Quadrature by Parity Asymptotic eXpansions (QPAX) for light scattering by high aspect ratio plasmonic particle

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Abstract

The study of scattering by a high aspect ratio particle has important applications in sensing and plasmonic imaging. To illustrate the effect of particle's narrowness (that can be related to parity properties) and the need for adapted methods (in the context of boundary integral methods), we consider the scattering by a penetrable, high aspect ratio ellipse. This problem highlights the main challenge and provides valuable insights to tackle general high aspect ratio particles. We find that boundary integral operators are nearly singular due to the collapsing geometry to a line segment. We show that these nearly singular behaviors lead to qualitatively different asymptotic behaviors for solutions with different parities. Without explicitly taking this into account, computed solutions incur large errors. We introduce the Quadrature by Parity Asymptotic eXpansions (QPAX) that effectively and efficiently addresses these issues. We demonstrate the effectiveness of QPAX through several numerical examples.

Keywords: Boundary integral methods; asymptotic analysis; numerical quadrature; scattering.

1 Problem setting

Consider a penetrable high aspect ratio ellipse D characterized by some material property $\varsigma_- \in \mathbb{C}$. Typically, the plasmonic case corresponds to $\Re(\varsigma_-) < 0$, where ς_- represents the inverse of the dielectric permittivity of the particle made of a noble metal such as gold or silver. The ellipse is surrounded by vacuum (characterized by $\varsigma_+ = 1$). The associated scattering problem is given by the transmission problem: Find $u_+ \in \mathscr{C}^2(E := \mathbb{R}^2 \setminus \bar{D})) \cup \mathscr{C}^1(\mathbb{R}^2 \setminus D)$ such that $u_- \in \mathscr{C}^2(D) \cup \mathscr{C}^1(\bar{D})$ such that, $\Delta u_+ + k_+^2 u_+ = 0$ in E, $\Delta u_- + k_-^2 u_- = 0$ in D, $u_+ = u_-$ and $\varsigma_+ \partial_n u_+ = \varsigma_- \partial_n u_-$ on ∂D. We denote $u_\pm = u^{\mathsf{in}} + u_\pm^{\mathsf{sc}}$ the total fields, $u_\pm^{\mathsf{sc}}$ the scattered fields, u^{in} is the incident field, ∂_n is the normal derivative. Consider a wavenumber $k > 0$, we define $k_\pm = k/\sqrt{\varsigma_\pm}$. We also require u_+^{sc} to satisfy the Sommerfeld radiation condition, and we assume that $(\varsigma_-, \varsigma_+)$ are such that the problem is well-posed. Using the representation formula [1] and the transmission conditions on ∂D, we write

$$\begin{aligned} u_+ &= u^{\mathsf{in}} + \mathcal{K}_+^H[u_+] - \mathcal{S}_+^H[\partial_n u_+] \qquad \text{in } E,\\ u_- &= -\mathcal{K}_-^H[u_+] + \frac{\varsigma_+}{\varsigma_-}\mathcal{S}_-^H[\partial_n u_+] \qquad \text{in } D, \end{aligned}$$

where $\mathcal{K}_\pm^H$, $\mathcal{S}_\pm^H$, are the double-layer potentials, single-layer potentials, associated to the considered Helmholtz equations, respectively. To study scattering by a high aspect ratio particle, we consider the ellipse defined according to $y(t) = (\varepsilon\cos(t), \sin(t))$, $t \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$, with $0 < \varepsilon \ll 1$, and we study the asymptotic limit $\varepsilon \to 0^+$. Given $x \in \mathbb{R}^2 \setminus \partial D$, 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). When $y = y(s)$ for $s \in \mathbb{T}$, we find that the unknown fields on the boundary, $(u_+(s), v_+(s)) := (u_+(y(s)), \partial_{n_y} u_+(y(s))|y'(s)|)$, satisfy the system

$$\begin{bmatrix} \frac{\mathrm{I}}{2} - \mathscr{K}_+^H & \mathscr{S}_+^H \\ \frac{\mathrm{I}}{2} + \mathscr{K}_-^H & -\frac{\varsigma_+}{\varsigma_-}\mathscr{S}_-^H \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} u^{\mathsf{in}} \\ 0 \end{bmatrix}, \qquad (1)$$

with $\mathscr{S}_\pm^H[v](s) = \frac{\mathrm{i}}{4}\int_{\mathbb{T}} \mathsf{H}_0^{(1)}(k_\pm r_\varepsilon^s(t) v(t)\,\mathrm{d}t$,

$$\mathscr{K}_\pm^H[u](s) = \frac{\mathrm{i}\pi k_\pm}{2}\int_{\mathbb{T}} r_\varepsilon^s(t)\,\mathsf{H}_1^{(1)}(k_\pm\, r_\varepsilon^s(t))\; K_\varepsilon^L(s,t)\; u(t)\,\mathrm{d}t,$$

with $r_\varepsilon^s(t) = |y(s) - y(t)|$, $\mathsf{H}_m^{(1)}$ the Hankel function of the first kind of order m, and K_ε^L the Laplace's double-layer potential kernel

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

The kernel K_ε^L is sharply peaked at the *reflection-points* along the semi-major axis of the ellipse, $s+t \equiv \pi\,[2\pi]$: $K_\varepsilon^L(s,t) = -\frac{1}{4\pi\varepsilon}$. This peak is enhanced as the ellipse collapses ($\varepsilon \to 0$).

This sharp peak leads to nearly singular integral operators in the boundary integral equation system (1). Not addressing this behavior gives large errors when using standard quadrature rules such as Kress' Product Quadrature Rule (PQR), as plotted in Fig. 1.

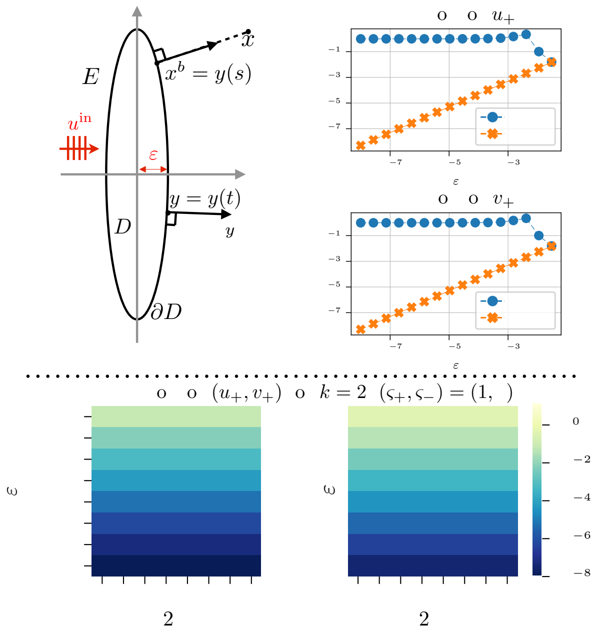

Figure 1: (Top left) Sketch and notations of the problem. (Top right) Error with respect to ε when approximating the solution (u_+, v_+) of (1) using PQR, QPAX (leading order), $k = 2$, $(\varsigma_+, \varsigma_-) = (1, 4)$, and $N = 128$ quadrature points. The analytic solution is computed using Mathieu functions [2]. (Bottom) Error for (u_+, v_+) for various ε, N.

2 Parity asymptotic expansions

We rewrite system (1) as $A_\varepsilon U_\varepsilon = F_\varepsilon$, we perform an asymptotic expansion about $\varepsilon = 0$. The leading order gives us

$$A_\varepsilon = \begin{bmatrix} \Pi_{\mathsf{ev}} & S_0^+ \\ \Pi_{\mathsf{od}} & -\frac{\varsigma_+}{\varsigma_-} S_0^- \end{bmatrix} + \mathcal{O}(\varepsilon),$$

$$U_\varepsilon = \begin{bmatrix} u_0^+ \\ v_0^+ \end{bmatrix} + \mathcal{O}(\varepsilon),\ F_\varepsilon = \begin{bmatrix} u^{\mathsf{in}}(0, \sin(s)) \\ 0 \end{bmatrix} + \mathcal{O}(\varepsilon).$$

where $S_0^\pm$ are integral operators that can be found following [2, Section 4] (along with order 1 terms). Above, Π_{ev}, Π_{od}, denotes the projection onto even, odd function with respect to the semi-major axis of the ellipse, respectively: $\Pi_{\mathsf{ev}}[\mu](s) = \frac{\mu(s)+\mu(\pi-s)}{2}$, $\Pi_{\mathsf{od}}[\mu](s) = \frac{\mu(s)-\mu(\pi-s)}{2}$, $\mu \in \mathscr{C}^0(\mathbb{T})$, $s \in \mathbb{T}$. Thus, there is an underlying nearly singular behavior to address at the reflection-points, and parity decomposition (namely even/odd properties with respect to reflection-points) is necessary to accurately compute the field on the boundary : problem $A_\varepsilon U_\varepsilon = F_\varepsilon$ may be ill-posed if one considers only even or odd F_ε. Quadratures such as PQR are well adapted to treat weakly singular integrals involved in (1) (e.g. [1]), but do not treat the parity or the close evaluation problem. To address these, we introduce the Quadrature by Parity Asymptotic eXpansions (QPAX) [2], a modification of PQR as follows: split the fields and the operators obtained from the previous linear system into their even and odd parts, discretize the systems obtained with asymptotic expansions (accuracy depends on the expansions truncation's order), use PQR on weakly singular integrals involved in the systems, and spectral methods on the rest. Considering an $\mathcal{O}(\varepsilon)$ expansion, we expect the error to decrease linearly as $\varepsilon \to 0$, for any number of quadrature points. To validate the method we plot in Figure 1 the errors in log obtained with PQR ('•' line) and QPAX ('+' line), for a classical penetrable ellipse ($\varsigma_- > 0$) where one can compute an analytic solution (codes available on GitHub). Results show that QPAX approximation effectively addresses the inherent parity in the nearly singular behaviors associated with this high aspect ratio ellipse. QPAX efficiently computes near-fields in plasmonic cases as well (but no analytic solution is available).

3 Future work

The above approach can be carried out for more general high aspect ratio particles where two distinct asymptotic behaviors along reflection-points must be addressed carefully. Extensions to three-dimensional high aspect ratio particles are considered, starting with axisymmetric high aspect ratio particles.

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