepsilon \to 0^+$ (following the expected order from Eq. (17)). However when f is odd, the relative error is large and comparable to PTR for all values of ε . Thus, the MTR is only effective for solving Eq. (11) when f is even.

3.3. Quadrature by parity asymptotic expansions (QPAX). It is clear from previous results that we must explicitly take into account the qualitative differences between even and odd boundary data to fully address the nearly singular behavior of K^L . In what follows, we develop a numerical method based on the asymptotic expansions for even and odd parities. We call this new method Quadrature by Parity Asymptotic expansions (QPAX).

We now rewrite Eq. (11) as $\mathscr{L}[\mu](s) = f(s)$, with $\mathscr{L}[\mu](s) = \left(\frac{1}{2}I - \mathscr{K}^L\right)[\mu](s)$, and

(19)
$$\mathscr{K}^{L}[\mu](s) := \int_{\mathbb{T}} K^{L}(s, t; \varepsilon) \mu(t) \, \mathrm{d}t, \quad s \in \mathbb{T}.$$

We write a formal asymptotic expansion of the operator $\mathscr{L} \sim \sum_{q \in \mathbb{N}} \varepsilon^q \mathscr{L}_q$ as $\varepsilon \to 0^+$. Using standard matched asymptotic techniques, one obtains the following result (the proof is given in Appendix B.1) [8]:

Lemma 2. The integral operator \mathscr{K}^L admits the following expansion $\mathscr{K}^L[\mu] = \mathscr{K}_0^L[\mu] + \varepsilon \mathscr{K}_1^L[\mu] + \phi(\varepsilon)$, for $\mu \in \mathscr{C}^2(\mathbb{T})$, where

$$\mathscr{K}_{0}^{L}[\mu](s) = -\frac{1}{2}\mu(\pi - s) \quad and \quad \mathscr{K}_{1}^{L}[\mu](s) = -\frac{1}{2\pi}\int_{\mathbb{T}}\mathsf{E}_{\pi - s}[\mu](t)\,\mathrm{d}t$$

with $(s,t) \mapsto \mathsf{E}_s[\mu](t) \in \mathscr{C}(\mathbb{T}^2)$ defined by

(20)
$$\mathsf{E}_{s}[\mu](t) = \begin{cases} \frac{\mu(s+t) - 2\mu(s) + \mu(s-t)}{2(1-\cos(t))} & \text{if } t \neq 0 [2\pi] \\ \mu''(s) & \text{if } t = 0 [2\pi] \end{cases}.$$

Lemma 2 requires at least \mathscr{C}^2 regularity for μ to define the continuous function E_s in Eq. (20) (which we will assume for the rest of the paper). Using Lemma 2, we obtain

(21)
$$\mathscr{L}_0[\mu](s) = \frac{\mu(s) + \mu(\pi - s)}{2}$$
 and $\mathscr{L}_1[\mu](s) = \frac{1}{2\pi} \int_{\mathbb{T}} \mathsf{E}_{\pi - s}[\mu](t) \, \mathrm{d}t.$

From Eq. (21), we directly have $\mathscr{L}_0[\mu] = \mu_{\text{ev}}$ and $\mathscr{C}_{\text{od}}(\mathbb{T}) \subset \ker(\mathscr{L}_0)$, therefore $\mathscr{L}_0[\mu] = f$ is ill-posed for $f \in \mathscr{C}(\mathbb{T})$. If we assume that the right-hand side $f = \sum_{q \in \mathbb{N}} \varepsilon^q f_q$ and the density $\mu = \sum_{q \in \mathbb{N}} \varepsilon^q \mu_q$ have a smooth expansion, we will only be able to solve for the even part. For the odd part, the solution is not smooth as $\varepsilon \to 0^+$ and we need to consider a different asymptotic expansion. This change is also motivated by the fact that the analytical solution given in Eq. (14) admits an odd part of order ε^{-1} as $\varepsilon \to 0^+$. To take this limit behavior into account, we use the following two asymptotic expansions for the even and odd parts of $\mu = \mu_{\text{ev}} + \mu_{\text{od}}$:

$$\mu_{\mathsf{ev}} = \sum_{q \in \mathbb{N}} \varepsilon^q \, \mu_q^{\mathsf{ev}} \quad \text{and} \quad \mu_{\mathsf{od}} = \frac{1}{\varepsilon} \, \mu_{-1}^{\mathsf{od}} + \sum_{q \in \mathbb{N}} \varepsilon^q \, \mu_q^{\mathsf{od}}.$$

One can show that the operator \mathscr{L} preserves even and odd parity: $(\mathscr{L}[\mu])_{\text{ev/od}} = \mathscr{L}[\mu_{\text{ev/od}}]$. Using this result, we then substitute these expansions into $\mathscr{L}[\mu_{\text{ev}} + \mu_{\text{od}}] = \sum_{q \in \mathbb{N}} \varepsilon^q (f_q^{\text{ev}} + f_q^{\text{od}})$, and obtain to leading order

(22)
$$\mathscr{L}_0[\mu_0^{\text{ev}}] = f_0^{\text{ev}}, \qquad \mathscr{L}_0[\mu_1^{\text{ev}}] + \mathscr{L}_1[\mu_0^{\text{ev}}] = f_1^{\text{ev}}, \quad \text{and} \quad \mathscr{L}_1[\mu_{-1}^{\text{od}}] = f_0^{\text{od}}.$$

The operator \mathscr{L}_0 is invertible on $\mathscr{C}_{ev}(\mathbb{T})$ (it is the identity operator). The nullspace of \mathscr{L}_1 is simply the set of constant functions (see Lemma 6). Therefore \mathscr{L}_1 is invertible on $\mathscr{C}_{od}(\mathbb{T})$. Using Eq. (22), we get

$$\mu_0^{\mathsf{ev}} = f_0^{\mathsf{ev}}, \qquad \mu_1^{\mathsf{ev}} = f_1^{\mathsf{ev}} - \mathscr{L}_1[f_0^{\mathsf{ev}}], \quad \text{and} \quad \mu_{-1}^{\mathsf{od}} = (\mathscr{L}_1)^{-1}[f_0^{\mathsf{od}}].$$

In practice we compute the approximation $\mu \simeq \mu^{\text{asy}} = \mu^{\text{asy}}_{\text{ev}} + \mu^{\text{asy}}_{\text{od}}$ with

(23)
$$\mu_{\mathsf{ev}}^{\mathsf{asy}} = f_{\mathsf{ev}} - \varepsilon \, \mathscr{L}_1[f_{\mathsf{ev}}] \quad \text{and} \quad \mu_{\mathsf{od}}^{\mathsf{asy}} = \frac{1}{\varepsilon} \, (\mathscr{L}_1)^{-1}[f_{\mathsf{od}}].$$

Based on the chosen ansatz, we anticipate the following relative errors:

$$\frac{\|\mu_{\mathsf{ev}} - \mu_{\mathsf{ev}}^{\mathrm{asy}}\|_{\mathrm{L}^{\infty}(\mathbb{T})}}{\|\mu_{\mathsf{ev}}\|_{\mathrm{L}^{\infty}(\mathbb{T})}} = \mathcal{O}\left(\varepsilon^{2}\right) \quad \text{and} \quad \frac{\|\mu_{\mathsf{od}} - \mu_{\mathsf{od}}^{\mathrm{asy}}\|_{\mathrm{L}^{\infty}(\mathbb{T})}}{\|\mu_{\mathsf{od}}\|_{\mathrm{L}^{\infty}(\mathbb{T})}} = \mathcal{O}\left(\varepsilon\right).$$

We now turn to the discretization, for which we will need to separate even and odd parts. From Lemma 6, we find that for any $m \in \mathbb{Z}$,

$$\mathcal{L}_1 [\cos(mt)](s) = (-1)^{m+1} m \cos(ms), \quad \mathcal{L}_1 [\sin(mt)](s) = (-1)^m m \sin(ms).$$

Using these two relations, we define the discretized operators \mathbb{L}_1^{ev} and \mathbb{L}_1^{od} as follows. Given 2N uniformly spaced grid points starting at $-\frac{\pi}{2}$ (bottom of the narrow ellipse), one can simply use the half grid to define the even and odd parts. Let C_{N+1} denote the $(N+1)\times(N+1)$ matrix corresponding to the discrete cosine transform with the following entries,

$$(\mathsf{C}_{N+1})_{i,0} = \sqrt{\frac{2}{N}} \frac{1}{2}, \qquad (\mathsf{C}_{N+1})_{i,j} = \sqrt{\frac{2}{N}} \cos\left(\frac{ij\pi}{N}\right), \qquad (\mathsf{C}_{N+1})_{i,N} = \sqrt{\frac{2}{N}} \frac{(-1)^i}{2},$$

for $(i,j) \in [0,N]^2$. In terms of C_{N+1} , we define \mathbb{L}_1^{ev} according to

(24)
$$\mathbb{L}_{1}^{ev} = \mathsf{C}_{N+1} \operatorname{diag}(0, 1, \dots, N) \; \mathsf{C}_{N+1}.$$

Let S_{N-1} denote the $(N-1) \times (N-1)$ matrix corresponding to the discrete sine transform with entries

$$(\mathsf{S}_{N-1})_{i,j} = \sqrt{\frac{2}{N}} \sin\left(\frac{ij\pi}{N}\right),$$

for $(i,j) \in [1,N-1]^2$. In terms of S_{N-1} , we define $\mathbb{L}_1^{\sf od}$ according to

(25)
$$\mathbb{L}_{1}^{\text{od}} = \mathsf{S}_{N-1} \operatorname{diag}(-1, -2, \dots, -(N-1)) \; \mathsf{S}_{N-1}$$

We now use these asymptotic results to develop a numerical method to solve Eq. (11). Given the Dirichlet boundary data f, we first compute the vectors,

$$\boldsymbol{f}_{N+1}^{\text{ev}} = (f_{\text{ev}}(s_i))_{i \in [\![0,N]\!]} = \left(\frac{1}{2}f(s_i) + \frac{1}{2}f(\pi - s_i)\right)_{i \in [\![0,N]\!]},$$

and

$$\boldsymbol{f}_{N-1}^{\text{od}} = (f_{\text{od}}(s_i))_{i \in [\![1,N-1]\!]} = \left(\frac{1}{2}f(s_i) - \frac{1}{2}f(\pi - s_i)\right)_{i \in [\![1,N-1]\!]},$$

where $s_i = i\Delta t - \frac{\pi}{2}$, $i \in [0, 2N - 1]$, are the PTR quadrature points. Next, we compute the numerical approximation of Eq. (23) through evaluation of

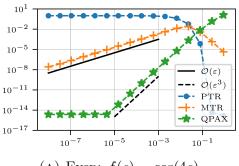
$$\boldsymbol{\mu}_{N+1}^{\mathsf{ev}} = \boldsymbol{f}_{N+1}^{\mathsf{ev}} - \varepsilon \, \mathbb{L}_1^{\mathsf{ev}} \boldsymbol{f}_{N+1}^{\mathsf{ev}} \quad \text{and} \quad \boldsymbol{\mu}_{N-1}^{\mathsf{od}} = \varepsilon^{-1} \, \left(\mathbb{L}_1^{\mathsf{od}} \right)^{-1} \boldsymbol{f}_{N-1}^{\mathsf{od}}.$$

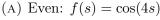
With these results, we compute the approximation

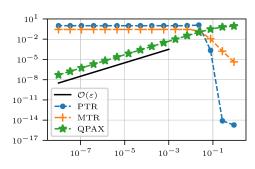
(26)
$$\mu(s_i) \approx \begin{cases} \left(\boldsymbol{\mu}_{N+1}^{\text{ev}}\right)_i & i = 0, N \\ \left(\boldsymbol{\mu}_{N+1}^{\text{ev}}\right)_i + \left(\boldsymbol{\mu}_{N-1}^{\text{od}}\right)_i & i \in \llbracket 1, N - 1 \rrbracket, \\ \left(\boldsymbol{\mu}_{N+1}^{\text{ev}}\right)_{2N-i} + \left(\boldsymbol{\mu}_{N-1}^{\text{od}}\right)_{2N-i} & i \in \llbracket N + 1, 2N - 1 \rrbracket. \end{cases}$$

We denote μ_{2N} to be the 2N vector whose entries are given by Eq. (26).

In Fig. 3 we show the relative error, $\|\boldsymbol{\mu}_{2N} - \boldsymbol{\mu}_{\text{ana}}\|_{\infty} / \|\boldsymbol{\mu}_{\text{ana}}\|_{\infty}$ (with $\boldsymbol{\mu}_{\text{ana}}$ the vector denoting discrete analytic solution at the quadrature points computed via Eq. (14)) as a function of ε using PTR, MTR, and QPAX to compute the solution of Eq. (11). All codes are publicly available on Github [22]. For these results, the number of quadrature points for all methods is 2N = 64. The results in the left plot are for the even source $f(s) = \cos(4s)$ and the results in the right plot are for the odd source $f(s) = \sin(5s)$. Results indicate, as expected, that the error made by QPAX is $\mathcal{O}(\varepsilon^2)$ for an even source and $\mathcal{O}(\varepsilon)$ for an odd source. For the considered even sources, we have taken the two-term asymptotic approximation in Eq. (23) which leads to the $\mathcal{O}(\varepsilon^3)$ because the second-order term vanishes. From the parity asymptotic expansions we found that the odd part contributes globally to the nearly singular behavior. It is the reason why the MTR (based only on local inner expansion) fails for odd sources.







(B) Odd: $f(s) = \sin(5s)$

FIGURE 3. Results for relative error as a function of ε in the numerical solution of the boundary integral equation for the Dirichlet problem for Laplace's equation in a high aspect ratio ellipse for PTR (blue curves with " \bullet " symbols), MTR (orange curves with "+" symbols), and QPAX (green curves with " \star " symbols). All of these results were computed using 2N=64 quadrature points. In the left plot, we show relative error for the even source $f(s)=\cos(4s)$ and in the right plot, we show relative error results for the odd source $f(s)=\sin(5s)$. The solid black line represents the $\mathcal{O}(\varepsilon)$ convergence slope and the dashed black line represents the $\mathcal{O}(\varepsilon^3)$ convergence slope.

Remark 3. For simplicity, we have explicitly used a spectral decomposition to discretize the operator \mathcal{L}_1 . This is obtained using Lemma 6. Other discretizations are possible as long as we split the expansion as in Eq. (23). For example Chebyshev nodes on interval $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ may be appropriate since the operator \mathcal{L}_1 is diagonalizable on $\mathscr{C}^2_{\text{ev/od}}(\mathbb{T})$.

4. QPAX FOR SCATTERING BY A HIGH ASPECT RATIO ELLIPSE

From the discussion on the Dirichlet problem for Laplace's equation in a high aspect ratio ellipse, we found that it is necessary to consider different asymptotic expansions for the even and odd parts of the solution. We now extend those results to the scattering problem by a sound-hard, high aspect ratio ellipse.

We rewrite Eq. (6) on the high aspect ratio ellipse as $\mathscr{L}^H[u] = u^{\text{in}}$ with $\mathscr{L}^H := \frac{1}{2}I - \mathscr{K}^H$ and the operator $\mathscr{K}^H[\mu](s) = \int_{\mathbb{T}} K(s,t;\varepsilon)\mu(t) \,dt$. Using Eq. (7), we write the kernel of \mathscr{K}^H as $K(s,t;\varepsilon) = H(z_{\varepsilon}(s,t)) \,K^L(s,t;\varepsilon)$ where

$$z_{\varepsilon}(s,t) := k \, r(s,t;\varepsilon) = 2 \, k \, \left| \sin\left(\frac{s-t}{2}\right) \right| \, \sqrt{\cos\left(\frac{s+t}{2}\right)^2 + \varepsilon^2 \sin\left(\frac{s+t}{2}\right)^2},$$

and H denotes the continuous function $H(z) := \frac{i\pi}{2} z H_1^{(1)}(z)$. Although H is continuous, its derivative has a logarithmic singularity at s = t (i.e. z = 0). To address this singularity in the derivative, we use [23, Section. 10.8] to decompose H according to

$$H(z) = \Psi(z) - \frac{z \operatorname{J}_1(z)}{2} \ln \left(\frac{4z^2}{k^2} \right),$$

where Ψ is an analytic function on \mathbb{C} satisfying $\Psi(0) = 1$ and $\Psi'(0) = 0$. Then we split the integral operator according to $\mathscr{K}^H = \mathscr{K}^{\Psi} + \mathscr{K}^{\ln}$ where

(27a)
$$\mathscr{K}^{\Psi}[\mu](s) = \int_{\mathbb{T}} K^{L}(s, t; \varepsilon) \ \Psi(z_{\varepsilon}(s, t)) \ \mu(t) \, \mathrm{d}t,$$

(27b)
$$\mathscr{K}^{\ln}[\mu](s) = -\frac{1}{2} \int_{\mathbb{T}} K^{L}(s,t;\varepsilon) \ z_{\varepsilon}(s,t) \, \mathsf{J}_{1}(z_{\varepsilon}(s,t)) \ln\left(\frac{4z_{\varepsilon}(s,t)^{2}}{k^{2}}\right) \ \mu(t) \, \mathrm{d}t.$$

We now state two useful Lemmas.

Lemma 4. The integral operator \mathscr{K}^{Ψ} defined in Eq. (27a) admits the expansion $\mathscr{K}^{\Psi}[\mu] = \mathscr{K}_0^{\Psi}[\mu] + \varepsilon \mathscr{K}_1^{\Psi}[\mu] + o(\varepsilon)$, for $\mu \in \mathscr{C}^2(\mathbb{T})$, where

$$\mathscr{K}_{0}^{\Psi}[\mu](s) = -\frac{1}{2}\mu(\pi - s) \quad and \quad \mathscr{K}_{1}^{\Psi}[\mu](s) = -\frac{1}{2\pi}\int_{\mathbb{T}}\mathsf{E}_{\pi - s}[\psi_{s}\,\mu](t)\,\mathrm{d}t$$

with $\psi_s(t) = \Psi\left(2k \left|\sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right)\right|\right)$, and E_s defined in Eq. (20).

Lemma 5. The integral operator \mathcal{K}^{\ln} defined in Eq. (27b) admits the expansion $\mathcal{K}^{\ln}[\mu] = \varepsilon \mathcal{K}_1^{\ln}[\mu] + \phi(\varepsilon)$, for $\mu \in \mathscr{C}^2(\mathbb{T})$, where

$$\mathscr{K}_1^{\ln}[\mu](s) = \frac{1}{2\pi} \int_{\mathbb{T}} \left[\phi_s \,\mu\right]_{\mathsf{ev}}(t) \,\ln\left(4\sin\left(\frac{s-t}{2}\right)^2\right) \mathrm{d}t$$

with

(28)
$$\phi_{s}(t) = \begin{cases} k \left| \frac{\sin\left(\frac{s-t}{2}\right)}{\cos\left(\frac{s+t}{2}\right)} \right| J_{1}\left(2k \left| \sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right) \right|\right) & \text{if } t \not\equiv \pi - s\left[2\pi\right] \\ 2k^{2} \sin\left(\frac{s-t}{2}\right)^{2} & \text{if } t \equiv \pi - s\left[2\pi\right] \end{cases}.$$

The proof of the expansion of \mathcal{K}^{Ψ} , \mathcal{K}^{\ln} , defined in Eq. (27a), Eq. (27b), can be found in Appendix B.2, Appendix B.3, respectively. Using Lemma 4 and Lemma 5 we can write the asymptotic expansion of the integral operator $\mathcal{L}^{H} = \mathcal{H}_{0} + \varepsilon \mathcal{H}_{1} + o(\varepsilon)$ where

(29a)
$$\mathscr{H}_0[\mu](s) = \frac{\mu(s) + \mu(\pi - s)}{2} = \mu_{\text{ev}}(s)$$

(29b)
$$\mathscr{H}_1[\mu](s) = \frac{1}{2\pi} \int_{\mathbb{T}} \mathsf{E}_{\pi-s}[\psi_s \, \mu](t) \, \mathrm{d}t - \frac{1}{2\pi} \int_{\mathbb{T}} [\phi_s \, \mu]_{\mathsf{ev}} \ln\left(4\sin\left(\frac{s-t}{2}\right)^2\right) \, \mathrm{d}t.$$

Similar to the Dirichlet problem for the Laplace's equation, we have $\ker(\mathscr{H}_0) = \mathscr{C}_{\sf od}(\mathbb{T})$ and the leading order problem $\mathscr{H}_0[u] = u^{\sf in}$ is not well-posed on $\mathscr{C}(\mathbb{T})$. As a consequence we need to separate the even and odd terms to solve $\mathscr{L}^H[u] = u^{\sf in}$. We write the source term as $f(s) = u^{\sf in}(y(s)) = u^{\sf in}(\varepsilon \cos(s), \sin(s))$, and we expand $f = f_{\sf ev} + f_{\sf od}$ with $f_{\sf ev} = \sum_{q \in \mathbb{N}} \varepsilon^q f_q^{\sf ev}(s)$ and $f_{\sf od} = \sum_{q \in \mathbb{N}} \varepsilon^q f_q^{\sf od}(s)$. To highlight the parity scales, we write as before $u = u_{\sf ev} + u_{\sf od}$ with the ansatz

(30)
$$u_{\text{ev}} = \sum_{q \in \mathbb{N}} \varepsilon^q u_q^{\text{ev}} \quad \text{and} \quad u_{\text{od}} = \frac{1}{\varepsilon} u_{-1}^{\text{od}} + \sum_{q \in \mathbb{N}} \varepsilon^q u_q^{\text{od}}$$

as $\varepsilon \to 0^+$. For the high aspect ratio ellipse, the expansions of the source term give us

(31a)
$$f_0^{\text{ev}}(s) = u^{\text{in}}(0, \sin(s)), \qquad f_1^{\text{ev}}(s) = 0,$$

(31b)
$$f_0^{\text{od}}(s) = 0,$$
 $f_1^{\text{od}}(s) = \cos(s) \, \partial_x u^{\text{in}}(0, \sin(s)).$

Contrary to Laplace's problem, the scattering problem is always well-posed, we know that $u_{-1}^{\text{od}} \equiv 0$, and $f_0^{\text{od}} \equiv 0$ is expected. However ill-posedness of the asymptotic problem as $\varepsilon \to 0^+$ remains (but it is subtle): note that the leading order term of f_{od} is $\mathcal{O}(\varepsilon)$ while the one for u_{od} is $\mathcal{O}(1)$. It is the reason why we still shift the power index of ε . To obtain leading behavior of the solution of $\mathscr{L}^H[u] = u^{\text{in}}$, we replace \mathscr{L}^H by $\mathscr{H}_0 + \varepsilon \mathscr{H}_1$, substitute the expansions for u_{ev} and u_{od} defined Eq. (30), and use the fact that \mathscr{L}^H (and consequently $\mathscr{H}_0, \mathscr{H}_1$) preserves parity. In the end we obtain similar equations as Eq. (22): $\mathscr{H}_0[u_0^{\text{ev}}] = f_0^{\text{ev}}, \mathscr{H}_0[u_1^{\text{ev}}] = -\mathscr{H}_1[f_0^{\text{ev}}]$, and $\mathscr{H}_1[u_0^{\text{od}}] = f_1^{\text{od}}$. In practice we simply to compute

(32a)
$$u_{\text{ev}}^{\text{asy}}(s) = u^{\text{in}}(0, \sin(s)) - \varepsilon \,\mathcal{H}_1\left[u^{\text{in}}(0, \sin(s))\right],$$

(32b)
$$u_{\text{od}}^{\text{asy}}(s) = \mathcal{H}_1^{-1} \left[\cos(s) \, \partial_x u^{\text{in}}(0, \sin(s)) \right],$$

we obtain an asymptotic approximation $u \simeq u^{\rm asy} = u^{\rm asy}_{\rm ev} + u^{\rm asy}_{\rm od}$ in the limit as $\varepsilon \to 0^+$, whose error is $\phi(\varepsilon)$. As for the Laplace case, we anticipate the following relative errors:

$$\frac{\|u_{\mathsf{ev}} - u_{\mathsf{ev}}^{\mathsf{asy}}\|_{\mathsf{L}^{\infty}(\mathbb{T})}}{\|u_{\mathsf{ev}}\|_{\mathsf{L}^{\infty}(\mathbb{T})}} = \mathcal{O}\left(\varepsilon^{2}\right) \quad \text{and} \quad \frac{\|u_{\mathsf{od}} - u_{\mathsf{od}}^{\mathsf{asy}}\|_{\mathsf{L}^{\infty}(\mathbb{T})}}{\|u_{\mathsf{od}}\|_{\mathsf{L}^{\infty}(\mathbb{T})}} = \mathcal{O}\left(\varepsilon\right).$$

We now introduce a numerical method for computing Eq. (32). This method modifies the product Gaussian quadrature rule by Kress [17] for two-dimensional scattering problems. Using the PTR quadrature points $s_n = t_n = n\Delta t - \pi/2$ for $n \in [0, 2N - 1]$ with $\Delta t = \pi/N$, Kress' Gaussian product quadrature rule (PQR) is given by

(33)
$$\int_{\mathbb{T}} K(s_i, t; \varepsilon) u(t) dt \approx \sum_{j=0}^{2N-1} \left[R_{|N-j|}^{(N)} K_1(s_i, t_j) + \Delta t K_2(s_i, t_j) \right] u_j,$$

with

$$K_1(s,t;\varepsilon) = -\frac{1}{2}z_{\varepsilon}(s,t) J_1(z_{\varepsilon}(s,t))K^L(s,t;\varepsilon),$$

and

$$K_2(s,t;\varepsilon) = \frac{1}{2} z_{\varepsilon}(s,t) \left[i\pi \, \mathsf{H}_1^{(1)}(z_{\varepsilon}(s,t)) + \mathsf{J}_1(z_{\varepsilon}(s,t)) \ln \left(4 \sin \left(\frac{s-t}{2} \right)^2 \right) \right] K^L(s,t;\varepsilon).$$

Here, J_1 is the Bessel function of first kind and of order one and K^L is given in Eq. (8). The quadrature weights in Eq. (33) are given by

(34)
$$R_k^{(N)} := -\frac{(-1)^k \pi}{N^2} - \frac{2\pi}{N} \sum_{m=1}^{N-1} \frac{1}{m} \cos\left(\frac{mk\pi}{N}\right), \quad k \in [0, N].$$

Using this quadrature rule within a Nyström method to solve Eq. (6), we obtain

(35)
$$\frac{1}{2}u_i - \sum_{j=0}^{2N-1} \left[R_{|N-j|}^{(N)} K_1(s_i, t_j) + \frac{\pi}{N} K_2(s_i, t_j) \right] u_j = u^{\mathsf{in}}(s_i), \quad i \in [0, 2N-1].$$

This PQR explicitly addresses the weak singularity in the derivative in K on s = t due to the Hankel function $\mathsf{H}_1^{(1)}$. However, it does not address the nearly singular behavior due to K^L , so we do not expect it to work well for the high aspect ratio ellipse.

We can easily modify the PQR method to include the modification we derived in Section 3.2 based on the asymptotic expansion for K^L . First, we observe that $K_1 = \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0^+$, so it does not exhibit any nearly singular behavior. Consequently, we do not need to modify that part of the PQR. However, K_2 exhibits a nearly singular behavior as $\varepsilon \to 0^+$, so we write

$$\int_{\mathbb{T}} K_2(s_i, t; \varepsilon) u(t) dt \approx -\frac{1}{\pi} \arctan\left(\frac{\Delta t}{4\varepsilon}\right) u_{-i[2N]} + \Delta t \sum_{\substack{j=0\\j \neq -i[2N]}}^{2N-1} K_2(s_i, t_j; \varepsilon) u_j.$$

Incorporating this modification into the Nyström method into Eq. (35), we obtain

(36)
$$\frac{1}{2}u_{i} - \sum_{j=0}^{2N-1} R_{|N-j|}^{(N)} K_{1}(s_{i}, t_{j})u_{j} + \frac{1}{\pi} \arctan\left(\frac{\Delta t}{4\varepsilon}\right) \mu_{-i [2N]} - \Delta t \sum_{\substack{j=0\\j \neq -i [2N]}}^{2N-1} K_{2}(s_{i}, t_{j}; \varepsilon) u_{j} = u^{\mathsf{in}}(s_{i}),$$

for $i \in [0, 2N - 1]$. We call Eq. (36) the modified product quadrature rule (MPQR). We expect MPQR to fail when considering an odd source term.

We now modify PQR further to extend QPAX to solve Eq. (6). Using Eq. (29), we define the discretized even operator \mathbb{H}_1^{ev} and the discretized odd operator \mathbb{H}_1^{od} as follows. First, we split $\mathbb{H}_1^{\text{ev/od}} = \mathbb{H}_{1,\psi}^{\text{ev/od}} - \mathbb{H}_{1,\ln}^{\text{ev/od}}$ into the two parts corresponding to the two integrals in Eq. (29). As before, we make use of the first half of the quadrature points to create the even and odd discrete operators. The entries for $\mathbb{H}_{1,\psi}^{\text{ev}}$ are given by

$$\left(\mathbb{H}^{\mathrm{ev}}_{1,\psi}\right)_{i,j} = \left(\mathbb{L}^{\mathrm{ev}}_1\right)_{i,j} \, \psi_{s_i}(t_j), \quad (i,j) = [\![0,N]\!]^2,$$

and the entries of $\mathbb{H}_{1,\psi}^{\mathsf{od}}$ are given by

$$(\mathbb{H}_{1,\psi}^{\text{od}})_{i,j} = (\mathbb{L}_1^{\text{od}})_{i,j} \psi_{s_i}(t_j), \quad (i,j) = [1, N-1]^2,$$

with \mathbb{L}_1^{ev} given in Eq. (24) and \mathbb{L}_1^{od} given in Eq. (25). One can check that the entries of $\mathbb{H}_{1,\ln}^{\text{ev/od}}$ are given by

$$\left(\mathbb{H}_{1,\ln}^{\text{ev}}\right)_{i,j} = \left(W_{N+1}^{\text{ev}}\right)_{i,j} \frac{\phi_{s_i}(t_j) + \phi_{s_i}(\pi - t_j)}{2}, \qquad (i,j) = [\![0,N]\!]^2,$$

$$\left(\mathbb{H}_{1,\ln}^{\text{od}}\right)_{i,j} = \left(W_{N+1}^{\text{ev}}\right)_{i,j} \frac{\phi_{s_i}(t_j) - \phi_{s_i}(\pi - t_j)}{2} \qquad (i,j) = [1, N-1]^2,$$

respectively, where W_{N+1}^{ev} is the matrix of Kress weights for integrating even functions defined by

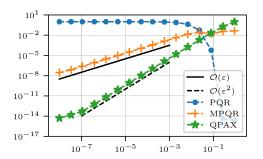
$$W_{N+1}^{\mathsf{ev}} = \mathsf{C}_{N+1} \, \operatorname{diag}\left(0, -\frac{2\pi}{1}, -\frac{2\pi}{2}, \dots, -\frac{2\pi}{N}\right) \, \mathsf{C}_{N+1}$$

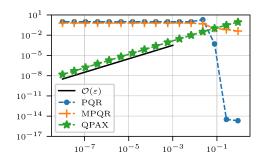
with C_{N+1} denoting the same matrix of the discrete cosine transform used in Eq. (24). As for the Laplace case, from Eq. (32), we obtain the approximation of the unknowns $\boldsymbol{u}_{N+1}^{\text{ev}} \approx (u_{\text{ev}}(s_i))_{i \in \mathbb{I}_{0,N}}$ and $\boldsymbol{u}_{N-1}^{\text{od}} \approx (u_{\text{od}}(s_i))_{i \in \mathbb{I}_{1,N-1}}$ as

$$oldsymbol{u}_{N+1}^{\mathsf{ev}} = oldsymbol{f}_{N+1}^{\mathsf{ev}} - arepsilon \, \mathbb{H}_{1}^{\mathsf{ev}} oldsymbol{f}_{N+1}^{\mathsf{ev}} \quad ext{and} \quad oldsymbol{u}_{N-1}^{\mathsf{od}} = \left(\mathbb{H}_{1}^{\mathsf{od}} \right)^{-1} oldsymbol{f}_{N-1}^{\mathsf{od}}$$

where $\mathbf{f}_{N+1}^{\text{ev}} = \left(u^{\text{in}}(0,\sin(s_i))\right)_{i\in[0,N]}$ and $\mathbf{f}_{N-1}^{\text{od}} = \left(\cos(s_i)\,\partial_x u^{\text{in}}(0,\sin(s_i))\right)_{i\in[1,N-1]}$. Then, we recombine the even and odd parts using Eq. (26) to obtain the approximation vector \mathbf{u}_{2N} .

We now study the relative error $\|\mathbf{u}_{2N} - \mathbf{u}_{\text{ana}}\|_{\infty} / \|\mathbf{u}_{\text{ana}}\|_{\infty}$ (with \mathbf{u}_{ana} the vector denoting discrete analytic solution at the quadrature points computed via Eq. (37)) as a function of ε made by PQR, MQPR, and QPAX. All codes are publicly available on Github [22]. In Fig. 4, we show these relative errors for $u^{\text{in}}(x,y) = \text{Mc}_3^{(1)}(\xi,q) \cos_3(\eta,q)$ which produces a purely even source on the boundary (left plot) and $u^{\text{in}}(x,y) = \text{Ms}_2^{(1)}(\xi,q) \sec_2(\eta,q)$ which produces a purely odd source on the boundary (right plot). For these results, the number of quadrature points is fixed at 2N = 64 for all of the approximations. These results mimic what we had seen for the Dirichlet problem for Laplace's equation in a high aspect ratio ellipse. Here, the PQR approximation produces large errors as $\varepsilon \to 0^+$ because it does not account for the nearly singular behavior of the integral operator for a high aspect ratio ellipse. For an even source, the relative error of the MPQR exhibits an $\mathcal{O}(\varepsilon)$, but it does not work well for an odd source. In contrast, the relative error of the QPAX approximation exhibits, as anticipated, an $\mathcal{O}(\varepsilon^2)$ behavior for the even source and an $\mathcal{O}(\varepsilon)$ behavior for the odd source. Hence, the QPAX approximation effectively addresses the inherent parity in the nearly singular behavior associated with this high aspect ratio ellipse.



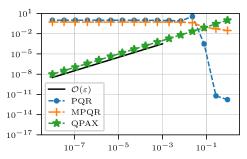


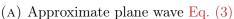
(A) Even source: $u^{\text{in}}(x,y) = \text{Mc}_3^{(1)}(\xi,q) \text{ ce}_3(\eta,q)$ (B) Odd source: $u^{\text{in}}(x,y) = \text{Ms}_2^{(1)}(\xi,q) \text{ se}_2(\eta,q)$

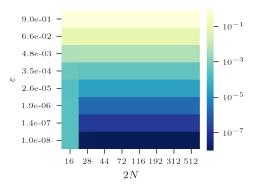
FIGURE 4. Results for relative error as a function of ε in the numerical solution of the boundary integral equation for scattering by a sound-hard, high aspect ratio ellipse for PQR (blue curves with " \bullet " symbols), MPQR (orange curves with "+" symbols), and QPAX (green curves with " \star " symbols). All of these results were computed using 2N=64 quadrature points. The left plot shows results for an incident field that produces an even source on the boundary and the right plot shows results for an incident field that produces an odd source on the boundary. The black line represents the $\mathcal{O}(\varepsilon)$ convergence slope and the dashed black line represents the $\mathcal{O}(\varepsilon^2)$ convergence slope.

Because the relative error for the QPAX approximation for odd parity exhibits an $\mathcal{O}(\varepsilon)$ behavior, we expect that it exhibits an $\mathcal{O}(\varepsilon)$ behavior for a general incident field. To verify that this is indeed true, we show in Fig. 5a the relative error with respect to the infinity norm as a function of ε for the approximate plane wave given by Eq. (3). This incident field has both even and odd components. Again we see that PQR and MPQR do not work well for this problem. In contrast, the relative error exhibited by QPAX is $\mathcal{O}(\varepsilon)$ as expected.

It appears that the QPAX approximation is effective for studying scattering by a high aspect ratio ellipse. Thus, we evaluate its relative error with respect to the infinity norm as a function



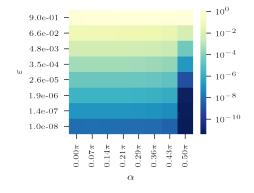


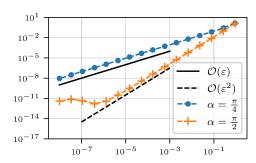


(B) Relative error for QPAX

FIGURE 5. (Left) Relative error as in Fig. 4, but for the approximate plane wave incident field given in Eq. (3). (Right) The relative error for QPAX (log scale) plotted as a function of the number of quadrature points, 2N, and the high aspect ratio parameter, ε , for the approximate plane wave incident field given in Eq. (3).

of ε and 2N in Fig. 5b. Results show the effectiveness of the QPAX approximation over a range of aspect ratios and computational resolutions. The relative error for 2N=16 appears to saturate as $\varepsilon \to 0^+$. For that case, the fields on the boundary are underresolved with that number of quadrature points leading to a dominating aliasing error. For all other cases, we observe that the relative error behaves as $\mathcal{O}(\varepsilon)$ as $\varepsilon \to 0^+$. Results in Fig. 6 show that the performance of the QPAX method does not depend on the direction $d=(\cos(\alpha),\sin(\alpha))$ of the incident field. We consider u^{in} defined in Eq. (3) where we choose $\alpha_m^{\text{in}}=2\,\mathrm{i}^m\,\cos_m(\frac{\pi}{2}-\alpha,q)$ and $\beta_m^{\text{in}}=2\,\mathrm{i}^m\,\sin_m(\frac{\pi}{2}-\alpha,q)$, $\alpha\in[0,\frac{\pi}{2}]$. Note that the choice $\alpha=\frac{\pi}{2}$ is a special case: the incident field is even with respect to the major axis of the ellipse, therefore the odd part of the solution vanishes, leading to an $\mathcal{O}(\varepsilon^2)$ relative error. Thus, the QPAX approximation is highly effective (accurate) and efficient (requiring modest resolution) for scattering problems by a high aspect ratio ellipse.





(B) Plane waves of incidence $\alpha = \left\{\frac{\pi}{4}, \frac{\pi}{2}\right\}$

(A) Relative error for QPAX with respect to α , ε .

FIGURE 6. (Left) Plot of the relative error for the QPAX method with respect to $0 \le \alpha \le \frac{\pi}{2}$, $10^{-8} \le \varepsilon \le 0.9$, and 2N = 64. (Right) Plot of the relative error for the QPAX method with respect to $\alpha = \left\{\frac{\pi}{4}, \frac{\pi}{2}\right\}$, $10^{-8} \le \varepsilon \le 0.9$, and 2N = 64.

5. Conclusions

We have studied two-dimensional sound-hard scattering by a high aspect ratio ellipse using boundary integral equations. In the limit as $\varepsilon \to 0^+$ (where ε^{-1} denotes the aspect ratio), the integral operator in the boundary integral equation exhibits nearly singular behavior corresponding to the collapsing of the ellipse to a line segment. This nearly singular behavior leads to large errors when solving the boundary integral equation.

By performing an asymptotic analysis of the integral operator for a high aspect ratio ellipse we find that two different scalings due to parity are needed to solve the boundary integral equation. By introducing two different asymptotic expansions for even and odd parity solutions, we identify the leading behavior of the solution. We first study the Dirichlet problem for Laplace's equation in a high aspect ratio ellipse to identify these behaviors. Upon determining the correct asymptotic expansions for the different parities, we introduce a numerical method which we call Quadrature by Parity Asymptotic eXpansions (QPAX) that effectively and efficiently solves this problem. We then extend QPAX for the scattering problem.

Our results show that the relative error (defined with respect to the infinity norm) exhibits an $\mathcal{O}(\varepsilon^2)$ behavior for even parity problems, and an $\mathcal{O}(\varepsilon)$ behavior for odd parity problems. Thus, in general, the relative error for QPAX exhibits an $\mathcal{O}(\varepsilon)$ behavior. In contrast, other methods we have used that do not explicitly take into account the parity of solutions may or may not work for even parity problems, but do not work for odd parity problems.

By identifying the different asymptotic behaviors due to parity and developing an effective and efficient method to compute them, we have identified and addressed an elementary issue in scattering by high aspect ratio particles. While we have concentrated our efforts on the sound-hard problem, one can easily extend our method to sound-soft, and penetrable obstacles. What we have found here will certainly play an important role in any extensions to three-dimensional problems involving general high aspect ratio particle shapes, for example. It is for these reasons that we believe that this analysis is useful for the study of scattering by high aspect ratio particles.

APPENDIX A. ANALYTICAL SOLUTION FOR SCATTERING BY A SOUND-HARD ELLIPSE

Boundary value problem Eq. (1) can be solved analytically as follows. We define the elliptical coordinates $(\xi, \eta) \in \mathbb{R}_+^* \times \mathbb{T}$ as

$$x = c_{\varepsilon} \sinh(\xi) \sin(\eta)$$
 and $y = c_{\varepsilon} \cosh(\xi) \cos(\eta)$,

where $c_{\varepsilon} = \sqrt{1 - \varepsilon^2}$ is a parameter defining the focus of the ellipse. The boundary in these coordinates is $\{\xi_{\varepsilon}\} \times \mathbb{T}$, where $\xi_{\varepsilon} = \operatorname{artanh}(\varepsilon)$. Using these elliptical coordinates, the Helmholtz equation becomes

$$(\partial_{\xi\xi} + \partial_{\eta\eta})u^{\mathsf{sc}} + \frac{c_{\varepsilon}^2 k^2}{2}(\cosh(2\xi) - \cos(2\eta))u^{\mathsf{sc}} = 0,$$

it admits two sets of solutions: $\{\mathsf{Mc}_m^{(i)}(\xi,q)\,\mathsf{ce}_m(\eta,q)\}_{m\geq 0}$, $\{\mathsf{Ms}_m^{(i)}(\xi,q)\,\mathsf{se}_m(\eta,q)\}_{m\geq 1}$ with $q=c_\varepsilon^2k^2/4$ and m integer. Here, ce and se denote the angular Mathieu functions of order m, and $\mathsf{Mc}^{(i)}$ and $\mathsf{Ms}^{(i)}$ denote the radial Mathieu function of order m and i^{th} -kind. Using [23, Sec. 28.20(iii)], we find that only $\mathsf{Mc}_m^{(3)}$ and $\mathsf{Ms}_m^{(3)}$ satisfy the Sommerfeld radiation condition. Thus, the scattered field is given by

(37)
$$u^{\text{sc}}(\xi, \eta) = \sum_{m=0}^{\infty} \alpha_m \operatorname{Mc}_m^{(3)}(\xi, q) \operatorname{ce}_m(\eta, q) + \sum_{m=1}^{\infty} \beta_m \operatorname{Ms}_m^{(3)}(\xi, q) \operatorname{se}_m(\eta, q),$$

with the coefficients α_m and β_m to determine by requiring a sound-hard boundary condition on ∂D to be satisfied. For a given incident field, $u^{\text{in}}(\xi_{\varepsilon}, \eta)$, we have for the sound-hard problem,

$$\alpha_m = \frac{-1}{\operatorname{Mc}_m^{(3)}{}'(\xi_\varepsilon,q)\,\pi} \int_0^{2\pi} \sqrt{\sin(\eta)^2 + \varepsilon^2 \mathrm{cos}(\eta)^2} \,\partial_n u^{\mathrm{in}}(\xi_\varepsilon,\eta) \,\operatorname{ce}_m(\eta,q) \,\mathrm{d}\eta$$

and

$$\beta_m = \frac{-1}{\mathsf{Ms}_{\bullet}^{(3)'}(\xi_{\varepsilon}, q) \, \pi} \int_0^{2\pi} \sqrt{\sin(\eta)^2 + \varepsilon^2 \mathrm{cos}(\eta)^2} \, \partial_n u^{\mathsf{in}}(\xi_{\varepsilon}, \eta) \, \mathsf{se}_m(\eta, q) \, \mathrm{d}\eta.$$

APPENDIX B. MATCHED ASYMPTOTIC EXPANSIONS

In this Appendix we provide matched asymptotic expansions of the double-layer potential for Laplace and Helmholtz equation.

B.1. Proof of Lemma 2.

Proof. We rewrite Eq. (19) as

$$\mathscr{K}^{L}[\mu](s) = -\frac{\varepsilon}{2\pi} \int_{-s}^{2\pi - s} \frac{\mu(t)}{1 + \varepsilon^2 - (1 - \varepsilon^2)\cos(s + t)} \,\mathrm{d}t,$$

so that when using the change of variable $t = \pi - s + x$ we have

$$\mathscr{K}^{L}[\mu](s) = -\frac{\varepsilon}{2\pi} \int_{-\pi}^{\pi} \frac{\mu(\pi - s + x)}{1 + \varepsilon^2 - (1 - \varepsilon^2)\cos(x)} \, \mathrm{d}x.$$

The above operator is then a nearly singular integral about $x \equiv 0$ [2π]. Introducing $\delta > 0$ such that $\varepsilon = \phi(\delta)$, we split the integral $\mathcal{K}^L[\mu](s) = \mathcal{K}^{\text{inn}}[\mu](s) + \mathcal{K}^{\text{out}}[\mu](s)$ with

(38a)
$$\mathscr{K}^{\text{inn}}[\mu](s) := \frac{-\varepsilon}{2\pi} \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \frac{\mu(\pi - s + x)}{1 + \varepsilon^2 - (1 - \varepsilon^2)\cos(x)} \, \mathrm{d}x,$$

(38b)
$$\mathscr{K}^{\text{out}}[\mu](s) := \frac{-\varepsilon}{2\pi} \int_{I_{\delta}} \frac{\mu(\pi - s + x)}{1 + \varepsilon^2 - (1 - \varepsilon^2)\cos(x)} \, \mathrm{d}x,$$

with $I_{\delta} = (-\pi, \pi) \setminus \left(-\frac{\delta}{2}, \frac{\delta}{2}\right)$ and we look for the leading order terms of the above integrals as $\delta, \varepsilon \to 0^+$. Note that the inner term $\mathscr{K}^{\text{inn}}[\mu](s) = I_{\delta}(\varepsilon)$ defined in Section 3.2, then following the same procedure (using the change of variable $x = \varepsilon X$ and expanding about $\varepsilon = 0$ then $\delta = 0$), we obtain

(39)
$$\mathcal{K}^{\text{inn}}[\mu](s) = -\frac{1}{\pi} \arctan\left(\frac{\delta}{4\varepsilon}\right) \mu(\pi - s) + \mathcal{O}(\delta\varepsilon)$$
$$= -\frac{1}{2}\mu(\pi - s) + \frac{4}{\pi}\mu(\pi - s)\frac{\varepsilon}{\delta} + \mathcal{O}\left(\frac{\varepsilon^{3}}{\delta^{3}}\right) + \mathcal{O}(\delta\varepsilon).$$

For the outer term $\mathcal{K}^{\text{out}}[\mu](s)$, we first expand the integrand for $x \not\equiv 0$ [2 π], leading to

$$\mathcal{K}^{\text{out}}[\mu](s) = \frac{-\varepsilon}{2\pi} \int_{I_{\delta}} \frac{\mu(\pi - s + x)}{1 - \cos(x)} \left[1 + \mathcal{O}\left(\frac{\varepsilon^{2}}{\tan(\frac{x}{2})^{2}}\right) \right] dx$$

$$= \frac{-\varepsilon}{2\pi} \int_{I_{\delta}} \frac{\mu(\pi - s + x)}{1 - \cos(x)} dx + \mathcal{O}\left(\frac{\varepsilon^{3}}{\delta^{3}}\right).$$
(40)

Let us note that $x \mapsto (1 - \cos(x))^{-1}$ is an even function (in the classic sense) over I_{δ} . We define $\nu(x) = \mu(\pi - s + x)$ and we split $\nu = \nu_{+} + \nu_{-}$ into its *classic* even and odd parts $\nu_{\pm} = \frac{1}{2}(\nu(x) \pm \nu(-x))$, we then obtain

$$\begin{split} \int_{I_{\delta}} \frac{\nu(x)}{1 - \cos(x)} \, \mathrm{d}x &= \int_{I_{\delta}} \frac{\nu_{+}(x)}{1 - \cos(x)} \, \mathrm{d}x \\ &= \nu_{+}(0) \int_{I_{\delta}} \frac{1}{1 - \cos(x)} \, \mathrm{d}x + \int_{I_{\delta}} \frac{\nu_{+}(x) - \nu_{+}(0)}{1 - \cos(x)} \, \mathrm{d}x \\ &= \frac{2\nu_{+}(0)}{\tan(\frac{\delta}{4})} + \int_{I_{\delta}} \frac{\nu_{+}(x) - \nu_{+}(0)}{1 - \cos(x)} \, \mathrm{d}x \end{split}$$

Note that $\mathsf{E}_{\pi-s}[\mu]$ defined in Eq. (20) extends the function

$$x \mapsto \frac{\nu_+(x) - \nu_+(0)}{1 - \cos(x)} = \frac{\mu(\pi - s + x) - 2\mu(\pi - s) + \mu(\pi - s - x)}{2(1 - \cos(x))}$$

to a continuous function in $\mathscr{C}(\mathbb{T})$. We write (using some rescaling and expansion about $\varepsilon = 0$)

$$\int_{I_{\delta}} \frac{\nu_{+}(x) - \nu_{+}(0)}{1 - \cos(x)} dx = \int_{-\pi}^{\pi} \mathsf{E}_{\pi - s}[\mu](x) dx - \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \mathsf{E}_{\pi - s}[\mu](x) dx$$
$$= \int_{-\pi}^{\pi} \mathsf{E}_{\pi - s}[\mu](x) dx + \mathcal{O}(\delta)$$

because $\mathsf{E}_{\pi-s}[\mu]$ is bounded on $\left(-\frac{\delta}{2},\frac{\delta}{2}\right)$. Using the fact that

$$\frac{2}{\tan(\frac{\delta}{4})}\nu_{+}(0) = 8\mu(\pi - s)\frac{1}{\delta} + O(\delta),$$

combining all of the above results we obtain

(41)
$$\mathscr{K}^{\text{out}}[\mu](s) = -\frac{4}{\pi}\mu(\pi - s)\frac{\varepsilon}{\delta} - \frac{\varepsilon}{2\pi} \int_{-\pi}^{\pi} \mathsf{E}_{\pi - s}[\mu](x) \, \mathrm{d}x + \mathcal{O}\left(\frac{\varepsilon^3}{\delta^3}\right) + \mathcal{O}(\delta\varepsilon).$$

Finally plugging Eq. (39) and Eq. (41) into $\mathscr{K}^{L}[\mu](s)$, and choosing δ such that $\mathcal{O}\left(\frac{\varepsilon^{3}}{\delta^{3}}\right) + \mathcal{O}(\delta\varepsilon) = \mathcal{O}(\varepsilon)$ (for example $\delta = \sqrt{\varepsilon}$) we obtain

$$\mathscr{K}^{L}[\mu](s) = -\frac{1}{2}\mu(\pi - s) - \frac{\varepsilon}{2\pi} \int_{-\pi}^{\pi} \mathsf{E}_{\pi - s}[\mu](x) \, \mathrm{d}x + \mathcal{O}(\varepsilon).$$

B.2. Proof of Lemma 4.

Proof. We have the expansion

(42)
$$z_{\varepsilon}(s,t) = \begin{cases} 2k \left| \sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right) \right| + \mathcal{O}(\varepsilon^{2}) & \text{if } s+t \not\equiv \pi \left[2\pi\right] \\ 2k \left|\cos(s)\right| \varepsilon & \text{if } s+t \equiv \pi \left[2\pi\right] \end{cases}$$

using $\Psi'(0) = 0$, we get $\Psi(z_{\varepsilon}(s,t)) = \Psi\left(2k \left|\sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right)\right|\right) + \mathcal{O}(\varepsilon^2)$. Then, we obtain $\mathscr{K}^{\Psi}[\mu](s) = \mathscr{K}^{L}[\Psi\left(2k \left|\sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right)\right|\right)\mu](s) + \mathcal{O}\left(\varepsilon^2\mathscr{K}^{L}[\mu](s)\right)$, then we apply Lemma 2 to \mathscr{K}^{L} and use $\Psi(0) = 1$ to finish the proof.

Lemma 6. Consider \mathcal{L}_1 defined in Eq. (21). For all $m \in \mathbb{Z}$, we have

$$\mathscr{L}_1[e^{imt}](s) = -|m| e^{im(\pi-s)}.$$

Proof. From the expression of Eq. (21), we obtain

$$\mathscr{L}_1[e^{imt}](s) = -\frac{e^{im(\pi - s)}}{2\pi} \int_{\mathbb{T}} \left[\frac{\sin\left(\frac{|m|t}{2}\right)}{\sin\left(\frac{t}{2}\right)} \right]^2 dt.$$

We recognize the Fejér kernel and we get the result using [23, Eq. (1.15.16)].

B.3. Proof of Lemma 5.

Proof. Recall from Eq. (27b) we have

$$\mathscr{K}^{\ln}[\mu](s) = -\frac{1}{2} \int_{\mathbb{T}} K^{L}(s,t;\varepsilon) \ z_{\varepsilon}(s,t) \, \mathsf{J}_{1}(z_{\varepsilon}(s,t)) \ln \left(\frac{4z_{\varepsilon}(s,t)^{2}}{k^{2}} \right) \ \mu(t) \, \mathrm{d}t.$$

We start by showing that $K^L(s,t;\varepsilon)$ $z_{\varepsilon}(s,t)$ $\mathsf{J}_1(z_{\varepsilon}(s,t))$ is regular as $\varepsilon \to 0^+$. From the definition of J_1 , see [23, Section. 10.2(ii)], there exists an analytic function Φ such that $\mathsf{J}_1(z) = z\Phi(z)$ and $\Phi(0) = \frac{1}{2}$. Using Φ and Eq. (42), we get

$$K^{L}(s,t;\varepsilon) z_{\varepsilon}(s,t) \mathsf{J}_{1}(z_{\varepsilon}(s,t)) = K^{L}(s,t;\varepsilon) z_{\varepsilon}(s,t)^{2} \Phi(z_{\varepsilon}(s,t))$$
$$= -\frac{\varepsilon k^{2}}{\pi} \sin\left(\frac{s-t}{2}\right)^{2} \Phi\left(2k \left|\sin\left(\frac{s-t}{2}\right)\cos\left(\frac{s+t}{2}\right)\right|\right) + \mathcal{O}(\varepsilon^{2}).$$

We then rewrite

(43)
$$\ln\left(\frac{4z_{\varepsilon}(s,t)^{2}}{k^{2}}\right) = \ln\left(4\sin\left(\frac{s-t}{2}\right)^{2}\right) + \ln\left(4\cos\left(\frac{s+t}{2}\right)^{2} + 4\varepsilon^{2}\sin\left(\frac{s+t}{2}\right)^{2}\right).$$

Using Lemma 7 and the function $\phi_s(t) = 2k^2 \sin\left(\frac{s-t}{2}\right)^2 \Phi\left(2k \left|\sin\left(\frac{s+t}{2}\right)\cos\left(\frac{s+t}{2}\right)\right|\right)$ introduced in Eq. (28) we obtain

$$\mathcal{K}^{\ln}[\mu](s) = \frac{\varepsilon}{2\pi} \left[\int_{\mathbb{T}} \phi_s(t)\mu(t) \ln\left(4\sin\left(\frac{s-t}{2}\right)^2\right) dt + \int_{\mathbb{T}} \phi_s(t)\mu(t) \ln\left(4\cos\left(\frac{s+t}{2}\right)^2\right) dt \right]$$
$$= \frac{\varepsilon}{2\pi} \int_{\mathbb{T}} [\phi_s \, \mu]_{\text{ev}}(t) \ln\left(4\sin\left(\frac{s-t}{2}\right)^2\right) dt$$

where we used the change of variable $t = \pi - x$ in the second integral, leading to the even representation of $\phi_s \mu$.

Lemma 7. For $f \in \mathscr{C}^{\infty}(\mathbb{T})$, and $s \in \mathbb{T}$, we have the following asymptotic expansion

$$\int_{\mathbb{T}} f(t) \ln\left(4\cos\left(\frac{s+t}{2}\right)^2 + 4\varepsilon^2\sin\left(\frac{s+t}{2}\right)^2\right) dt = \int_{\mathbb{T}} f(t) \ln\left(4\cos\left(\frac{s+t}{2}\right)^2\right) dt + \mathcal{O}(1)$$

$$as \ \varepsilon \to 0^+.$$

Proof. Using the change of variable $t = \pi - s + x$, we then split the integral

$$\int_{-\pi}^{\pi} f(\pi - s + x) \ln \left(4 \cos \left(\frac{s+t}{2} \right)^2 + 4\varepsilon^2 \sin \left(\frac{s+t}{2} \right)^2 \right) dx = \mathcal{F}^{\text{inn}} + \mathcal{F}^{\text{out}}$$

with

$$\mathcal{F}^{\text{inn}} = \int_{-\delta}^{\delta} f(\pi - s + x) \ln\left(4\cos\left(\frac{s+t}{2}\right)^2 + 4\varepsilon^2\sin\left(\frac{s+t}{2}\right)^2\right) dx,$$

$$\mathcal{F}^{\text{out}} = \int_{I_{\delta}} f(\pi - s + x) \ln\left(4\cos\left(\frac{s+t}{2}\right)^2 + 4\varepsilon^2\sin\left(\frac{s+t}{2}\right)^2\right) dx$$

where $I_{\delta} = [-\pi, \pi] \setminus (-\delta, \delta)$, and δ is a parameter such that $\delta \to 0^+$ with $\varepsilon = \phi(\delta)$. We now use classic techniques from matched asymptotic expansions (see for instance Appendix B.1). For the inner expansion, we remark that, as $\varepsilon \to 0^+$, we have

$$\left| \ln \left(4 \cos \left(\frac{s+t}{2} \right)^2 + 4\varepsilon^2 \sin \left(\frac{s+t}{2} \right)^2 \right) \right| \le 2 \left| \ln(2\varepsilon) \right|$$

which gives $\mathcal{F}^{\text{inn}} = \mathcal{O}(\delta |\ln(\varepsilon)|)$. Then for the outer expansion, setting $x = s + t - \pi$ and using the fact that

$$\ln\left(4\cos\left(\frac{s+t}{2}\right)^2 + 4\varepsilon^2\sin\left(\frac{s+t}{2}\right)^2\right) = \ln\left(4\sin\left(\frac{x}{2}\right)^2\right) + \mathcal{O}\left(\varepsilon^2\tan\left(\frac{x}{2}\right)^{-2}\right)$$

we obtain

$$\mathcal{F}^{\text{out}} = \int_{I_{\delta}} f(\pi - s + x) \ln\left(4\sin\left(\frac{x}{2}\right)^{2}\right) dx + \mathcal{O}\left(\frac{\varepsilon^{2}}{\delta^{3}}\right)$$
$$= \int_{-\pi}^{\pi} f(\pi - s + x) \ln\left(4\sin\left(\frac{x}{2}\right)^{2}\right) dx + \mathcal{O}\left(\delta \left|\ln\delta\right|\right) + \mathcal{O}\left(\frac{\varepsilon^{2}}{\delta^{3}}\right)$$

One concludes by remarking that we can choose $\delta \to 0$ (for example $\delta = \sqrt{\varepsilon}$) such that $\mathcal{O}\left(\delta \left|\ln(\varepsilon)\right|\right) + \mathcal{O}\left(\delta \left|\ln\delta\right|\right) + \mathcal{O}\left(\frac{\varepsilon^2}{\delta^3}\right) = \mathcal{O}(1).$

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