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# Outgoing solutions to the scalar wave equation in helioseismology

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**Abstract:** This report studies the construction and uniqueness of physical solutions for the time-harmonic scalar wave equation arising in helioseismology. Intuitively speaking, physical solutions are characterized by their  $L^2(\mathbb{R}^3)$ -boundedness in the presence of absorption, while without, by their profile at infinity approximated by *outgoing* spherical waves (or retarded). For brevity, we unite these two families (with and without absorption) under the label ‘outgoing’ or ‘physical’. The definition of outgoing solutions to the equation in consideration or their construction and uniqueness has not been discussed before in the context of helioseismology. In our work, we use the Liouville transform to conjugate the original equation to a potential scattering problem for Schrödinger operator, with the new problem containing a Coulomb-type potential. Under assumptions (in terms of density and background sound speed) generalizing ideal atmospheric behavior, for  $\gamma \neq 0$ , we obtain existence and uniqueness of variational solutions using only basic techniques in analysis. For  $\gamma = 0$ , under the same assumptions, the theory of long-range scattering with singular potentials is employed to construct the resolvent by means of Limiting Absorption Principle (LAP). Solutions obtained in this manner are characterized uniquely by a Sommerfeld-type radiation condition at a new wavenumber denoted by  $k$ . The appearance of this wavenumber is only clear after applying the Liouville transform. Another advantage of the conjugated form is that it makes appear the Whittaker functions, when ideal atmospheric behavior is extended to the whole domain  $\mathbb{R}^3$  or outside of a sphere. This allows for the explicit construction of the outgoing Green kernel and the exact Dirichlet-to-Neumann map and hence reference solutions and radiation boundary condition. In addition, the role played by  $k$  in radiation condition and asymptotic expansion of the solution suggests that  $k$  should be the more natural choice to use as gauge function in approximating the exact nonlocal radiation condition. This perspective gives rise to a simpler family of radiation boundary conditions. To supplement the theoretical discussion, some preliminary numerical tests are carried out to investigate the robustness of this new family, compared to those already existent in literature which were obtained in terms of the original complex frequency  $\omega$ .

**Key-words:** Coulomb potential, long-range scattering, short-range scattering, perturbation theory, spectral theory, limiting absorption principle, Whittaker functions, helioseismology, outgoing solution, outgoing fundamental solution, outgoing Green kernel, radiation condition, Schrödinger equation, Liouville transform, absorbing boundary condition, exact Dirichlet-to-Neumann map, radiation impedance coefficients.

# Solutions sortantes pour l'équation des ondes scalaires en héliosismologie

**Résumé :** Ce rapport étudie la construction et l'unicité des solutions pour l'équation des ondes harmoniques scalaire dans un problème d'héliosismologie. De façon intuitive, les solutions physiques sont caractérisées par le fait qu'elles soient bornées en  $L^2(\mathbb{R}^3)$  en présence d'absorption ( $\gamma \neq 0$ ), et, en son absence ( $\gamma = 0$ ), par leur profil à l'infini approché par une onde sortante (ou retardée) sphérique. Nous unissons ces deux familles sous l'appellation 'sortante' ou 'physique'. La définition des solutions sortantes pour notre équation, ou leur construction et unicité n'a jamais été abordée pour le cas de l'héliosismologie. Dans notre travail, nous utilisons la transformée de Liouville pour conjuguer l'équation originale et obtenir un problème de diffusion pour l'opérateur de Schrödinger, avec un potentiel de type Coulomb. Sous des hypothèses (relatives à la densité et à la vitesse du son dans le milieu) généralisant un comportement atmosphérique idéal, nous obtenons, pour  $\gamma \neq 0$ , l'existence et l'unicité pour les solutions variationnelles en utilisant les techniques d'analyse standard. Pour  $\gamma = 0$ , la théorie de diffusion longue portée pour les potentiels singuliers est utilisée pour construire le résolvant à partir du principe d'absorption limite. Les solutions obtenues ainsi sont caractérisées de façon unique par une condition de radiation de type Sommerfeld, associée à un nouveau nombre d'onde  $k$ . L'apparition de ce nombre d'onde n'est seulement claire qu'après avoir appliqué la transformée de Liouville. Un autre avantage de la forme conjuguée est qu'elle fait apparaître les fonctions Whittaker, lorsque le modèle atmosphérique idéal est étendu sur tout  $\mathbb{R}^3$  ou en dehors d'une sphère. Cela permet de construire explicitement le noyau de Green sortant et la condition Dirichlet-to-Neumann exacte; et ainsi les solutions de référence et les conditions aux limites de radiation. De plus, le rôle de  $k$  dans la condition de radiation, et le développement asymptotique de la solution montre que  $k$  est un choix plus naturel pour la fonction de jauge dans l'approximation de la condition de radiation non-locale exacte. Cela nous donne une famille simple pour les conditions aux limites de radiation. Pour compléter les résultats analytiques, des exemples numériques sont mis en place pour tester la robustesse de cette nouvelle famille, et la comparer avec celles existantes dans la littérature, qui sont obtenues avec la fréquence original  $\omega$ .

**Mots-clés :** Potentiel de Coulomb, théorie de la perturbation, théorie spectrale, fonction Whittaker, héliosismologie, solutions fondamentales sortantes, noyau de Green, condition de radiation, équation de Schrödinger, transformée de Liouville, conditions au limite absorbantes, Dirichlet vers Neumann exact.

# 1 Introduction

In this report, we give a theoretical exposition to construct physical solutions of the linear scalar wave equation arising in helioseismology with unknown  $u_{\text{orig}}$  and source  $f_{\text{orig}}$ ,

$$-\frac{\omega^2}{\rho c^2} u_{\text{orig}} - \nabla \cdot \left( \frac{1}{\rho} \nabla u_{\text{orig}} \right) = f_{\text{orig}} \quad \text{in } \mathbb{R}^3. \quad (1.1)$$

The equation models the propagation of acoustic waves in the Sun's interior and atmosphere, where  $c$  denotes the sound speed, and  $\rho$  the density. This is a Helmholtz equation with variable coefficients and is obtained under simplifying assumptions from the original vectorial problem, cf. [15] and discussion in Remark 1. Absorption is prescribed in the form of a complex frequency<sup>1</sup>  $\omega \in \mathbb{C}$ ,

$$\omega = \sqrt{1 + i\gamma} \omega_0, \quad \omega_0 \in \mathbb{R}^+ \text{ and } \gamma \in \mathbb{R}. \quad (1.2)$$

Here,  $\gamma$  is called the absorption and the square root branch  $\sqrt{\cdot}$  is chosen so that  $\text{Im } \sqrt{\cdot} \geq 0$ , see definition in (4.11b). Intuitively speaking, ‘physical’ solutions, in the presence of absorption ( $\gamma \neq 0$ ), are characterized by their decay to zero at infinity; in mathematical terms, they belong to  $L^2(\mathbb{R}^3)$ . When absorption tends to zero, they display oscillatory behavior; the retarded ‘physical’ solutions are chosen so that they consist of only outgoing spherical waves, which is however a delicate theoretical task.

Under the assumption that outside of compact set,  $c$  is constant and  $\rho$  exponentially decay, called **Atmo** model, in [5], the first author and collaborators constructed radiation boundary conditions for equation (1.1) when  $\gamma > 0$ , in order to obtain a numerical approximation (using finite element discretization) of the physical solution that exists in the whole  $\mathbb{R}^3$ . Our work complements and extends theoretically the numerical experiments in [5] by, under assumptions generalizing the **Atmo** model, providing a theoretical definition of the ‘outgoing’ solution for  $\gamma \geq 0$ , and justifying the existence and uniqueness of such a solution. The analysis shines light on the structure of the solution,

$$\exp(\psi) \times \frac{1}{r} \times \exp(\pm i\phi_\omega) \times (\text{bounded part}). \quad (1.3)$$

This consists of a real exponential part represented by  $e^\psi$  with  $\psi$  a real function, an oscillatory part described by a phase function  $\phi_\omega$  depending on  $\omega$ , and a bounded part. The exponential real part  $e^\psi$  is common to all solutions, while it is the  $+$  or  $-$  in the oscillatory part that will distinguish between bounded and non-bounded function when  $\gamma \neq 0$ , and between outgoing and incoming solution when  $\gamma = 0$ . Because of this, in order to establish existence and uniqueness of solution, it is more natural to conjugate  $e^\psi$  out of (1.3). This is one of the intuitions of our approach. We start with the same equation considered in [5], but however use the Liouville transformation to rewrite it as a potential scattering problem with Schrödinger operator. In particular, if  $u_{\text{orig}}$  solves (1.1), then  $u = \rho^{-1/2} u_{\text{orig}}$  solves

$$-\Delta u + \mathbf{q}(x) u - \frac{\omega^2}{c^2} u = \rho^{1/2} f_{\text{orig}}, \quad (1.4)$$

with

$$\mathbf{q}(x) := \rho^{1/2}(x) \Delta \rho^{-1/2}(x), \quad x \in \mathbb{R}^3. \quad (1.5)$$

Instead of having a first order perturbation of  $-\Delta$ , we only have zero-th order one.

Thanks to the Liouville transform, one can apply the theory of potential scattering for time independent Schrödinger equation and obtain well-posedness for the conjugated problem (1.4) when  $\gamma = 0$ . Even in the simplest (but important) case in helioseismology, the **Atmo** model, the potential  $\mathbf{q}$  (1.5) contains a repulsive Coulomb-like potential, i.e. a slowly-decay potential with a singularity at the origin, and places the problem in the more challenging type of potential scattering. However, with some assumptions on  $\rho$  and  $c$  (while still more general than **Atmo**), the slow decay of the potential is dealt with by the machinery

<sup>1</sup>This can also be of the form

$$\omega = \sqrt{1 + i \frac{2i\gamma}{\omega_0}} \omega_0, \quad \omega_0 \in \mathbb{R}^+ \text{ and } \gamma \in \mathbb{R}.$$

of long-range potential scattering by Ikebe and Saito, cf., e.g. [39]. The results obtained are not only the existence of solution, but also resolvent bound, asymptotic expansion of solution cf. (3.88), as well as radiation condition (3.87). Each of the two latter properties can be used to characterize the uniqueness of the outgoing solution. There are slight modifications in applying the theory which as stated in [39] only deals with real potential, while in our case, the potential can be complex due to the term  $\frac{\omega^2}{c^2}$ .

The framework of potential scattering gives rise to the normalized wavenumber  $k$ , which has implication in numerical approximation, in particular radiation boundary condition. The defined ‘outgoing’ conjugated solution is shown to satisfy a Sommerfeld-type radiation condition with in terms of  $k$  (and not the original  $\omega/c$ ). This gives a new perspective in approximating the transparent boundary condition, with the right gauge function in terms of  $k$ . In [5],  $\omega$  and small angle of incidence in terms of  $\omega$  are used as gauge function, and are called there ‘parameters of interest’. Due to the length of the report, we only restrict ourselves to preliminary tests of radiation boundary condition for the case **Atmo**. However, we expect that in the general case (under applicable assumption), the simplest condition  $\partial_r u - iku = 0$  should work as well as the zeroth-order Sommerfeld radiation condition (cf. [4, Sec 4.3]) for the Helmholtz equation. In addition, at the same order of approximation (of the nonlocal impedance coefficients), working with  $k$  gives simpler radiation impedance coefficients with better performance (in terms of error compared to the reference coefficients which are Dirichlet-to-Neumann (D-t-N) or nonlocal transparent one).

Another important advantage of working with Schrödinger equation is the natural link with the Whittaker functions. In the case where one extends the behavior of ‘ideal atmospheric’ to the whole domain, i.e.  $\rho$  is exactly described by a decaying exponential and  $c$  constant, one has explicit description of the outgoing Schwartz kernel for the resolvent in terms of Whittaker functions, and when the **Atmo** hypothesis are assumed outside of a sphere, one has explicit description of the analytical solution using the same family of special function. The role played by the Whittaker functions is not as easy to recognize in the original form (1.1). In the second problem, once analytical solutions are obtained, one not only has the true reference solution, and but also the *exact* Dirichlet-to-Neumann map. The latter acts as the true reference radiation impedance coefficient, which was lacked in [5], and thus has implication in numerical implementation and evaluation of RBCs.

Liouville transformation was used in [30] to study the Calderón’s inverse conductivity problem with an inhomogeneous conductivity, see also [28, 3]. In the context of helioseismology, this is the first time to our knowledge<sup>2</sup> that theoretical consideration and justification of the well-posed of the outgoing solution is done. This transformation is also mentioned in recent work, cf. e.g. [40, 15, 13], or [29] in one form or another, however it is used either for bounded domain, or it is not used to construct radiation boundary condition. For more discussion on some recent appearance using this transformation, we refer to the introduction of Section 2 and Remark 1–2. The second novelty of the work is in using Liouville transformation and exploiting the theory of potential scattering to give a rigorous justification for the existence of the outgoing solutions, as well as the asymptotic expansion and radiation condition. The latter is used to characterize the uniqueness of outgoing solutions. As mentioned above, with the recognition of the presence of the Whittaker function family in the problem, if the **Atmo** model is imposed on the whole domain or outside of a sphere, one has explicit description of the analytical solutions. This provides an accurate way to evaluate the performance of an approximate radiation boundary condition, and adds to the novelty of the current work. Lack of the true D-t-N, a numerical approximation was employed in [5] to create a reference solution. This however is only applicable in the case of absorption. Since absorption is a natural physical phenomenon, the numerical reference solution is sufficient. However, numerically, this type of numerical approximation will create troubles at very small absorption.

The organization of the report is as follows. We first describe in more details the Liouville transform in Section 2 and introduce the generalized form of the problem in (2.19). Section 3 is devoted to discussion of well-posedness of the physical solution. In the presence of absorption ( $\gamma \neq 0$ ), a straightforward proof is given to obtain the existence and uniqueness of variational solution, cf. Proposition 1 and Proposition 2. At zero absorption ( $\gamma = 0$ ), we first extract elements of the theory of scattering with long-range and

<sup>2</sup>At the update of the second version of the report, we learn of the preprint [1] which also works with the conjugated problem and allow for a Coulomb-type potential. They consider the problem **S+Atmo** in the context of inverse problem of helioseismology. Instead of using the Whittaker functions, they use the Coulomb wave functions, which are normalized version of Whittaker functions.



singular potentials needed for our consideration, and then, in Subsection 3.3 apply them to the case of the conjugated problem. The constructed resolvent is given in (3.69) for  $\gamma > 0$  and for  $\gamma = 0$  in two approaches, cf. (3.71) and (3.84), while the asymptotic expansion and radiation condition are stated in (3.87) and (3.88). In Section 4, having the expression of the outgoing Green kernel, cf. (4.70), we give an explicit construction and uniqueness proof of the solution in the spirit of Colton and Kress's scattering theory for Helmholtz operator in [12], cf. Prop 17. In particular, when  $\gamma = 0$ , the uniqueness is defined in terms of several equivalent radiation conditions, cf. Prop 18, one of which is the classic Sommerfeld-type radiation condition. The exact Dirichlet-to-Neumann map is also obtained, as well as additional results such as Rellich-type uniqueness theorem, cf. Lemma 20 and expansion of solution in spherical harmonics, cf. Prop 21. Section 5 rephrases all results of the conjugated problem as those for the original one (1.1). In Section 6, we construct new radiation boundaries using the new gauge function  $k$  and provide a few preliminary tests to show that it is more advantageous and correct to work with the wavenumber  $k$ . More in-depth numerical experiments will appear in a second report.

## 2 Reduction to time-harmonic Schrödinger equation via Liouville transform

In this section, we first describe the Liouville transformation and then describe how the theory of long-range scattering for Schrödinger equation can be applied to the resulting problem. Let us introduce the transformation. Denote by  $\mathcal{L}_{\text{orig}}$  the original operator

$$\mathcal{L}_{\text{orig}} u := -\nabla \cdot (\rho^{-1} \nabla u) - \frac{\omega^2}{\rho c^2} u, \quad (2.1)$$

which gives rise to the original problem (1.1),

$$\mathcal{L}_{\text{orig}} u_{\text{orig}} = f_{\text{orig}}. \quad (2.2)$$

One applies the change of variable

$$u := \rho^{-1/2} u_{\text{orig}}. \quad (2.3)$$

The new unknown  $u$  solves the conjugated problem

$$\mathcal{L} u = \rho^{1/2} f_{\text{orig}}, \quad (2.4)$$

with conjugated operator  $\mathcal{L}$  defined as

$$\mathcal{L} := \rho^{-1/2} \mathcal{L}_{\text{orig}} \rho^{1/2} = -\Delta - \frac{\omega^2}{c^2} + q(x). \quad (2.5)$$

This is a Schrödinger operator with potential

$$q(x) := \rho^{1/2} \Delta \rho^{-1/2}, \quad x \in \mathbb{R}^3. \quad (2.6)$$

For algebraic derivation of this, see Prop. 24 in Appendix A.

This transformation was used in [30] to study the Calderón's inverse conductivity problem with an inhomogeneous conductivity, see also [3, p.10] or [2, Section 7.2.2 p.100]. More recently and in the context of helioseismology, the approach to work with the Schrödinger equation is employed in [29, Eqn 1.4] for inversion in time-distance helioseismology, and in [40] for helioseismic holography. While our potential decays slowly at infinity, in [29], the conjugated problem is a perturbation of  $-\Delta$  by a potential of compact support, and the scattering theory for this type of potentials can be found in e.g. [12, Chapter 8]. This assumption is also implied in [40], since only the Green kernel of the free Laplacian is employed there. In spherical symmetry, the Liouville transform is more or less the usual ODE technique to remove first-order derivatives. It is in this form that is mentioned in [13], see Remark 2, however the remaining work of [13] uses the original equation; see further discussion on this point in Section 6 and Remark 27.

## 2.1 The conjugated potential

We study in more details the potential  $\mathbf{q}$  (2.6). Denote by  $\partial_r$  the radial part of the gradient

$$\partial_r := \frac{x}{|x|} \cdot \nabla. \quad (2.7)$$

We also define the function

$$\alpha(x) := -\frac{\partial_r \rho}{\rho(x)}. \quad (2.8)$$

We can write the potential  $\mathbf{q}$  (2.6) as (cf. Proposition (25) of Appendix A).

$$\begin{aligned} \mathbf{q}(x) &:= \frac{3}{4} \left\| \frac{\nabla \rho}{\rho} \right\|^2 - \frac{1}{2} \frac{\Delta \rho}{\rho} \\ &= \frac{\alpha^2(x)}{4} + \frac{\partial_r \alpha(x)}{2} + \frac{\alpha(x)}{|x|} + \frac{1}{|x|^2} \left( \frac{3 \|\nabla_{\mathbb{S}^2} \rho\|^2}{4 \rho^2(x)} - \frac{\Delta_{\mathbb{S}^2} \rho}{2 \rho(x)} \right), \end{aligned} \quad (2.9)$$

where  $\mathbb{S}^2$  denotes the unit sphere. Spherical symmetry (i.e. with all coefficients depending only on  $r = |x|$ ) is an important assumption in many applications, including helioseismology, which in this context is called the **1D-background** model cf. [13, Sect 2.2] or **1.5D** problem cf. [15, Sect 6.1]. In this case, the background density and sound speed are radial, i.e.  $\rho(x) = \rho(|x|)$  and  $c(x) = c(|x|)$ , thus so is  $\alpha(x)$  defined in (2.8). In helioseismology, the quantity  $\frac{1}{\alpha(r)}$  is called *the density scale height* denoted by  $H(r)$ , cf. [13, Eqn 12],

$$\alpha(x) = \alpha(r) = -\frac{\rho'(r)}{\rho(r)} := \frac{1}{H(r)}. \quad (2.10)$$

The potential  $\mathbf{q}$  simplifies to,

$$\mathbf{q}(r) = \frac{\alpha^2(r)}{4} + \frac{\alpha'(r)}{2} + \frac{\alpha(r)}{r} = \frac{1}{4 H^2(r)} \left( 1 - 2 H'(r) + \frac{4 H(r)}{r} \right). \quad (2.11)$$

In addition, the quantity  $\mathbf{q}(r) c^2(r)$  is called the *cut-off frequency*,

$$\omega_c^2(r) := \frac{c^2(r)}{4 H^2} \left( 1 - 2 H'(r) + \frac{4 H(r)}{r} \right). \quad (2.12)$$

## 2.2 The long-range behavior in Model Atmo

In order to investigate the invertibility by means of potential scattering theory, two important elements have to be kept in mind: the growth/decay of a potential at infinity and its local integrability. We restrict ourselves to cases that are applicable in helioseismology, and use as a basis of generalization the potential  $\mathbf{q}$  resulting from the model **S + Atmo**, cf. [5], in particular its decay at infinity (in the atmosphere) and the local integrability (in the interior of the Sun). In this model, the interior of the Sun is described by  $\rho$  and  $c$  following the model **S** [10] while the atmosphere is described by an exponentially decaying density and constant sound speed, called ideal atmospheric behavior or simply the **Atmo** model, cf. [13, Sec. 2.3]. Concretely, in terms of the scaled radius  $r = \frac{R}{R_\odot}$  with  $R_\odot$  the radius of the sun,

$$\rho(r) := \begin{cases} \rho_{\mathbf{S}}(r) & , r \leq R_a \\ \rho_{\mathbf{S}}(R_a) e^{-\alpha_\infty(r-R_a)} & , r > R_a \end{cases} \quad \text{and} \quad c(r) := \begin{cases} c_{\mathbf{S}}(r) & , r \leq R_a \\ c_\infty & , r > R_a \end{cases}, \quad (2.13)$$

with

$$\rho_{\mathbf{S}} > \rho_0 > 0 \quad , \quad c_{\mathbf{S}} > c_0 > 0. \quad (2.14)$$

The extension into the atmosphere is achieved by continuing density  $\rho$  to be exponential decay at the same rate at end of model **S**, while the sound speed  $c$  is smoothly extended to a constant  $c_\infty$ . For  $\mathcal{C}^1$  continuity, we require that

$$c_{\mathbf{S}}(R_a) = c_\infty \quad , \quad \frac{d}{dr} \rho_{\mathbf{S}}|_{r=R_a}^- = -\alpha_\infty \rho_{\mathbf{S}}(R_a) \quad \Rightarrow \quad \alpha_\infty = \frac{1}{H(R_a)}.$$

In Figure 1, we plot the radial profile of the density and velocity using (2.13) with  $R_a = 1.000699$ ,  $c_\infty = 6.867 \text{ km s}^{-1}$ , and  $\alpha_\infty = 6663.62$ . In Figure 2, we plot the corresponding  $\alpha$  from (2.10). We observe that the profile of density and velocity in the Sun decreases rapidly below the surface of the Sun which is indicated at scaled radius  $r = 1$ . It results in a sharp increase in  $\alpha$ , cf. Figure 2, which, in addition, shows an oscillatory pattern when we zoom.

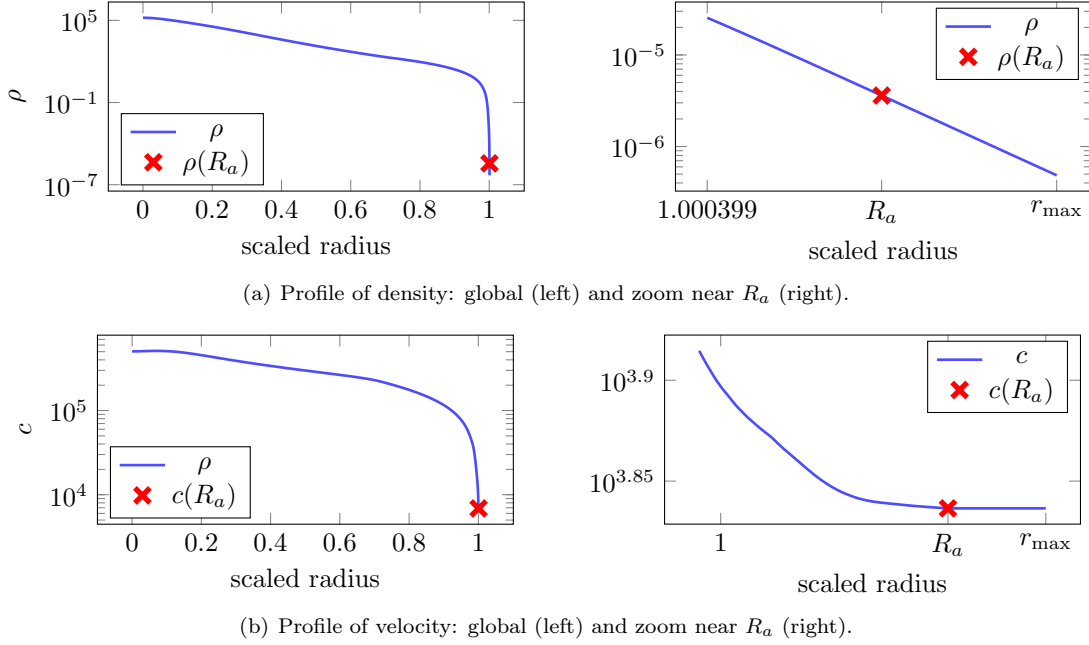


Figure 1: Profile of density and velocity in the model **S+Atmo** on  $r \leq r_{\max} = 1.001$ . The interior of the Sun,  $r < R_a = 1.000699$ , is described by model **S** [10] and extended into the atmosphere by (2.13).

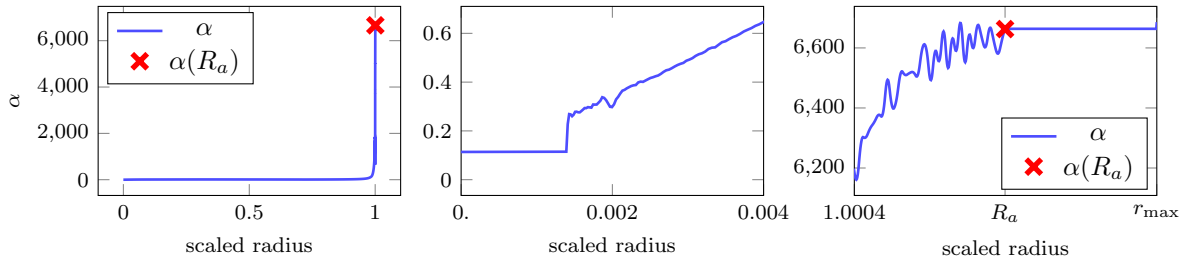


Figure 2: Profile of the inverse of density scale-height  $\alpha$  from (2.10) in the model **S+Atmo** shown on the whole interval  $r \leq r_{\max}$  (on the left) and zoomed (on the right) near  $R_a$ . This plot shows that  $\alpha$  is positive and is constant for  $r \geq R_a$ . In addition, near  $r = 0$ ,  $\alpha$  is strictly positive, which means that the resulting potential  $q$  (2.11) not only has a Coulomb-type potential but also a weak-singularity at  $r = 0$ , cf. (2.15) and (2.16).

We next consider the form of the conjugated  $\mathcal{L}$  in each region.

- In the atmosphere i.e.  $r > R_a$ ,  $\alpha(r) = \alpha_\infty$ , hence  $\alpha'(r) = 0$ , while  $c = c_\infty$ . The potential  $q$  is simplified to,

$$q(x) = \frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{r}, \quad |x| \geq R_a.$$

We write the conjugated operator into a normalized form, which reflects that in addition to the energy

level (0<sup>th</sup> term), there is also a perturbation by a Coulomb potential,

$$\rho^{1/2} \mathcal{L}_{\text{orig}} \rho^{-1/2} = -\Delta - \underbrace{\left( \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} \right)}_{\text{energy level}} + \underbrace{\frac{\alpha_\infty}{|x|}}_{\text{Coulomb potential}}, \quad |x| \geq R_a. \quad (2.15)$$

- In the interior, i.e.  $|x| < R_a$ , we simply have

$$\rho^{1/2} \mathcal{L}_{\text{orig}} \rho^{-1/2} = -\Delta - \frac{\omega^2}{c^2} + \frac{\alpha^2(r)}{4} + \frac{\alpha'(r)}{2} + \frac{\alpha(r)}{r}. \quad (2.16)$$

In this region, it is the integrability of the potential that matters. The last term potentially carries a singularity; however under the assumption that  $\alpha$  is continuous, this term remains integrable in  $\mathbb{R}^3$ , i.e., it is  $L^1(\mathbb{R}^3)$ .

Before further discussion, we need to give the definition of long-range versus short-range potentials.

**Definition 1** (long-range). *A long-range potential  $V_L$  is a  $C^3$ -function that decays slower than  $|x|^{-1}$  at infinity,*

$$|\partial^m V_L(x)| \leq C(1 + |x|)^{-\delta - |\alpha|}, \quad \delta \in (0, 1], \quad 0 \leq m \leq 3. \quad \triangle$$

**Definition 2** (short-range). *A short-range potential  $V_S$  decays strictly faster than  $|x|^{-1}$ , in particular*

$$|V_S(x)| \leq C(1 + |x|)^{-1-\delta}, \quad \delta \in (0, 1]. \quad \triangle$$

## 2.3 Generalization

The results in this report are applied to a generalization of model **S+Atmo** under the following assumptions.

1. Background density  $\rho$  is decreasing globally<sup>3</sup> so that the inverse density scale height ( $\alpha$ ) is non-negative.
2. Background sound speed  $c$  and density  $\rho$  do not oscillate at infinity and have limiting scalar values, denoted by

$$\alpha_\infty := \lim_{r \rightarrow \infty} \alpha; \quad \alpha'_\infty := \lim_{r \rightarrow \infty} \alpha'; \quad c_\infty := \lim_{r \rightarrow \infty} c. \quad (2.17)$$

We define the normalized wave number  $k^2$  which gathers contributions at zero-th order and the limiting value  $s$  of the potentials,

$$k^2 = \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2}. \quad (2.18)$$

3. In the atmosphere, background density  $\rho$  and sound speed  $c$  are extended in a way so that the conjugated operator is a perturbation of  $-\Delta - k^2$  by at most a Coulomb potential and a short-range one, as shown in (2.19). However, it suffices for the current application to assume<sup>4</sup> that  $c$  is equal to a constant  $c_\infty > 0$  outside of a compact set.

With these assumptions, the conjugated operator (2.5) can be put into the following normalized form,

$$\begin{aligned} \rho^{1/2} \mathcal{L}_{\text{orig}} \rho^{-1/2} = & -\Delta - \underbrace{\left( \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2} \right)}_{\substack{\text{energy level} \\ k^2}} + \underbrace{\frac{\alpha(x)}{|x|}}_{\substack{\text{Coulomb-like} \\ \text{potential}}} - \underbrace{\omega^2 \left( \frac{1}{c^2} - \frac{1}{c_\infty^2} \right)}_{\substack{\text{compactly supported} \\ \text{perturbation } p_1(x)}} \\ & + \underbrace{\left( \frac{\alpha^2}{4} + \frac{\partial_r \alpha}{2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2} \right)}_{\substack{\text{short-range perturbation} \\ p_2(x)}} + \underbrace{\frac{1}{|x|^2} \left( \frac{3 \|\nabla_{\mathbb{S}^2} \rho\|^2}{4 \rho^2(x)} - \frac{\Delta_{\mathbb{S}^2} \rho}{2 \rho(x)} \right)}_{\substack{\text{short-range perturbation} \\ p_3(x)}}. \end{aligned} \quad (2.19)$$

<sup>3</sup>In fact, we only need  $\rho$  to decrease outside of a compact set, see Remark 7.

<sup>4</sup>However, the same result can be obtained for the case where  $\frac{1}{c^2} - \frac{1}{c_\infty^2}$  is short-range cf. Remark 16 or even long-range, cf. Remark 13.

In the next section we will construct the resolvent for  $\mathcal{L}$  in the presence of and without attenuation. The latter case is done by means of long-range scattering theory. After some preparation, the results for  $\mathcal{L}$  are given at the end in Subsection 3.3. The resolvent is given in (3.69) for  $\gamma > 0$  and for  $\gamma = 0$  in two approaches, cf. (3.71) and (3.84), while the asymptotic expansion and radiation condition, each of which can be used to characterize the uniqueness of the constructed solution, are stated in (3.87) and (3.88). The corresponding results for the conjugated problem are interpreted for the original one (1.1) in Section 5.

**Remark 1.** *In the frequency domain, the scalar wave equation is obtained from the original vectorial equation modeling small perturbations from a background described by Euler equation, cf. [15, Eqn 2–3] also [40, Eqn 3.1],*

$$-(\omega_0 + i\tilde{\gamma} + i\mathbf{v} \cdot \nabla)^2 \boldsymbol{\xi} - \frac{1}{\rho} \nabla(\rho c^2 \nabla \cdot \boldsymbol{\xi}) + \text{gravity terms} = \mathbf{f}. \quad (2.20)$$

Here, in addition to the sound speed  $c$  and density, there is also the effect of the background flow  $\mathbf{v}$ , and  $\mathbf{f}$  is the source. If one neglects gravity terms and second-order terms in  $\gamma$  and  $\mathbf{v}$ , upon taking the divergence and under the assumption of slow variations of  $\mathbf{v}$ ,  $c$  and  $\gamma$  compared to the wavelength, one obtains the simplified scalar equation, cf. [15, Section 2.2 Eqn 5–7],

$$-\frac{\omega^2}{c} \tilde{u} - 2i \frac{\omega_0}{c} \mathbf{v} \cdot \nabla \tilde{u} - \nabla \cdot \left( \frac{1}{\rho} \nabla(\rho c \tilde{u}) \right) = \nabla \cdot \mathbf{f}, \quad (2.21)$$

in terms of unknown

$$\tilde{u} := c \nabla \cdot \boldsymbol{\xi}.$$

To solve (2.21) using a FEM discretization, [15] works with another unknown, [15, Eqn 63]

$$u_{\text{orig}} := \rho c \tilde{u} = \rho c^2 \nabla \cdot \boldsymbol{\xi}.$$

This is also the unknown used in [5] and [13]. In terms of this unknown, the equation (2.21) becomes, cf. [15, Eqn 64]

$$-\frac{\omega^2}{\rho c^2} u_{\text{orig}} - 2i \frac{\omega_0}{c} \mathbf{v} \cdot \nabla \left( \frac{u_{\text{orig}}}{\rho c} \right) - \nabla \cdot \left( \frac{1}{\rho} \nabla u_{\text{orig}} \right) = \nabla \cdot \mathbf{f}.$$

In absence of flow i.e.  $\mathbf{v} = 0$ , this is our starting equation (1.1), which is also the one considered in [5, Eqn 2.1] and [13, Eqn 1]. In [40], another type of unknown is employed (following Lamb 1909 and Deubner and Gough 1984),

$$u := \rho^{-1/2} u_{\text{orig}} = \rho^{1/2} c^2 \nabla \cdot \boldsymbol{\xi},$$

which solves, cf. [40, Eqn (3.3)],

$$-\Delta u - \frac{\omega^2}{c^2} u + \rho^{1/2} \Delta \rho^{-1/2} u - 2i \frac{\omega_0}{\rho^{1/2} c} \rho \mathbf{v} \cdot \nabla \left( \frac{u}{\rho^{1/2} c} \right) = \rho^{1/2} \nabla \cdot \mathbf{f}. \quad (2.22)$$

This amounts to working with the Liouville change of variable (2.3). In the absence of flow, this reduces<sup>5</sup> to the Schrödinger equation (2.4)–(2.6) studied in the current work.  $\triangle$

**Remark 2.** *In the radial case, Liouville transform reduces to the usual technique in ODE to remove the first order derivatives. There are two equivalent approaches.*

- One first applies the Liouville change of variable  $\rho^{-1/2} u_{\text{orig}} = u$ , then carries out separation of variables. One next eliminates the first order derivatives in the ODE in the radial variable  $r$ , which in this case only contains  $\frac{2}{r} \partial_r$  (the first order term of the radial Laplacian). The final unknown is  $w$  with  $u = r^{-1} w$ . In relation to the original unknown,  $w = r \rho^{-1/2} u_{\text{orig}}$ . The details of the computation are listed in Section 4.

<sup>5</sup>There is although a difference with [40, Eqn (3.3)]. We start with the same source  $f$  (in [40, Eqn 3.1] and (2.20)), however our source in the reduced equation (2.22) is  $\rho^{1/2} \nabla \cdot \mathbf{f}$ , while in [40, Eqn (3.3)] is  $\rho^{1/2} c^2 \nabla \cdot \mathbf{f}$ .

- Equivalently, starting from the original equation in 3D (2.2), one first does a separation of variables, and then eliminates the first order terms in the resulting ODE (in the variable  $r$ ), which in this case is  $(\frac{2}{r} + \alpha_\infty) \frac{d}{dr}$ . This amounts to doing all-at-once the change of unknown  $w = r\rho^{-1/2}u_{\text{orig}}$ . The details of the computation are listed in Appendix A.2. This approach is also mentioned in [13, Eq. (8)], however was not exploited to construct radiation boundary conditions, see further discussion in Section 6 and Remark 27.  $\triangle$

### 3 General discussion of well-posedness

In this section, we construct the resolvent of the conjugated operator  $\mathcal{L}$  (2.5). There are three main parts to the discussion:

1. in the first part (Subsection 3.1), we study the existence and uniqueness of solution for problem of the form

$$\left(-\Delta + \frac{\alpha(x)}{|x|} + \mathfrak{p}(x) - \mathbf{k}^2\right) u = f \quad (3.1)$$

and

$$\left(-\Delta + \frac{\alpha(x)}{|x|} + \mathfrak{p}(x) - \frac{\omega^2}{c(x)^2}\right) u = f. \quad (3.2)$$

These arise from the normalized form (2.19) of the conjugated operator  $\mathcal{L}$  discussed in previous section. When  $\text{Im } \mathbf{k}^2 \neq 0$ , we obtain well-posedness in  $H^1(\mathbb{R}^3)$ , for the variational problem (3.1) and (3.2), by using basic analysis tools such as ellipticity and coercitivity, and Lax-Milgram theory for sesquilinear forms. These results are stated in Theorem 1 and 2 respectively.

Although the well-posedness results for variational solutions are sufficient for applications (in particular for consideration with finite element discretization), for problem (3.1), in Subsection 3.1.4, we will also state stronger results given by Kato and Kato-Rellich's perturbation theory for self-adjoint operators. Much stronger and further-reaching, these results describe the invertibility of the problem in terms of the spectrum of the operator. We will only cite important theorems following mostly e.g. [17]. Under necessary assumptions, with  $\mathfrak{p}_m = \min_{x \in \mathbb{R}^3} \mathfrak{p} \leq 0$ , we will show that  $[\mathfrak{p}_m, +\infty)$  and thus  $\mathbb{R}^+ := [0, \infty)$  is contained in the spectrum, see Figure 3 and 4. It is also noted that criterion of being in  $H^1(\mathbb{R}^3)$  defines the physical solutions in the presence of absorption.

2. In the second part (Subsection 3.2), we state results from short-range and long-range scattering for  $-\Delta + V - \lambda$  with real potential  $V$  which is either short-range or long-range, respectively. Solution as  $\text{Im } \mathbf{k}^2 \rightarrow 0$  are obtained as limiting of solutions off the spectrum, in a process called limiting absorption principle (LAP). In the current convention, the physical solutions, called 'outgoing' are obtained by approaching the spectrum from above, i.e.  $\text{Im } \mathbf{k}^2 \rightarrow 0^+$ . These solutions are shown to satisfy radiation condition, which are then used to define them uniquely. There are three important elements:

- the existence of the above limit in certain function spaces as one approaches the spectrum, which gives the existence of 'outgoing' solution.
- These solutions satisfy certain radiation condition.
- Their uniqueness under the radiation condition is intimately connected to the absence of positive eigenvalues.

To show the LAP for short-range potentials, perturbation theory with respect to  $-\Delta$  (the Agmon-Jensen-Kato approach) can be used. This however excludes long-range potentials, and theory has to be redone, and is replaced by e.g. the long-range scattering theory by Ikebe and Saito. Since the theory is extremely technical and elaborate, we will only state the main results, following the exposition of [39]. For radiation conditions, we will follow the exposition of [43].

3. In the third part (Subsection 3.3), we put together the results of the first two to obtain the resolvent of conjugated operator  $\mathcal{L}$ . Slight adaptations have to be made due to the dependence on frequency  $\omega$  of the term  $\frac{\omega^2}{c^2}$  and the singularity at zero of Coulomb-type potential  $\frac{\alpha(x)}{|x|}$ . The construction of the

resolvent is given in (3.69) for  $\gamma > 0$  and for  $\gamma = 0$  in two approaches, cf. (3.71) and (3.84), while the asymptotic expansion and radiation condition are stated in (3.87) and (3.88).

### 3.1 Well-posedness of variational problem in the presence of absorption

#### 3.1.1 Recall of basic analysis tools

This subsection serves to recall some basic notions and facts (e.g. ellipticity and coercitivity) needed for the well-posedness of a generic variational problem (off the spectrum) in Subsection 3.1.2–3.1.3,

$$\begin{aligned} &\text{for } \ell \in \mathcal{H}^*, \text{ find } u \in \mathcal{H} \text{ so that} \\ &\mathbf{d}(u, v) = \ell(v) \quad , \quad \forall v \in \mathcal{H}. \end{aligned} \quad (3.3)$$

With the superscript  $*$  denoting the dual (i.e. the space of bounded linear functional on  $\mathcal{H}$ ), we have written

$$\mathcal{H} := H^1(\mathbb{R}^3) \quad , \quad \mathcal{V} := L^2(\mathbb{R}^3) \quad , \quad \mathcal{H}^* := H^1(\mathbb{R}^3)^*.$$

**$\mathcal{H}$ -ellipticity** A sesquilinear form  $\mathbf{d}$  is continuous if there exists  $d > 0$ ,

$$\mathbf{d}(u, v) \leq d \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}}, \quad (3.4)$$

and is  $\mathcal{H}$ -ellipticity if, cf. [37, Eqn (2.43)],

$$\exists \sigma \in \mathbb{C}, |\sigma| = 1, c > 0 \quad : \quad |\operatorname{Re} \sigma \mathbf{d}(u, u)| \geq c \|u\|_{H^1(\mathbb{R}^3)}. \quad (3.5)$$

Given  $\mathcal{H}$ -ellipticity of a sesquilinear form  $\mathbf{c}$ , we have

$$c \|u\|_{\mathcal{H}}^2 \leq |\operatorname{Re} (\sigma \mathbf{d}(u, u))| \leq |\sigma \mathbf{d}(u, u)| \leq |\mathbf{d}(u, u)|. \quad (3.6)$$

For a continuous and  $\mathcal{H}$ -elliptic sesquilinear form, the solvability of the variational problem (3.3) follows from Riesz representation theorem, since (3.5) and (3.6) imply that  $\mathbf{c}$  defines an inner product on  $\mathcal{H}$  with a norm that is equivalent to  $\|\cdot\|_{\mathcal{H}}$ . Or, we can also apply Lax-Milgram cf. [37, Lem 2.1.51]. In addition, if  $\ell(v) = \mathbf{a}(u, v)$  for all  $v \in \mathcal{H}$ , then

$$c \|u\|_{\mathcal{H}}^2 \leq |\ell(u)| \leq \|\ell\|_{\mathcal{H}^*} \|u\|_{\mathcal{H}}.$$

With  $c$  the constant from (3.5), we obtain the bound for the unique solution  $u \in \mathcal{H}$ .

$$\|u\|_{\mathcal{H}} \leq \frac{1}{c} \|\ell\|_{\mathcal{H}^*}. \quad (3.7)$$

**$\mathcal{H}$ -coercitivity** If a continuous sesquilinear form  $\mathbf{d} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  satisfies the Gårding inequality,

$$\operatorname{Re} (\mathbf{d}(u, u) + \langle Tu, u \rangle_{\mathcal{H}^*, \mathcal{H}}) > \min \{ |\operatorname{Re} k^2|, 1 \} \|u\|_{\mathcal{H}}^2, \quad (3.8)$$

with  $T : \mathcal{H} \rightarrow \mathcal{H}^*$  a compact operator, we have Fredholm alternative, cf. [19, Thm 5.3.10]. This means

- either for each  $\ell \in \mathcal{H}^*$ , variational problem (3.3) associated to  $\mathbf{d}$  has a unique solution, or
- there exists a finite-dimensional kernel space  $\mathcal{N} = \{u \in \mathcal{H} \mid \mathbf{d}(u, v) = 0, \forall v \in \mathcal{H}\}$ , and there exists solution to the inhomogeneous problem (3.3) with right-hand side  $\ell \in \mathcal{H}^*$  if and only if  $\ell(u) = 0$  for  $u \in \mathcal{N}$ .

**Hardy inequality** Due to the presence of the Coulomb potential, we will also need Hardy inequality, cf. [43, 1.4.2]

$$\int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx \leq \frac{4}{d-2} \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx \quad , \quad u \in H^1(\mathbb{R}^d), d \geq 3. \quad (3.9)$$

### 3.1.2 Well-posedness result version 1

For  $k^2 \in \mathbb{C}$  with  $\text{Im } k^2 \neq 0$ , we consider the variational problem on  $\mathbb{R}^3$  corresponding to problem

$$\left( -\Delta + \frac{\alpha(x)}{|x|} + p(x) - k^2 \right) u = f, \quad (3.10)$$

under the following assumptions.

Function  $\alpha(x)$  and  $p(x)$  are nonnegative, bounded and measurable functions, i.e.

$$0 \leq \alpha(x) \leq \alpha_M < \infty, \quad 0 \leq p(x) \leq p_M < \infty. \quad (3.11)$$

**Remark 3.** Note that in the current form and with the assumption  $\alpha > 0$ , the potential  $V(x) := \frac{\alpha(x)}{|x|} + p(x)$  is allowed to be singular at the origin.  $\triangle$

Define sesquilinear form

$$\begin{aligned} \mathbf{a} : \mathcal{H} \times \mathcal{H} &\rightarrow \mathbb{C} \\ \mathbf{a}(u, v) &:= \int_{\mathbb{R}^3} (\nabla u) \cdot (\nabla \bar{v}) dx + \int_{\mathbb{R}^3} \left( -k^2 + \frac{\alpha(x)}{|x|} + p(x) \right) u \bar{v} dx. \end{aligned} \quad (3.12)$$

The variational problem associated to (3.10) reads

$$\begin{aligned} \text{For } \ell \in \mathcal{H}^*, \text{ find } u \in \mathcal{H} \text{ such that} \\ \mathbf{a}(u, v) = \ell(v), \quad \forall v \in \mathcal{H}. \end{aligned} \quad (3.13)$$

Below, we will establish  $\mathcal{H}$ -ellipticity of  $\mathbf{a}$  when  $k^2 \in \mathbb{C} \setminus \mathbb{R}^+$  under hypothesis (3.11).

**Proposition 1.** The sesquilinear form  $\mathbf{a}$  (3.12) with assumptions (3.11) has the following properties.

- The mapping  $\mathbf{a} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  is continuous.
- When  $k^2 \in \mathbb{C} \setminus \mathbb{R}^+$ ,  $\mathbf{a}$  is  $\mathcal{H}$ -elliptic with constants in (3.5) given by

$$\begin{aligned} \text{Re } k^2 > 0 : \quad \sigma &:= \frac{\beta}{|\beta|}, \quad c = \frac{\delta}{|\beta|} = \frac{|\text{Im } k^2|}{|k^2 + i|} \quad \text{with } \beta = \delta + i \frac{\delta \text{Re } k^2 + \delta}{\text{Im } k^2}, \\ \text{Re } k^2 < 0 : \quad \sigma &:= 1, \quad c = \min \{ |\text{Re } k^2|, 1 \}. \end{aligned} \quad (3.14)$$

As a result of this, when  $k^2 \in \mathbb{C} \setminus \mathbb{R}^+$ , the variational problem (3.13) has a unique solution  $u \in \mathcal{H}$ , satisfying estimates

$$\|u\|_{\mathcal{H}} \leq C \|\ell\|_{\mathcal{H}^*}, \quad \text{with } C = \begin{cases} \frac{|k^2 + i|}{|\text{Im } k^2|}, & \text{Re } k^2 \geq 0 \\ \frac{1}{\min \{ |k^2|, 1 \}}, & \text{Re } k^2 < 0 \end{cases}. \quad (3.15)$$

**Remark 4.** In the language of spectral and perturbation theory, a potential  $V = \frac{\alpha(x)}{|x|} + p(x)$  with  $\alpha$  and  $p$  satisfying hypothesis (3.11) is in the Kato-Rellich class  $(L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3))$ . With such a potential  $V$ , operator  $H_V := -\Delta + V(x)$  with domain  $D(H) = H^2(\mathbb{R}^3)$  is self-adjoint, thus has real spectrum. In addition, if  $V$  is positive (which is the case under the current assumption (3.11)), then the spectrum  $\sigma(H_V) \subset [0, \infty)$ . To further determine the structure of the spectrum in  $[0, \infty)$ , we need more hypothesis on the behavior of  $V$  at infinity. For example, if in addition,  $V \rightarrow 0$  as  $|x| \rightarrow \infty$  then Kato theory gives that  $\sigma(H_V) = \sigma_{\text{ess}}(H_V) = [0, \infty)$ . This is the case if we assume additionally in (3.11) that  $p \rightarrow 0$  as  $|x| \rightarrow \infty$ . See further discussion in subsubsection 3.1.4.  $\triangle$



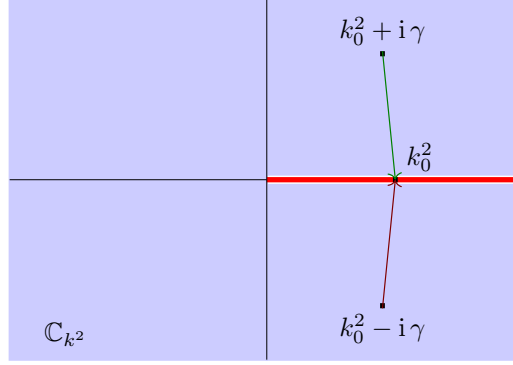


Figure 3: Under hypothesis (3.11), for  $k^2 \in$  the highlighted region in blue  $\mathbb{C} \setminus \mathbb{R}^+$ , Prop 1 states that the variational problem to  $(-\Delta + V(x) - k^2)u = f$  with  $f \in \mathcal{H}^*$  has a unique solution  $u \in \mathcal{H}$ .

*Proof. Continuity:* Under the assumption that  $\alpha(x)$  is bounded and using Hardy's inequality (3.9) in dimension 3,

$$\left\| \frac{u(x)}{|x|} \right\|_{\mathcal{V}} \leq 2 \|\nabla u\|_{\mathcal{V}},$$

to bound

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|\alpha(x)|}{|x|} |u(x)| |\bar{v}(x)| dx &\leq \alpha_M \left\| \frac{u(x)}{|x|} \right\|_{\mathcal{V}} \|v(x)\|_{\mathcal{V}} \\ &\leq 2\alpha_M \|\nabla u\|_{\mathcal{V}} \|v(x)\|_{\mathcal{V}}, \end{aligned} \quad (3.16)$$

and thus obtain the bound defining the continuity of  $\mathbf{a}$  in  $\mathcal{H} \times \mathcal{H}$ ,

$$\begin{aligned} |\mathbf{a}(u, v)| &\leq \|\nabla u\|_{\mathcal{V}} \|\nabla v\|_{\mathcal{V}} + (|k^2| + \|\mathbf{p}\|_{\infty}) \|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}} + 2\|\alpha\|_{\infty} \|\nabla u\|_{\mathcal{V}} \|v\|_{\mathcal{V}} \\ &\leq (1 + |k^2| + \mathbf{p}_M + 2\alpha_M) \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}}. \end{aligned} \quad (3.17)$$

**Ellipticity:** The real and imaginary of  $\mathbf{a}(u, u)$  are given by

$$\begin{aligned} \operatorname{Re} \mathbf{a}(u, u) &= \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( -\operatorname{Re} k^2 + \frac{\alpha + |x| \mathbf{p}(x)}{|x|} \right) |u|^2 dx; \\ \operatorname{Im} \mathbf{a}(u, u) &= - \int_{\mathbb{R}^3} (\operatorname{Im} k^2) |u|^2 dx. \end{aligned}$$

$\operatorname{Re} k^2 < 0$  In this case, we immediately have the bound

$$|\operatorname{Re} \mathbf{a}(u, u)| \geq \int_{\mathbb{R}^3} |\nabla u|^2 dx + |\operatorname{Re} k^2| \int_{\mathbb{R}^3} |u|^2 dx \geq \min\{|\operatorname{Re} k^2|, 1\} \|u\|_{\mathcal{H}}^2. \quad (3.18)$$

$\operatorname{Re} k^2 \geq 0$  For  $\delta > 0$ , consider a complex number  $\beta = \beta_1 + i\beta_2$ ,  $\beta_2 \in \mathbb{R}$ ,

$$\begin{aligned} &\operatorname{Re} (\beta \mathbf{a}(u, v)) \\ &= \beta_1 \operatorname{Re} \mathbf{a}(u, v) - \beta_2 \operatorname{Im} \mathbf{a}(u, v) \\ &= \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} (\beta_2 \operatorname{Im} k^2 - \beta_1 \operatorname{Re} k^2) |u|^2 dx + \int_{\mathbb{R}^3} \frac{\beta_1 (\alpha(x) + |x| \mathbf{p}(x))}{|x|} |u|^2 dx. \end{aligned}$$

Using the fact that  $\alpha(x) > 0$  and  $\mathbf{p}(x) > 0$ , we obtain the lower bound

$$\operatorname{Re} (\beta \mathbf{a}(u, v)) \geq \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} (\beta_2 \operatorname{Im} k^2 - \beta_1 \operatorname{Re} k^2) |u|^2 dx.$$

We will choose  $\beta_1, \beta_2$  so that each integrand in the above sum is positive, e.g.

$$\beta_1 = \delta \quad , \quad \beta_2 := \frac{\beta_1 \operatorname{Re} k^2 + \delta}{\operatorname{Im} k^2} . \quad (3.19)$$

With this choice,

$$\operatorname{Re} \left( \beta \mathbf{a}(u, v) \right) > \delta \int_{\mathbb{R}^3} |\nabla u|^2 dx + \delta \int_{\mathbb{R}^3} |u|^2 dx = \delta \|u\|_{\mathcal{H}}^2 .$$

For the second to last inequality we have used that  $\alpha \geq 0$ . In this way, combined with (3.18), we have shown the  $\mathcal{H}$ -ellipticity of  $\mathbf{a}$  with constants given in (3.14).  $\square$

**Remark 5.** We cite the result of [24, Prop. 14.1 p.47] which gives the meromorphic continuation of the resolvent. Consider  $R(\omega) = (-\Delta + V - \omega)^{-1}$ . The resolvent  $R(\omega) : H^{-2} \rightarrow L^2$  is a holomorphic operator function for  $\omega \in \mathbb{C} \setminus ([0, \infty) \cup \Sigma)$  where  $\Sigma$  is a discrete set in  $[V_0, 0)$ . In a neighborhood of every point  $\omega_j$  then the resolvent admits the Laurent expansion

$$R(\omega) = -\frac{P_j}{\omega - \omega_j} + R_j(\omega),$$

where  $P_j$  is an orthogonal projection in  $L^2$  with a finite-dimensional range and  $R_j(\omega) : H^{-2} \rightarrow L^2$  is holomorphic. The range of  $P_j$  consists of eigenfunctions

$$(-\Delta + V - \omega) \psi = \omega_j \psi \quad , \quad \psi \in \operatorname{Range} P_j .$$

### 3.1.3 Well-posedness result version 2

We extend the result of Proposition 1 by allowing  $\mathbf{p}$  to have a negative lower bound, and let  $\omega^2$  be perturbed by a function which is constant outside of a compact set. We consider

$$\left( -\Delta + \frac{\alpha(x)}{|x|} + \mathbf{p}(x) - \frac{\omega^2}{c^2(x)} \right) u = f . \quad (3.20)$$

We impose the following assumptions:

- The function  $\alpha(x)$  is bounded nonnegative measurable,

$$0 \leq \alpha(x) \leq \alpha_M < \infty . \quad (3.21)$$

- The function  $\mathbf{p}(x)$  is bounded and measurable. In addition, it is allowed to take on negative values but on a compact set, outside of which  $\mathbf{p}$  is positive.

$$\mathbf{p}(x) = \mathbf{p}_c(x) + \mathbf{p}_l(x) ,$$

$$\text{with } \mathbf{p}_m \leq \mathbf{p}_c(x) \leq \mathbf{p}_M < \infty \quad , \quad \operatorname{Supp} \mathbf{p}_c \subset \mathcal{B} \quad , \quad -\infty < \mathbf{p}_m \leq 0 , \quad (3.22)$$

$$\text{and } 0 < \mathbf{p}_l < \mathbf{p}_M .$$

- The function  $c(x)$  is bounded, strictly positive, and is equal to a constant  $c_\infty > 0$  outside of a compact set  $\mathcal{B}$ ,

$$0 < c_m < c(x) < c_M < \infty \quad , \quad \operatorname{Supp} (1 - c_\infty) c(x) \subset \mathcal{B} . \quad (3.23)$$

The associated sesquilinear form is given by

$$\begin{aligned} \mathbf{a} : \mathcal{H} \times \mathcal{H} &\rightarrow \mathbb{C} \\ \mathbf{a}(u, v) &:= \int_{\mathbb{R}^3} (\nabla u) \cdot (\nabla \bar{v}) dx + \int_{\mathbb{R}^3} \left( -\frac{\omega^2}{c^2(x)} + \frac{\alpha(x)}{|x|} + \mathbf{p}(x) \right) u \bar{v} dx . \end{aligned} \quad (3.24)$$

The associated variational problem associated to (3.20) reads

$$\begin{aligned} \text{For } \ell \in \mathcal{H}^*, \text{ find } u \in \mathcal{H} \text{ such that} \\ \mathbf{a}(u, v) = \ell(v) \quad , \quad \forall v \in \mathcal{H}. \end{aligned} \quad (3.25)$$

We recall the Sobolev space notations  $\mathcal{H}$ ,  $\mathcal{V}$  and introduce  $H_0^1(\mathcal{B})$  for a compact subset  $\mathcal{B}$ ,

$$\mathcal{H} := H^1(\mathbb{R}^3), \quad \mathcal{V} := L^2(\mathbb{R}^3) \quad , \quad H_0^1(\mathcal{B}) := \{u \in \mathcal{H} \mid \text{Supp } u \subset \bar{\mathcal{B}}\}. \quad (3.26)$$

We will show that if  $\omega^2 \in \mathbb{C} \setminus ([0, \infty) \cup S)$  for a discrete subset  $S$  of  $(-\mathfrak{p}_m, 0]$ , the variational problem (3.25) has unique solution. Compared with Theorem 1, for which  $\mathfrak{p}_m = 0$ , the difference here is in the interval  $[\mathfrak{p}_m, 0]$  where there will be discrete eigenvalues.

**Proposition 2.** *Under assumptions (3.21)–(3.23), sesquilinear form  $\mathbf{a}$  (3.24) has the following properties.*

- The mapping  $\mathbf{a} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  is continuous.
- When  $\omega^2 \in \mathbb{C} \setminus [\mathfrak{p}_m \mathfrak{c}_M^2, \infty)$ ,  $\mathbf{a}$  is  $\mathcal{H}$ -elliptic. When  $\omega^2 < \mathfrak{p}_m \mathfrak{c}_M^2$ , the constants  $\mathcal{H}$ -ellipticity constants in (3.5) are

$$\sigma := 1 \quad \text{and} \quad c := \min \left\{ -\frac{\text{Re } \omega^2}{\mathfrak{c}_M^2} + \mathfrak{p}_m, 1 \right\}, \quad (3.27)$$

while for  $\text{Re } \omega^2 > \mathfrak{p}_m \mathfrak{c}_M^2$ , they are

$$\sigma := \frac{\beta}{|\beta|} \quad \text{and} \quad c := \frac{\delta}{|\beta|} \Rightarrow c = \frac{\text{Im } \omega^2}{|\omega^2 + i \mathfrak{c}_M^2 (1 - \mathfrak{p}_m)|}, \quad (3.28)$$

where for  $\delta > 0$ ,  $\beta$  is defined as,

$$\beta := \delta \frac{\omega^2 + i \mathfrak{c}_M^2 (1 - \mathfrak{p}_m)}{\text{Im } \omega^2}.$$

As a result of this, when  $\omega^2 \in \mathbb{C} \setminus [\mathfrak{p}_m \mathfrak{c}_M^2, \infty)$ , the variational problem (3.25) has a unique solution  $u \in \mathcal{H}$  with estimate

$$\|u\|_{\mathcal{H}} \leq C \|\ell\|_{\mathcal{H}^*} \quad , \quad \text{with} \quad C = \begin{cases} \frac{|\omega^2 + i \mathfrak{c}_M^2 (1 - \mathfrak{p}_m)|}{|\text{Im } \omega^2|} & , \quad \text{Re } \omega^2 \geq \mathfrak{p}_m \mathfrak{c}_M^2 \\ \frac{1}{\min \left\{ -\frac{\text{Re } \omega^2}{\mathfrak{c}_M^2} + \mathfrak{p}_m, 1 \right\}} & , \quad \text{Re } \omega^2 < \mathfrak{p}_m \mathfrak{c}_M^2 \end{cases}. \quad (3.29)$$

- For  $\omega^2 \in [\mathfrak{p}_m \mathfrak{c}_M^2, 0]$ , the Fredholm alternative holds for variational problem (3.25).

In fact, one can make a more precise statement: apart from a discrete set (possibly infinite)  $S \subset [\mathfrak{p}_m \mathfrak{c}_M^2, 0]$ ,  $A(\omega^2)$  is invertible. In addition,

$$\omega^2 \in S \quad , \quad \mathcal{N}(\omega^2) := \{u \in \mathcal{V} \mid A(\omega^2)u = 0\} \text{ is finite-dimensional.}$$

**Remark 6.** In the case of constant wavespeed  $\mathfrak{c}$ , the perturbation theory provides more precise results. In particular, with  $H_V := -\Delta + \frac{\alpha(x)}{|x|} + \mathfrak{p}(x)$ , if we impose in addition that  $\mathfrak{p} \rightarrow 0$  as  $|x| \rightarrow 0$  (which means that  $\mathfrak{p}_l \rightarrow 0$  in (3.22)), then  $S$  is the discrete spectrum  $\sigma_{\text{dis}}(H_V)$  and  $[0, \infty)$  is the essential spectrum  $\sigma_{\text{ess}}(H_V)$ . This means that in the case  $S$  is infinite, its only limiting point is 0. In this case,  $V = \frac{\alpha(x)}{|x|} + \mathfrak{p}(x)$  is called a Kato-potential (B.2) (i.e. of type  $L^2(\mathbb{R}^n) + L^2(\mathbb{R}^n)_\epsilon$ ).  $\triangle$

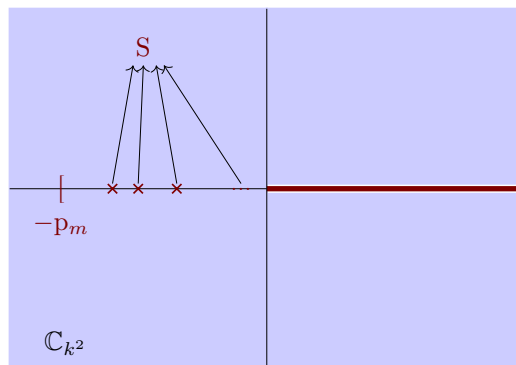


Figure 4: Illustration of results of Prop 2. Under hypothesis (3.21)–(3.23), for  $k^2 \in \mathbb{C} \setminus (\mathbf{S} \sqcup [0, \infty))$ , the variational problem to  $\left(-\Delta + \frac{\alpha(x)}{|x|} + \mathbf{p}(x) - \frac{\omega^2}{c^2(x)}\right) u = f$  for  $f \in \mathcal{H}^*$  has a unique solution  $u \in \mathcal{H}$ . Here  $\mathbf{p}_m := \min_{x \in \mathbb{R}} \mathbf{p}(x)$ ,  $\mathbf{c}_M := \max_{x \in \mathbb{R}} \mathbf{c}(x)$ , and the set  $\mathbf{S}$  represents a discrete (possibly infinite) set in the interval  $[-\mathbf{p}_m, 0)$ .

*Proof. Continuity statement:* As before, with  $\alpha(x)$  bounded, we bound the term involving  $\frac{\alpha}{|x|}$  of  $\mathbf{a}(u, v)$  using (3.16), and thus obtain the bound defining the continuity of  $\mathbf{a}$  in  $\mathcal{H} \times \mathcal{H}$ ,

$$\begin{aligned} |\mathbf{a}(u, v)| &\leq \|\nabla u\|_{\mathcal{V}} \|\nabla v\|_{\mathcal{V}} + \left( \frac{|\omega^2|}{\mathbf{c}_m^2} + \mathbf{p}_M \right) \|u\|_{\mathcal{V}} \|v\|_{\mathcal{V}} + 2\alpha_M \|\nabla u\|_{\mathcal{V}} \|v\|_{\mathcal{V}} \\ &\leq \left( 1 + \frac{|\omega^2|}{\mathbf{c}_m^2} + \mathbf{p}_M + 2\alpha_M \right) \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}}. \end{aligned} \quad (3.30)$$

**Ellipticity statement:** We develop the real and imaginary parts of  $\mathbf{a}(u, u)$

$$\begin{aligned} \operatorname{Re} \mathbf{a}(u, u) &= \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( -\frac{\operatorname{Re} \omega^2}{c^2(x)} + \mathbf{p}(x) \right) |u|^2 dx + \int_{\mathbb{R}^3} \frac{\alpha}{|x|} |u|^2 dx; \\ \operatorname{Im} \mathbf{a}(u, u) &= - \int_{\mathbb{R}^3} \frac{\operatorname{Im} \omega^2}{c^2(x)} |u|^2 dx. \end{aligned}$$

$\operatorname{Re} \omega^2 < \mathbf{p}_m \mathbf{c}_M^2$  Since  $\mathbf{c}_M^2 > 0$ , this condition can be written as

$$-\operatorname{Re} \omega^2 + \mathbf{p}_m \mathbf{c}_M^2 > 0 \Leftrightarrow -\frac{\operatorname{Re} \omega^2}{\mathbf{c}_M^2} + \mathbf{p}_m > 0 \Leftrightarrow \mathbf{p}_m \mathbf{c}_M^2 > \operatorname{Re} \omega^2. \quad (3.31)$$

Since  $\mathbf{p}_m \leq 0$  and  $\mathbf{c}^2 > 0$ , this also implies that

$$\operatorname{Re} \omega^2 < 0 \Leftrightarrow -\operatorname{Re} \omega^2 > 0.$$

In addition, since

$$0 < c^2(x) < \mathbf{c}_M^2, \quad \mathbf{p}(x) > \mathbf{p}_m,$$

we have

$$\frac{-\operatorname{Re} \omega^2}{c^2(x)} + \mathbf{p}(x) > \frac{-\operatorname{Re} \omega^2}{\mathbf{c}_M^2} + \mathbf{p}_m(x) > 0.$$

Under the current hypothesis (3.31), the lower bound is strictly positive. Together with the fact that  $\alpha > 0$ , we obtain the  $\mathcal{H}$ -ellipticity for  $\mathbf{a}$ ,

$$\begin{aligned} |\operatorname{Re} \mathbf{a}(u, u)| &\geq \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( \frac{-\operatorname{Re} \omega^2}{\mathbf{c}_M^2} + \mathbf{p}_m \right) |u|^2 dx \\ &\geq \min \left\{ -\frac{\operatorname{Re} \omega^2}{\mathbf{c}_M^2} + \mathbf{p}_m, 1 \right\} \|u\|_{\mathcal{H}}^2. \end{aligned} \quad (3.32)$$

$\boxed{\operatorname{Re} \omega^2 \geq \mathbf{p}_m \mathbf{c}_M \text{ and } \operatorname{Im} \omega^2 \neq 0}$  Consider a complex number  $\beta = \beta_1 + i\beta_2$ ,  $\beta_1 > 0$ ,  $\beta_2 \in \mathbb{R}$ ,

$$\begin{aligned} & \operatorname{Re}(\beta \mathbf{a}(u, v)) \\ &= \beta_1 \operatorname{Re} \mathbf{a}(u, v) - \beta_2 \operatorname{Im} \mathbf{a}(u, v) \\ &= \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( \frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}^2(x)} + \beta_1 \mathbf{p}(x) \right) |u|^2 dx + \int_{\mathbb{R}^3} \beta_1 \frac{\alpha}{|x|} |u|^2 dx. \end{aligned}$$

Using that  $\alpha \geq 0$ ,  $\mathbf{p}(x) > \mathbf{p}_m$ , and  $\beta_1 > 0$ .

$$\operatorname{Re}(\beta \mathbf{a}(u, v)) \geq \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( \frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}^2(x)} + \beta_1 \mathbf{p}_m \right) |u|^2 dx. \quad (3.33)$$

For  $\delta > 0$ , we define  $\beta_2$  as

$$\frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}_M^2} + \beta_1 \mathbf{p}_m = \delta \Leftrightarrow \beta_2 = \frac{\beta_1 (\operatorname{Re} \omega^2 - \mathbf{c}_M^2 \mathbf{p}_m) + \mathbf{c}_M^2 \delta}{\operatorname{Im} \omega^2}. \quad (3.34)$$

This also means that

$$\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2 = \mathbf{c}_M^2 \delta - \mathbf{c}_M^2 \beta_1 \mathbf{p}_m.$$

Since  $\mathbf{c}_M^2 > 0$ ,  $\delta > 0$ ,  $\beta_1 > 0$  and  $\mathbf{p}_m < 0$ , with  $\beta_2$  as defined by (3.34), we have

$$\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2 > \mathbf{c}_M^2 \delta.$$

This means that

$$\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2 > 0 \quad \text{and} \quad \frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}_M^2} > \delta.$$

As a result of this,

$$\frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}^2(x)} > \frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}_M^2} > \delta.$$

We use this to further bound the right-hand-side of inequality (3.33),

$$\begin{aligned} \operatorname{Re}(\beta \mathbf{a}(u, v)) &\geq \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \left( \frac{\beta_2 \operatorname{Im} \omega^2 - \beta_1 \operatorname{Re} \omega^2}{\mathbf{c}_M^2(x)} + \beta_1 \mathbf{p}_m \right) |u|^2 dx \\ &\stackrel{(3.34)}{=} \beta_1 \int_{\mathbb{R}^3} |\nabla u|^2 dx + \delta \int_{\mathbb{R}^3} |u|^2 dx. \end{aligned}$$

Upon choosing  $\beta_1 = \delta$ , we have

$$\operatorname{Re}(\beta \mathbf{a}(u, v)) > \delta \int_{\mathbb{R}^3} |\nabla u|^2 dx + \delta \int_{\mathbb{R}^3} |u|^2 dx = \delta \|u\|_{\mathcal{H}}^2. \quad (3.35)$$

With this choice and (3.34) for  $\beta_2$ ,

$$\beta = \delta \left( 1 + i \frac{\operatorname{Re} \omega^2 - \mathbf{c}_M^2 \mathbf{p}_m + \mathbf{c}_M^2}{\operatorname{Im} \omega^2} \right) = \delta \frac{\omega^2 + i \mathbf{c}_M^2 (1 - \mathbf{p}_m)}{\operatorname{Im} \omega^2}. \quad (3.36)$$

The above results, combined with (3.32) have shown the  $\mathcal{H}$ -ellipticity,  $\operatorname{Re}(\sigma \mathbf{a}(u, u)) \geq c \|u\|_{\mathcal{H}}$  with constants given by (3.27)–(3.28).

**Coercitivity statement** For the proof, we consider  $\omega^2$  with

$$\operatorname{Im} \omega^2 = 0 \quad , \quad \mathbf{p}_m \mathbf{c}_M^2 < \operatorname{Re} \omega^2 < 0. \quad (3.37)$$

We decompose  $\mathbf{a}$  as

$$\mathbf{a}(u, v) := \tilde{\mathbf{a}}(u, v) + \langle \mathcal{M}u, v \rangle_{\mathcal{H}^*, \mathcal{H}}$$

where

$$\begin{aligned} \tilde{\mathbf{a}} : \mathcal{H} \times \mathcal{H} &\rightarrow \mathbb{C} \\ \tilde{\mathbf{a}}(u, v) &:= \int_{\mathbb{R}^3} (\nabla u) \cdot (\nabla \bar{v}) dx + \int_{\mathbb{R}^3} \left( -\frac{\omega^2}{c^2(x)} + \frac{\alpha(x)}{|x|} + \mathbf{p}_l(x) \right) u \bar{v} dx. \end{aligned} \quad (3.38)$$

and  $\mathcal{M} : \mathcal{H} \rightarrow \mathcal{H}^*$  is the multiplication operator by  $\mathbf{p}_c$

$$\langle \mathcal{M} u, v \rangle_{\mathcal{H}^*, \mathcal{H}} = \int_{\mathbb{R}^3} \mathbf{p}_c u v dx.$$

Denote the associated operators to  $\mathbf{a}$  and  $\tilde{\mathbf{a}}$  by

$$\tilde{A}(\omega^2) := -\Delta - \frac{\omega^2}{c^2(x)} + \frac{\alpha(x)}{|x|} + \mathbf{p}_l(x) \quad ; \quad A(\omega^2) := \tilde{A}(\omega^2) + \mathcal{M}_{\mathcal{H} \rightarrow \mathcal{V}}. \quad (3.39)$$

The sesquilinear form  $\tilde{\mathbf{a}}$  (3.38) is  $\mathcal{H}$ -elliptic in this case. In fact, for  $-\operatorname{Re} \omega^2 > 0$ , using the assumption that  $\alpha > 0$  and  $\mathbf{p}_l > 0$ ,

$$\operatorname{Re} \tilde{\mathbf{a}}(u, u) > \int_{\mathbb{R}^3} |\nabla u|^2 dx + \int_{\mathbb{R}^3} \frac{(-\operatorname{Re} \omega^2)}{c_M} |u|^2 dx > \min\{|\operatorname{Re} \omega^2|, 1\} \|u\|_{\mathcal{H}}^2.$$

This also means the operator  $\tilde{A}(\omega^2)$  (3.39) is invertible with  $\tilde{A}(\omega^2)^{-1} : \mathcal{H}^* \rightarrow \mathcal{H}$  is bounded, which restricts to a bounded operator  $\tilde{A}(\omega^2)^{-1} : \mathcal{V} \rightarrow \mathcal{H}$ . In particular, for  $f \in \mathcal{V}$ ,

$$\|\tilde{A}^{-1} f\|_{\mathcal{H}} \leq C \|f\|_{\mathcal{H}^*} \leq C \|f\|_{\mathcal{V}}.$$

On the other hand, under the current assumption 3.22,  $\mathbf{p}_c$  is compactly supported in  $\mathcal{B}$ . We have the compactness of the embedding  $\mathbf{i} : H_0^1(\mathcal{B}) \hookrightarrow \mathcal{V}$ , cf. e.g. [23, Theorem 3.7] or [24, Thm 7.2], with  $H_0^1(\mathcal{B})$  defined in (3.26).

Weaker version: We have  $\mathcal{M}$  is a compact mapping,

$$\begin{aligned} \mathcal{M}_{\mathcal{H} \rightarrow \mathcal{H}^*} &= \underbrace{\mathbf{i}_{L^2(\mathbb{R}^3) \hookrightarrow (H^1(\mathbb{R}^3))'}}_{\text{continuous embedding}} \circ \underbrace{\mathbf{i}_{H_0^1(\mathcal{B}) \hookrightarrow L^2(\mathbb{R}^3)}}_{\text{compact embedding}} \circ \underbrace{\mathcal{M}_{H^1(\mathbb{R}^3) \rightarrow H_0^1(\mathcal{B})}}_{\text{continuous}}. \end{aligned}$$

As a result,  $\mathbf{a}$  satisfies the Gårding inequality,

$$\operatorname{Re} (\mathbf{c}(u, u) + \langle \mathcal{M} u, u \rangle_{\mathcal{H}^*, \mathcal{H}}) > \min\{|\operatorname{Re} \omega^2|, 1\} \|u\|_{\mathcal{H}}^2.$$

From here, we obtain Fredholm alternative for variational problem (3.25) under the current assumption, cf. subsection 3.1.1.

Stronger version: Since  $\tilde{A}(\omega^2)^{-1} : \mathcal{V} \rightarrow \mathcal{H}$  is bounded for  $\operatorname{Re} \omega^2 < 0$ , this means that

$$\mathbf{Q}^- := \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\}$$

is in the resolvent set  $\rho(\tilde{A})$ , and the function

$$\begin{aligned} \mathbf{Q}^- &\longrightarrow \mathcal{L}(\mathcal{V}, \mathcal{H}) \quad \text{is analytic} \\ \omega^2 &\mapsto \tilde{A}(\omega^2)^{-1}. \end{aligned} \quad (3.40)$$

Decompose by the operator  $A(\omega^2)$  as

$$A(\omega^2)_{\mathcal{H} \rightarrow \mathcal{V}} = \tilde{A}(\omega^2)_{\mathcal{H} \rightarrow \mathcal{V}} + \mathcal{M}_{\mathcal{H} \rightarrow \mathcal{V}} = \left( \mathbf{Id}_{\mathcal{V} \rightarrow \mathcal{V}} + \underbrace{\mathcal{M}_{\mathcal{H} \rightarrow \mathcal{V}} \tilde{A}(\omega^2)^{-1}_{\mathcal{V} \rightarrow \mathcal{H}}}_{= K(\omega^2) : \mathcal{V} \rightarrow \mathcal{V}} \right) \tilde{A}(\omega^2)_{\mathcal{H} \rightarrow \mathcal{V}}.$$

Hence,  $A(\omega^2) : \mathcal{H} \rightarrow \mathcal{V}$  is invertible if  $(\mathbf{Id} + K(\omega^2)) : \mathcal{V} \rightarrow \mathcal{V}$  is. From (3.40), the mapping  $K(\omega^2)$  is analytic on  $\mathbf{Q}^-$ . In addition, it is compact, being as a composition of continuous mappings with a compact one,

$$K(\omega^2)_{\mathcal{V} \rightarrow \mathcal{V}} = \underbrace{\mathbf{i}_{H_0^1(\mathcal{B}) \hookrightarrow \mathcal{V}}}_{\text{compact embedding}} \circ \underbrace{\mathcal{M}_{\mathcal{H} \rightarrow H_0^1(\mathcal{B})}}_{\text{continuous}} \circ \underbrace{\tilde{A}(\omega^2)^{-1}_{\mathcal{V} \rightarrow \mathcal{H}}}_{\text{continuous}}.$$

As a result, we can apply the analytic Fredholm theorem, cf. [34, Thm VI.14, p.201], to  $\mathbf{Id} + K(\omega^2)$ . The proof is finished by recalling that, in the ellipticity statement, we have shown that when  $\omega^2 \in \mathbb{Q}^- \setminus [\mathbf{p}_m, 0]$ ,  $\mathbf{a}$  is  $\mathcal{H}$ -elliptic, thus  $A(\omega^2)^{-1} : \mathcal{H} \rightarrow \mathcal{H}^*$  exists and is bounded, and restricts to a bounded map  $A(\omega^2)^{-1} : \mathcal{H} \rightarrow \mathcal{V}$ .

□

**Remark 7.** *With minimal modifications, the condition on the global positivity of  $\alpha$  can be relaxed to just being positive outside of a compact set but still finitely bounded below. For example with  $0 \leq \chi \leq 1$  a cut-off function  $\chi = 1$  in  $|x| \leq 1$  and  $|\chi| > 2$ , we can replace  $\alpha$  in the proof with  $(1 - \chi)\alpha$  and  $\mathbf{p}_c$  by  $\mathbf{p}_c + \chi\alpha$ . The lower bound  $\mathbf{p}$  is then  $\mathbf{p}_m = \inf_{x \in \mathbb{R}^3} \mathbf{p}_c + \chi\alpha$ .*

### 3.1.4 From the perspective of spectral theory and perturbation theory

We have shown that the operator  $-\Delta + V(x) - \mathbf{k}^2 : \mathcal{H} \rightarrow \mathcal{H}^*$  is invertible and with bounded inverse which restricts to bounded map  $(-\Delta + \mathbf{q}(x) - \mathbf{k}^2)^{-1} : \mathcal{V} \rightarrow \mathcal{H}$ . In the language of spectral theory, this means the spectrum of  $-\Delta + \mathbf{q}(x)$  is contained in  $[0, \infty)$ . Spectral theory goes beyond this result and provide more precise description of the spectrum. In particular, perturbation theory studies perturbations that preserve some property of the spectrum of the unperturbed operator. In the case of Schrödinger operator, one studies the spectrum of  $H_V = -\Delta + V(x)$  as a perturbation of the spectrum of  $\sigma(-\Delta)$ . One precise question is to determine the type of potential that would preserve first the self-adjointness and then the essential spectrum of  $-\Delta$ . Here, we focus on potentials that vanish at infinity, i.e.  $V \rightarrow 0$  as  $|x| \rightarrow \infty$ , as opposed to potential that grows at infinity as in the case of the harmonic oscillator, e.g.  $V = c|x|^2$ . More basis facts and definitions are recalled in Appendix B, here we summarize the important results for Schrödinger operator. Note that the potential of operator (3.1) under assumption (3.11) is Kato potentials (i.e. of type  $L^2(\mathbb{R}^n) + L^2(\mathbb{R}^n)_\epsilon$ , see (B.2)). An important example of the Kato class is the Coulomb potential, cf. [17, Example 14.8]. We defer further discussion for this case in Remark 23.

- As a result, cf. [17, Theorem 13.7],  $-\Delta + V$ , with  $V$  a real Kato-Rellich potential, is self-adjoint on domain  $D(\Delta) = H^2(\mathbb{R}^3)$ .

$$\sigma(H_V) \subset \mathbb{R} \quad , \quad \sigma(H_V) = \sigma_{\text{dis}}(A) \sqcup \sigma_{\text{ess}}(H_V);$$

$$\sigma_{\text{ess}}(H_V) = \{ \lambda \in \sigma(A) \mid \exists \{u_n\} \subset D(A), \|u\| = 1, u_n \xrightarrow{w} 0, (A - \lambda)u_n \xrightarrow{s} 0 \},$$

where  $\sqcup$  denotes the union of disjoint sets.

- More descriptions of the essential spectrum  $\sigma_{\text{ess}}(H_V)$  are obtained if decay at infinity is imposed for  $V$ ,

**Theorem 3** ([17, Thm 13.9]). *Assume that  $V$  is real and  $\Delta$ -bounded with relative  $\Delta$ -bound  $< 1$ , and that  $V(x) \rightarrow 0$  as  $\|x\| \rightarrow 0$ . Then  $H_V = -\Delta + V$  is self-adjoint on  $D(H + V) = H^2(\mathbb{R}^n)$  and*

$$\sigma_{\text{ess}}(H_V) = \sigma(-\Delta) = [0, \infty).$$

- By Theorem 14.9 [17], all real Kato potentials are relatively  $\Delta$ -compact. As a result, cf. [17, Cor. 14.10], for such a potential

$$\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0, \infty).$$

## 3.2 Construction and uniqueness of solution on the spectrum – Limiting Absorption Principle

The following discussion will use the weighted spaces  $L^2_\sigma(\mathbb{R}^3)$ , which consist of  $\psi \in L^2_{\text{loc}}(\mathbb{R}^3)$  with finite norm,

$$\|(1 + |x|)^{\sigma/2} \psi(x)\|_{L^2(\mathbb{R}^2)} < \infty.$$

**Theorem 4** (Weighted Sobolev embedding [24, Thm 2.5 p. 5]). *For  $s_1 > s_2$  and  $\sigma_1 > \sigma_2$  then embedding  $H^{s_1}_{\sigma_1} \subset H^{s_2}_{\sigma_2}$  is a compact operator.*

### 3.2.1 Short-range real-valued potentials

For  $H := \Delta + V(x)$  where  $V(x)$  only contains short-range perturbations. The outgoing resolvent is constructed based upon perturbation technique and uses the Born's splitting

$$H - k^2 = H_0 - k^2 + V = (H_0 - k^2) (\text{Id} + R_0(k^2) V).$$

For the rest of the discussion of short-range, we follow the exposition in [24]. The theory is also discussed in [39, Chapter 6 p.231].

**The free resolvent** The free resolvent can be constructed by using Fourier transform, cf. [24, Lemma 9.1]. Denote by  $\mathcal{R}_0(\lambda) := (-\Delta - \lambda)^{-1}$ . We have

$$\sigma(-\Delta) = \sigma_{\text{cont}}(-\Delta) = [0, \infty).$$

$\mathcal{R}_0(\lambda) : H^{-2} \rightarrow L^2$  is holomorphic for  $\lambda \in \mathbb{C} \setminus [0, \infty)$ , cf. [24, Lemma 9.1 ii.]. By using limiting absorption principle, one obtains the limit  $\mathcal{R}_0(\lambda_0 \pm i0)$ , for  $\lambda_0 > 0$ . Note that  $+i0$  stands for the limit when approaching from above the spectrum  $([0, \infty))$  and  $-i0$  from below. This also gives the limit  $\mathcal{R}_0(\lambda_0 \pm i0)$  as a bounded map between  $L^2_{-\sigma} \rightarrow L^2_{\sigma}$  for<sup>6</sup>  $\sigma > 0$ . In particular, for  $\psi \in L^2_{\sigma}$  with  $\sigma > \frac{1}{2}$ , cf. [24, p.72], we have

$$\| \mathcal{R}_0(k_0^2 \pm i\epsilon) \psi - \mathcal{R}_0(k_0^2 \pm i0) \psi \|_{L^2_{-\sigma}} \rightarrow 0, \quad \epsilon > 0.$$

In addition, by [24, Thm 18.3], with  $\sigma > \frac{1}{2}$ , the function

$$\begin{aligned} \{ \lambda \in \mathbb{C} : \text{Im } \lambda > 0 \} \setminus 0 &\rightarrow \mathcal{L}(L^2_{\sigma}, L^2_{-\sigma}) \text{ is continuous} \\ \lambda &\mapsto \mathcal{R}_0(\lambda). \end{aligned}$$

**Construction of the perturbed resolvent off the spectrum** ( $k^2 \in \mathbb{C} \setminus [0, \infty)$ ) Given the free resolvent at  $\lambda$  and the invertibility of  $1 + \mathcal{R}_0(\lambda)V$  in  $L^2(\mathbb{R}^3)$  for  $\beta > 0$  cf. [24, Prop 10.3], then  $\mathcal{R}(\lambda)$  can be constructed as a bounded map between  $L^2(\mathbb{R}^3)$  by using the Born splitting, cf. [24, Theorem 10.5 p. 33],

$$\mathcal{R}(\lambda) = (1 + \mathcal{R}_0(\lambda)V)^{-1} \mathcal{R}_0(\lambda). \quad (3.41)$$

The invertibility of  $\text{Id} + \mathcal{R}_0(\lambda)V$  is obtained by Fredholm theory, by first showing its compactness, cf. [24, Lemma 10.2], and then by showing that for  $\lambda \in \mathbb{C} \setminus [V_0, \infty)$ , the only solution in  $L^2$  to  $(H - \lambda)\psi = 0$  is the trivial one, cf. [24, Prop 10.3]. Note that, for the compactness, we only need some decay. In particular, we require for  $\lambda \in \mathbb{C} \setminus [0, \infty)$ , if  $V$  satisfies

$$V(x) \in \mathcal{C}(\mathbb{R}^3) \quad , \quad \sup_{x \in \mathbb{R}^3} (1 + |x|^2)^{\beta/2} |V(x)| < \infty \quad , \quad \beta > 0, \quad (3.42)$$

then  $R_0(k^2)V$  and  $V\mathcal{R}_0(k^2)$  are compact in  $L^2(\mathbb{R}^3)$ , cf. [24, Lemma 10.2]. By definition, a short-range decay requires  $\beta > 1$ . The resolvent is then extended as a meromorphic<sup>7</sup> function to  $[V_0, 0)$ , cf. [24, Prop 14.1].

**Construction of the perturbed resolvent on the spectrum**  $k^2 > 0$  : We will take limit as  $\lambda$  approaches the spectrum of the Born splitting (3.41), the result of which is given in [24, Theorem 19.2]. Here more decay requirement has to be imposed on the potential, i.e.

$$V(x) \in \mathcal{C}(\mathbb{R}^3) \quad , \quad \sup_{x \in \mathbb{R}^3} (1 + |x|^2)^{\beta/2} |V(x)| < \infty \quad , \quad \beta > 1. \quad (3.43)$$

Since one will need to show  $[\text{Id} + \mathcal{R}_0(\lambda_0 + \pm i\epsilon)V]^{-1} \rightarrow [\text{Id} + \mathcal{R}_0(\lambda_0 + \pm i0)V]^{-1}$ . This requires the following ingredients.

<sup>6</sup>Note that  $\sigma$  cannot be zero since  $[0, \infty)$  is continuous spectrum (thus lack of the existence of bounded inverse in  $L^2$ ).

<sup>7</sup>In fact, the function  $\mathbb{C} \setminus ((0, \infty) \cup \Sigma) \rightarrow \mathcal{L}(H^{-2}, L^2)$ ,  $\lambda \mapsto \mathcal{R}(\lambda)$  given by (3.41) is holomorphic. Here  $\Sigma \subset [V_0, 0)$  is a discrete set.



1. Limiting absorbing principle for the free resolvent, see discussion above.

2. The invertibility of  $\text{Id} + \mathcal{R}(\lambda \pm i0)V$  is obtained by Fredholm theory as follows.

- One first shows the compactness of  $\mathcal{R}(\lambda \pm i0)V$ . By [24, Lemm 19.1], for  $\beta > 1$  and  $k_0 > 0$ , we have<sup>8</sup>

$$\mathcal{R}_0(k_0^2 \pm i0)V : L_{-\sigma}^2 \longrightarrow L_{-\sigma}^2 \text{ is compact for } \sigma \in (\tfrac{1}{2}, \beta - \tfrac{1}{2}).$$

- Injectivity, if  $(1 + \mathcal{R}_0(\lambda \pm i0)V : L_{-\sigma}^2 \rightarrow L_{-\sigma}^2$  for  $k_0 > 0$ . We can apply Fredholm since  $\mathcal{R}_0(\lambda \pm i0)V$  is compact. This means for invertibility we need injectivity, i.e. that for  $k > 0$ , the problem

$$(-\Delta - k_0^2 + V(x))\psi = 0 \quad , \quad \psi \in L^2(\mathbb{R}^3),$$

only has trivial solution  $\psi = 0$ . This is given by applying Agmon's theorem which gives the decay of eigenfunction, cf. [24, Theorem 20.2] and then Kato's theorem giving the absence of the positive eigenvalues, cf. e.g. [24, Thm 15.1] or [39, Thm 1.1].

**Theorem 5** (Kato). *If the operator  $H = -\Delta + V$  is defined with  $V$  satisfying*

$$|v(x)| \leq C(1 + |x|)^{-\rho} \quad , \quad \rho > 1,$$

*or  $V$  continuous real function satisfying*

$$\lim_{|x| \rightarrow \infty} |x| V(x) = 0,$$

*then  $H$  does not have positive eigenvalues. That is if  $H\psi = \lambda\psi$  with  $\lambda > 0$  and  $\psi \in L^2$  then  $\psi = 0$ .*

As a result, one obtains the convergence of

$$(1 + \mathcal{R}_0(\lambda \pm i\epsilon)V)^{-1} \rightarrow (1 + \mathcal{R}_0(\lambda \pm i0)V)^{-1} \quad , \quad \epsilon > 0, \epsilon \rightarrow 0,$$

in the norm  $\mathcal{L}(L_{-\sigma}^2, L_{-\sigma}^2)$  and that, for  $\sigma > 1/2$ , cf. [24, Thm 19.2], the mapping

$$\begin{aligned} \{\lambda \in \mathbb{C} \mid \text{Im } \lambda \geq 0\} \setminus (\Sigma \cup \{0\}) &\longrightarrow \mathcal{L}(L_{-\sigma}^2, L_{-\sigma}^2) \text{ is continuous} \\ \lambda &\mapsto \mathcal{R}(\lambda). \end{aligned}$$

**Uniqueness and asymptotics of solutions** They follow from the properties of those given by the free resolvent. In particular, the solution given by  $\mathcal{R}(\lambda_0 \pm i0)$  is determined uniquely by the radiation condition cf. [39, Eqn 6.1.9 p. 233]

$$\lim_{r \rightarrow \infty} \int_{|x|=r} |\partial_r u(x) \mp i\lambda^{1/2} u(x)| dS_r = 0. \quad (3.44)$$

The uniqueness statement can be found in [39, Theorem 6.1.7 or Theorem 6.1.4 p. 233]. That the limiting solution satisfies the radiation condition is shown in [39, Theorem 4.4 and Cor 4.5], by using the asymptotics property of the free resolvent.

**Remark 8.** *One has another definition of outgoing solution. For  $u \in L_{loc}^2(\mathbb{R}^3)$ ,  $u$  is  $k_0$ -outgoing solution if*

$$u = -\mathcal{R}_0(k_0^2 + i0)f$$

*outside of some compact set for  $f \in L_{\sigma}^2(\mathbb{R}^3)$  with  $\sigma > 1/2$ , cf., e.g., [31, Definition 3.1].*

<sup>8</sup> This can be seen as follows. We first decompose the mapping from  $L_{-\sigma}^2 \rightarrow L_{-\sigma}^2$  as

$$L_{-\sigma}^2 \xrightarrow{V} L_{\sigma'}^2 \xrightarrow{\mathcal{R}_0(\lambda + i0)} H_{-\sigma'}^2 \xrightarrow{\text{Id}} L_{\sigma}^2.$$

Requirements have to be imposed on  $\sigma$ ,  $\sigma'$  and  $\beta$ , for the first two mappings to be continuous and the last one to be compact.

- The first mapping, under assumption (3.42), the multiplication operator by potential  $V$  is continuous if  $\sigma' + \sigma < \beta$ .
- The free resolvent on the spectrum  $\mathcal{R}_0(\lambda + i0)$  is continuous  $\sigma' > \frac{1}{2}$ , cf. [24, Thm 18.3 i]
- The embedding  $\text{Id}$  is continuous if  $\sigma' < \sigma$ .

This means

$$\frac{1}{2} < \sigma' < \sigma \quad , \quad \sigma' + \sigma < \beta \quad \Rightarrow \quad \beta > 1.$$

This explains why we need  $\beta > 1$ , equivalently that  $V$  is a continuous short-range potential.

### 3.2.2 Long-range real-valued potentials

We have seen in the previous discussion that in order to use perturbation theory with respect to  $-\Delta$  to obtain the limit on the spectrum of the resolvent of the  $H_V := -\Delta + V$ , one has to require that  $V$  decays faster than  $|x|^{-1}$  at infinity. This requirement is needed to obtain the compactness of the  $\mathcal{R}_0(\lambda + \pm iV)$ , which is a key ingredient in perturbation theory. The machinery has to be redone for slower decaying potentials, e.g. the work of Ikebe and Saito, or by Mourre's commutator method, cf. [39, p. 428] for the review of literature of LAP. We consider the equation of the form,

$$(-\Delta + V(x) - \lambda)u = f. \quad (3.45)$$

Define the resolvent at  $\lambda$  when it exists

$$\mathcal{R}(\lambda) := (-\Delta + V(x) - \lambda)^{-1}.$$

**Assumptions:** Real potential  $V$  is a *bounded* function, and for sufficient large  $|x|$ , admits a representation as a sum

$$V = V_S + V_L, \quad V = \overline{V}, \quad (3.46)$$

where  $V_S$  is a short-range potential with

$$V_S = O(|x|^{-\rho_s}) \quad , \quad \rho_s > 1 \quad , \quad |x| \rightarrow \infty, \quad (3.47)$$

and  $V_L$  a long-range one differential in  $|x|$ ,

$$V_L = O(|x|^{-\rho_l}) \quad , \quad \partial_r V_L = O(|x|^{-1-\rho_l}) \quad , \quad \rho_l > 0 \quad , \quad |x| \rightarrow \infty. \quad (3.48)$$

Using commutator estimates, it is shown, cf. [39] that the same radiation conditions as that for the short-range case, cf. (3.44), can be used to define uniquely a solution to (3.45),

$$\lim_{r \rightarrow \infty} \int_{|x|=r} |\partial_r u(x) \mp i\lambda^{1/2} u(x)| dS_r = 0. \quad (3.49)$$

**Theorem 6** (Uniqueness - [39, Thm 11.3.7]). *Assume that potential  $V$  satisfies (3.46)–(3.48). If  $u \in H_{loc}^2$  is a solution of  $-\Delta + V(x) - \lambda)u = 0$  and  $u$  satisfies one of the radiation condition (3.49), then  $u = 0$ .*

Note that also by commutator estimate technique and the notion of  $H$ -smooth of Kato<sup>9</sup>, the absence of positive eigenvalue is shown, in another word, the positive spectrum of  $-\Delta + V$  is absolutely continuous, cf. [39, Thm 11.1.1 and Cor 11.1.2].

**Theorem 7** (Existence by LAP - [39, Thm 11.3.6 – 11.3.7]). *Assume that potential  $V$  satisfies (3.46)–(3.48),  $f \in L_\sigma^2$ , and  $\sigma$  satisfies*

$$\frac{1}{2} < \sigma < \frac{3}{2} \quad , \quad \sigma < \rho_s - \frac{1}{2} \quad , \quad \sigma < \frac{1 + \rho_l}{2}. \quad (3.50)$$

Define the set

$$Q := \{\lambda = (k + i\epsilon)^2 \in \mathbb{C} \mid 0 < c_1 \leq k \leq c_2 \quad , \quad 0 < \epsilon \leq 1\}.$$

<sup>9</sup>For  $V$  admitting a long-range potential, we cite [39, Corollary 11.1.2]. It uses Kato's 'smoothness', cf. [39, Eq. 0.5.2 p. 30]. For a  $K$ -bounded operator  $G : \mathcal{H} \rightarrow C$

$$\sup_{\lambda \in X, \epsilon > 0} \|G(\mathcal{R}(\lambda + i\epsilon) - \mathcal{R}(\lambda - i\epsilon))G^*\| < \infty.$$

The main result is [39, Prop 0.5.3 p.30] which gives that if there exists an operator  $G$  that is  $K$ -smooth on Borel set  $X \subset \mathbb{R}$  with  $\text{Ker} G = \{0\}$ , then the spectrum of  $K$  is absolutely continuous on  $\overline{X}$ .

To apply to the case of Shrödinger equation: it is shown in [39, Thm 1.1] if  $Q$  is the operator of multiplication by  $(1 + r^2)^{-\sigma/2}$  with

$$\frac{1}{2} < \sigma < \frac{1}{2} \min\{\rho_s, 1 + \rho_l\}$$

then  $Q$  is  $H$ -smooth, and if  $\text{Ker } G$  is trivial then  $H$  is absolutely continuous on  $\overline{X}$ .

Then the function

$$\begin{aligned} u &: \mathbb{Q} \longrightarrow L^2_{-\sigma}(\mathbb{R}^n) \quad \text{is continuous.} \\ z &\mapsto u(z) := \mathcal{R}(z) \end{aligned}$$

Thus  $u(z)$  has boundary value along the cut  $[0, \infty)$ , denoted by  $u(\lambda_0 \pm i0)$ ,  $\lambda_0 > 0$ . This is a solution of

$$(-\Delta + V - \lambda_0)u = f.$$

In addition, it satisfies the following estimates

$$\begin{aligned} \|u(z)\|_{-\sigma} &\leq C \|f\|_{\sigma}; \\ \|u_r(z) - i\lambda^{1/2}u(z)\|_{\sigma-1} + \|\nabla^\perp u(z)\|_{\sigma-1} &\leq C \|f\|_{\sigma}, \end{aligned} \quad (3.51)$$

where  $C$  does not depend<sup>10</sup> on  $z \in \mathbb{Q}$ . In particular, the limiting solution satisfies

$$u_r(\lambda_0 \pm i0) \mp i\lambda_0^{1/2}u(\lambda_0 \pm i0) \in L^2_{\sigma-1}, \quad \lambda_0 > 0.$$

As a result of this, it satisfies the outgoing (incoming) radiation condition (3.49).

For other discussion of resolvent estimate in weighted  $L^2_\sigma$  spaces for LAP, we refer to the introduction of [42, p. 859–862].

**Theorem 8** ([14, Theorem 3.4]). *Assume that potential  $V$  satisfies (3.46)–(3.48). In addition, the long-range part  $V_L$  is  $\mathcal{C}^3$  with*

$$|\partial^m V_L| \leq c (1 + |x|)^{-\delta - |\beta|}, \quad \delta \in (0, 1], \quad 0 \leq |\beta| \leq 3.$$

With  $\lambda_0 > 0$ , for  $f \in L^2_\sigma$ ,  $\sigma > \frac{1}{2}$ , then<sup>11</sup>, with  $\mathcal{R}(\lambda) = (-\Delta - \lambda + V)^{-1}$ ,

$$\begin{aligned} (\mathcal{R}(\lambda_0 + i0)f)(x) &= \pi^{1/2}\lambda_0^{-1/4} \frac{e^{i\phi(x, \lambda_0)}}{|x|} \mathbf{a}_+\left(\frac{x}{|x|}\right) + o(|x|^{-1}), \\ (\partial_r \mathcal{R}(\lambda_0 + i0)f)(x) &= i\pi^{1/2}\lambda_0^{1/4} \frac{e^{i\phi(x, \lambda)}}{|x|} \mathbf{a} + \left(\frac{x}{|x|}\right) + o(|x|^{-1}), \end{aligned} \quad (3.52)$$

for some  $\mathbf{a}_+, \mathbf{a}_- \in L^2(\mathbb{S}^2)$  as  $|x| \rightarrow \infty$ . Here, the phase  $\phi(x, \lambda)$  is an exact or approximated solution to the eikonal equation

$$\|\nabla_x \phi(x, \lambda)\|^2 + V(x) = \lambda. \quad (3.53)$$

**Remark 9** (Sharp LAP). *We first note that in sharper form of LAP, the weighted  $L^2_\sigma$  spaces are replaced by the Agmon–Hörmander space  $\mathfrak{B}$  and  $\mathfrak{B}^*$  its dual (with respect to  $L^2(\mathbb{R}^3)$ ). The space  $\mathfrak{B}$  consists of functions  $f$  such that*

$$\|f\|_{\mathfrak{B}} := \left( \int_{|x| \leq 1} |f(x)| dx \right)^{1/2} + \sum_{k=0}^{\infty} \left( 2^k \int_{2^k \leq |x| \leq 2^{k+1}} |f(x)|^2 dx \right)^{1/2} < \infty. \quad (3.54)$$

Denote by  $\mathfrak{B}'$  its dual space with respect to  $L^2$ . Its norm is given by [39, Eqn. 6.3.2], with an equivalent form,

$$\|g\|_{\mathfrak{B}^*} := \sup_{r \geq 1} \left( \frac{1}{r} \int_{|x| \leq r} |g(x)|^2 ds \right)^{1/2}. \quad (3.55)$$

<sup>10</sup>In fact, the constant  $C$  does not depend on  $\lambda$  from compact subset of  $(\mathbb{C} \setminus \{0\}) \cap (\mathbb{C} \setminus [0, \infty))$ .

<sup>11</sup>We also have similar for the incoming solutions

$$\begin{aligned} (\mathcal{R}(\lambda - i0)f)(x) &= \pi^{1/2}\lambda^{-1/4} \frac{e^{-i\phi(x, \lambda)}}{|x|} \mathbf{a}_-\left(\frac{x}{|x|}\right) + o(|x|^{-1}); \\ (\partial_r \mathcal{R}(\lambda - i0)f)(x) &= i\pi^{1/2}\lambda^{1/4} \frac{e^{-i\phi(x, \lambda)}}{|x|} \mathbf{a}_-\left(\frac{x}{|x|}\right) + o(|x|^{-1}). \end{aligned}$$

Note that, cf. [39, p. 235],

$$L_\sigma^2 \subset \mathfrak{B} \subset L_{1/2}^2 \subset L^2 \subset L_{-1/2}^2 \subset \mathfrak{B}^* \subset L_{-\sigma}^2, \quad \sigma > 1/2. \quad (3.56)$$

Under the same assumption in cited Theorem 7, the resolvent estimate (3.51) can be replaced with

$$\|\mathcal{R}(\lambda)\|_{\mathfrak{B}, \mathfrak{B}^*} \leq C, \quad \text{Im } \lambda \neq 0. \quad \triangle$$

In the above cited theory, the potential  $V$  is assumed bounded. However, it can be allowed to develop some singularity. We comment on this extension in the following remark.

**Remark 10** (Scattering with long-range singular potential). *Due the existence of a Coulomb-like potential  $\frac{\alpha(x)}{|x|}$ , where  $\alpha$  is a continuous bounded function, we need to allow for singularity in  $V$ . However, we only need results for mild singularity. For this purpose, we will cite results of [42] which is for a more general problem: the magnetic potential. We will only need what is called the electric potential there, and set the magnetic potential to zero in the assumptions and results of [42]. We first use [42, Assumptions 1.5, 1.20–1.22], the real potential is decomposed into a short and bounded long-range one,*

$$V = V_L + V_S, \quad (3.57)$$

with assumptions,

$$V_S, V_L \in L_{loc}^1(\mathbb{R}^3), \quad \int (V_S + V_L) |u|^2 dx \leq \beta \int |\nabla u|^2 dx, \quad 0 < \nu < 1, \quad (3.58)$$

and for some  $c > 0$ ,  $r_0 > 0$  and  $\mu > 0$

$$\begin{aligned} \frac{|V_L|}{|x|} + (\partial_r V_L)_+ + |V_S| &\leq \frac{c}{|x|^{1+\mu}}, & \text{for } x \geq r_0; \\ V_L = (\partial_r V_L(x))_+ &= 0, & \text{if } |x| \leq r_0; \\ |V_S| &\leq \frac{c}{|x|^{2-\beta}}, & \text{for } |x| \leq r_0, \beta > 0. \end{aligned} \quad (3.59)$$

Here  $(\cdot)_+$  is the positive part. Note that there is a switch in sign convention compared to [42]. Setting the magnetic potential to be zero, for a fixed  $\lambda > 0$ , and all  $\lambda_0 > \lambda$ , theorem [42, Thm 1.7] gives that there exists a unique solution  $u \in H_{loc}^1(\mathbb{R}^3)$  of the equation

$$(-\Delta + V + \lambda_0)u = 0,$$

satisfying estimate

$$\lambda_0 \|u\|_{\mathfrak{B}^*}^2 + \|\nabla u\|_{\mathfrak{B}^*}^2 + \int \frac{|\nabla^\perp u|^2}{|x|} dx + \sup_{R>0} \frac{1}{R^2} \int_{|x|=R} |u|^2 d\sigma_R \leq C(\lambda) \|f\|_{\mathfrak{B}}, \quad (3.60)$$

and radiation condition with  $0 < \delta < 1$  with  $\delta < \mu$  (here  $\mu$  is in (3.58))

$$\int_{|x| \geq 1} \left| \nabla u - i\sqrt{\lambda_0} \frac{x}{|x|} u \right|^2 \frac{dx}{(1+|x|)^{1-\delta}} \leq C(\lambda) \|f\|_{L_{2+2\delta}^2}. \quad (3.61)$$

The solution is given as a limit of the sequence  $\mathcal{R}(\lambda_0 + i0)f$  as  $\epsilon \rightarrow 0^+$  in  $H_{loc}^1$ . Here  $\mathfrak{B}$  and its dual  $\mathfrak{B}^*$  are the Agmon-Hörmander spaces defined in (3.54)–(3.55). Note that  $\|\cdot\|_{\mathfrak{B}}$  and  $\|\cdot\|_{\mathfrak{B}^*}$  are denoted in [42] respectively by  $N_1(\cdot)$  and  $\|\cdot\|_1$ .  $\triangle$

**Remark 11** ( $L^2$ -type radiation condition). *The solution obtained by limiting absorption principle can be shown to satisfy a Sommerfeld-type radiation, which in turns defines its uniqueness. For more discussion of other forms of radiation condition see the introduction of [33, p.5]. We cite a result by Saito [36]. For*

$$V = p_{long}(x) + p_{short},$$

where  $p_{\text{short}}$  is a short-range potential, and  $p_{\text{long}}$  a bounded real function in  $\mathcal{C}^2(\mathbb{R}^3 \setminus \{0\})$

$$|\partial_x^\sigma p(x)| \leq c|x|^{-\sigma|x|} \quad , \quad |\sigma| \leq 2,$$

the solution given by limiting absorption principle satisfies radiation condition of the form,

$$\int_{\mathbb{R}^3} \left| \nabla u - i(\nabla \phi)u \right|^2 \frac{dx}{(1+|x|)^{1-\delta}} < +\infty, \quad (3.62)$$

where  $0 < \delta < 1$  is a fixed constant. Here, the phase  $\phi(x, \lambda)$  is an exact or approximate solution to the eikonal equation

$$\|\nabla_x \phi(x, \lambda)\|^2 + p_{\text{long}}(x) = \lambda.$$

In more recent results by [33, 43], the radiation condition is given in the form,

$$\int_{\mathbb{R}^3} \left| \nabla u - iV_\infty u \frac{x}{|x|} \right|^2 \frac{dx}{|x|} < +\infty, \quad (3.63)$$

where

$$V(x) \rightarrow V_\infty \quad , \quad x \rightarrow \infty.$$

For more discussion of other forms of radiation conditions, see the introduction of [36, 41, 33].  $\triangle$

### 3.3 Application to the conjugated operator

The goal of this section is to obtain the resolvent of the conjugated operator  $\mathcal{L} := \rho^{1/2} \mathcal{L}_{\text{orig}} \rho^{-1/2}$ , cf. (2.5). At the complex wave number  $\omega^2$  introduced in (1.2),

$$\omega = \mathfrak{g}_2(1 + i\gamma) \omega_0 \quad , \quad \text{where } \omega_0 \in \mathbb{R}^+ \text{ and } \gamma \in \mathbb{R},$$

where  $\mathfrak{g}_2$  is the branch of square root, cf. (4.11b). The normalized form (2.19) of  $\mathcal{L}$  is

$$\mathcal{L} = -\Delta - \mathbf{k}^2 + \frac{\alpha(x)}{|x|} + \mathbf{p}_2(x) + \mathbf{p}_3(x) + \omega^2 \mathbf{p}_1. \quad (3.64)$$

The involved potentials are

$$\begin{aligned} \mathbf{p}_1 &= -\frac{1}{c^2(x)} + \frac{1}{c_\infty^2} \quad ; \quad \alpha = \frac{\partial_r \rho}{\rho}; \\ \mathbf{p}_2 &= \frac{\alpha^2}{4} + \frac{\partial_r \alpha}{2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2}; \\ \mathbf{p}_3 &= \frac{1}{|x|^2} \left( \frac{3 \|\nabla_{\mathbb{S}^2} \rho\|^2}{4 \rho^2(x)} - \frac{\Delta_{\mathbb{S}^2} \rho}{2 \rho(x)} \right). \end{aligned}$$

Here, we work under the assumption that the potentials do not oscillate and have constant limits at infinity defined in (2.17),

$$\alpha_\infty := \lim_{r \rightarrow \infty} \alpha \quad ; \quad \alpha'_\infty := \lim_{r \rightarrow \infty} \partial_r \alpha \quad ; \quad c_\infty := \lim_{r \rightarrow \infty} c.$$

In addition,  $\mathbf{p}_1$  is smooth and compactly supported, while  $\mathbf{p}_2$  and  $\mathbf{p}_3$  are short-range potentials.  $\alpha$  is positive and bounded in  $L^2(\mathbb{R}^3)$ . The normalized wavenumber of the conjugated operator is defined in (2.18)

$$\mathbf{k}^2 = \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2}, \quad (3.65)$$

from the complex frequency  $\omega$ . When there is no attenuation, i.e. when  $\gamma = 0$ , the normalized wavenumber reduces to

$$\mathbf{k}_0^2 = \frac{\omega_0^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha'_\infty}{2}. \quad (3.66)$$

We introduce the following family of potentials,

$$\begin{aligned} V_0 &:= \frac{\alpha(x)}{|x|} + p_2(x) + p_3(x); \\ V_\beta &:= V_0 + \beta p_1. \end{aligned} \quad (3.67)$$

We also consider the following family of operators parametrized by complex numbers  $\beta$  and  $\lambda$ ,

$$\mathcal{L}_{\beta,\lambda} := -\Delta - \lambda + V_\beta. \quad (3.68)$$

We denote its resolvent by

$$\mathfrak{R}_\beta(\lambda) := (\mathcal{L}_{\beta,\lambda})^{-1} \quad \text{when it exists.}$$

Note that the conjugated operator (3.64) is

$$\mathcal{L} = \mathcal{L}_{\omega^2, k^2}, \quad \text{where } k \text{ is defined by (3.65).}$$

Our goal is to consider

$$\mathcal{L}^{-1} = \mathfrak{R}_{\omega^2}(k^2).$$

**Construction of solution for  $k^2 \in \mathbb{C} \setminus [0, \infty)$**  Recall that when  $\text{Im } \omega \neq 0$ , Prop 2 gives that

$$\mathfrak{R}_{\omega^2}(k^2) \in L^2(\mathbb{R}^3), \quad \omega^2 \in \mathbb{C} \setminus [0, \infty) \cup \Sigma, \quad (3.69)$$

where  $\Sigma$  is a discrete set in  $[a, 0)$ , with

$$a := \inf_{x \in \mathbb{R}^3} V_0, \quad c := \sup_{x \in \mathbb{R}^3} c.$$

**Construction of solution for  $k^2 \in (0, \infty)$**  It remains to define the resolvent at real parameters, i.e.

$$\mathfrak{R}_{\omega_0^2}(k_0^2).$$

We first make a remark regarding the real potentials  $V_0$  and  $V_{\omega_0^2}$  for fixed  $\omega_0^2$ .

**Remark 12.** Potential  $V_0$  (3.67) contains both short-range and long-range contribution. The presence of the Coulomb-like potential is dealt with by using the results of [42] discussed in Remark 10. We discuss briefly how potential (3.67) satisfies the required assumptions of this theory. Using a cut-off function<sup>12</sup>  $\chi \in C_c^\infty(\mathbb{R})$ , we first rewrite the Coulomb-like potential as

$$\frac{\alpha(x)}{|x|} = (1 - \chi(x)) \frac{\alpha(x)}{|x|} + \chi(x) \frac{\alpha}{|x|},$$

to separate out the singularity behavior at the origin and the slow decay at infinity. The compactly supported part  $\chi(x) \frac{\alpha(x)}{|x|}$ , which contains the Coulomb singularity, will be absorbed into the short range one, and leaves the slow decay at infinity to the long-range part of the potential. In particular,

$$V_0 = V_0^S + V_0^L, \quad V_0^L = (1 - \chi(x)) \frac{\alpha(x)}{|x|}. \quad (3.70)$$

It can be verified that potential  $V_0^L$  and  $V_0^S$  satisfy assumptions (3.58) with  $\mu$  in (3.58) equal to 1. On the other hand, the real potential  $V_{\omega^2}$  is only different from  $V_0$  by a compactly supported term which is smooth, we can use the same decompositions:

$$V_{\omega_0^2} = V_{\omega_0^2}^L + V_{\omega_0^2}^S, \quad V_{\omega_0^2}^L = V_0^L = (1 - \chi(x)) \frac{\alpha(x)}{|x|}.$$

with  $V_{\omega_0^2}^L$  and  $V_{\omega_0^2}^S$  also satisfying (3.58). △

<sup>12</sup>An example of  $\chi$  is  $\chi = 1$  for  $|x| \leq 1$  and  $\chi = 0$  for  $|x| \geq 2$ , and smoothly continued in between 1 and 2.

**Approach 1** For each fixed  $\omega_0^2$ , Remark 12 allows us to apply Theorem 1.7 of [42] to operator

$$-\Delta + V_{\omega_0^2},$$

which gives that the mapping

$$\begin{aligned} Q &\longrightarrow \mathcal{L}(\mathfrak{B}, \mathfrak{B}^*) \\ \lambda &\mapsto \left(-\Delta + V_{\omega_0^2} - \lambda\right)^{-1} \text{ is uniformly continuous.} \end{aligned}$$

Here

$$Q := \{\lambda \in \mathbb{C} \mid 0 < c_1 < \operatorname{Re} \lambda < c_2, \quad 0 \leq \operatorname{Im} \lambda \leq 1\}.$$

In particular, the boundary limit as  $\operatorname{Im} \lambda \rightarrow 0$  exists which gives a definition at  $\lambda = k_0^2$  for

$$\mathfrak{R}_{\omega_0^2}(k_0^2) := \left(-\Delta + V_{\omega_0^2} - (k_0^2 + i0)\right)^{-1}. \quad (3.71)$$

In addition, for  $f \in \mathfrak{B}$ ,  $\mathfrak{R}_{\omega_0^2}(k_0^2)f$  defines the unique solution  $u \in H_{\text{loc}}^1(\mathbb{R}^3)$  to

$$(-\Delta + V_{\omega_0^2} - \lambda)u = f, \quad \text{with } \lambda = k_0^2, \quad (3.72)$$

satisfying radiation condition (3.61) at  $\lambda = k_0^2$ ,

$$\int_{|x| \geq 1} \left| \nabla u - i k_0 \frac{x}{|x|} u \right|^2 \frac{dx}{(1 + |x|)^{1-\delta}} < \infty, \quad 0 < \delta < 1. \quad (3.73)$$

and asymptotic expansion (3.88) listed below.

**Remark 13.** In this approach,  $p_1$  does not have to be compactly supported, it only needs to decay no slower than a long-range potential.

**Approach 2** The difference here is to work solely with operator  $-\Delta - V_0$  and its resolvent  $\mathfrak{R}_0(\lambda)$  and use perturbation theory. The result is achieved in two steps.

**Step 1** By Remark 12, we can apply Theorem 1.7 of [42], cited in Remark 10, which gives that

$$\begin{aligned} Q &\longrightarrow \mathcal{L}(\mathfrak{B}, \mathfrak{B}^*) \\ \lambda &\mapsto (-\Delta + V_0 - \lambda)^{-1} \text{ is uniformly continuous,} \end{aligned} \quad (3.74)$$

and thus has boundary value as  $\operatorname{Im} \lambda \rightarrow 0^+$ . It defines a bounded inverse at  $\lambda = k_0^2$ ,

$$\mathfrak{R}_0(k_0^2) := \left(-\Delta + V_0 - (k_0^2 + i0)\right)^{-1} \in \mathcal{L}(\mathfrak{B}, \mathfrak{B}^*), \quad \sigma > 1/2. \quad (3.75)$$

In fact, with  $\Sigma'$  denoting a discrete set in  $[a, 0)$ , we have the definition of

$$\begin{aligned} \mathfrak{R}_0(\lambda) &\in \mathcal{L}(L^2(\mathbb{R}^3)) \quad , \quad \text{for } \lambda \in \mathbb{C} \setminus ([0, \infty) \cup \Sigma') \text{ with } \operatorname{Re} \lambda \geq 0; \\ \mathfrak{R}_0(\lambda) &\in \mathcal{L}(\mathfrak{B}, \mathfrak{B}^*) \quad , \quad \text{for } \lambda \in (0, \infty). \end{aligned} \quad (3.76)$$

In addition, for  $\lambda > 0$ ,  $\mathfrak{R}_0(\lambda)f$  defines the unique solution to  $(-\Delta + V_0 - \lambda)u = f$  satisfying radiation condition (3.61).

**Remark 14.** Note that the results in 10 gives the sharp form of LAP in the Agmon-Hörmander spaces  $\mathfrak{B}$  and its dual  $\mathfrak{B}^*$  (3.55). The current (weaker) result in weighed  $L^2$  space is obtained by using the inclusion of spaces (3.56).  $\triangle$

**Step 2** It remains to take care of the compact supported perturbation  $\omega^2 \mathbf{p}_1$ . We write  $-\Delta - V_\beta - \lambda$  as a perturbation of  $-\Delta - V_0 - \lambda$ ,

$$\begin{aligned} -\Delta - V_\beta - \lambda &= \left( \text{Id} + \beta \mathbf{p}_1 \mathfrak{R}_0(\lambda) \right) (-\Delta - V_0 - \lambda) \\ &= (-\Delta - V_0 - \lambda) \left( \text{Id} + \beta \mathfrak{R}_0(\lambda) \mathbf{p}_1 \right). \end{aligned} \quad (3.77)$$

This leads to the Born splitting

$$\mathfrak{R}_\beta(\lambda) = \left( \text{Id} + \beta \mathfrak{R}_0(\lambda) \mathbf{p}_1 \right)^{-1} \mathfrak{R}_0(\lambda). \quad (3.78)$$

**Remark 15.** Note that when  $\omega \in \lambda\mathbb{C} \setminus ([0, \infty) \cup \Sigma')$  with  $\beta = \omega^2$  and  $\lambda = \mathbf{k}^2$  defined in (3.65), using the Born splitting (3.78), we reobtain  $\mathfrak{R}_{\omega^2}(\mathbf{k}^2)$  in (3.69).  $\triangle$

We focus on the case when  $\beta = \omega_0^2$ ,

$$\mathfrak{R}_{\omega_0^2}(\lambda) = \left( \text{Id} + \omega_0^2 \mathfrak{R}_0(\lambda) \mathbf{p}_1 \right)^{-1} \mathfrak{R}_0(\lambda).$$

Given the existence of  $\mathfrak{R}_0(\lambda)$  in Step 1, cf. (3.76), it remains to justify the existence of the inverse of

$$\text{Id} + \omega_0^2 \mathfrak{R}_0(\mathbf{k}_0^2) \mathbf{p}_1.$$

We proceed as follows.

- Using the same argument for  $(-\Delta - \mathbf{k}_0^2)$  in Subsubsection 3.2.1, in particular Ingredient 2 and Footnote 8, we obtain that, for  $\vartheta > 2$  and  $\sigma \in (\frac{1}{2}, \vartheta - \frac{1}{2})$ , the mapping

$$\omega^2 \mathfrak{R}_0(\mathbf{k}^2) \mathbf{p}_1 : L_{-\sigma}^2 \longrightarrow L_{-\sigma}^2 \quad \text{is compact}.$$

Note that we have used Remark 14 which translates the fact that  $\mathfrak{R}_0(\mathbf{k}_0^2) \in \mathcal{L}(\mathfrak{B}, \mathfrak{B}^*)$  into  $\mathfrak{R}_0(\mathbf{k}_0^2) \in \mathcal{L}(L_{\sigma'}^2, L_{-\sigma'}^2)$  for  $\sigma' > \frac{1}{2}$ . Elliptic regularity gives that  $\mathfrak{R}_0(\mathbf{k}_0^2) \in \mathcal{L}(L_{\sigma'}^2, H^{2-\sigma'})$  for  $\sigma' > \frac{1}{2}$ , which is one of the ingredients needed, cf. Footnote 8.

- We now have a Fredholm operator, and we next verify for injectivity. We show that the homogeneous problem

$$\left( \text{Id} + \omega_0^2 \mathfrak{R}_0(\omega_0^2 + i0) \mathbf{p}_1 \right) \psi = 0, \quad (3.79)$$

only has trivial solution in  $L_{-\sigma}^2$  for  $\sigma \in (\frac{1}{2}, \vartheta - \frac{1}{2})$ . With the current  $\sigma$ , solution  $\psi$  has the following properties.

- We can rearrange (3.79) to rewrite  $\psi$  as an outgoing solution with right-hand-side  $g := \mathbf{p}_1 \psi$ ,

$$\psi = -\omega_0^2 \mathfrak{R}_0(\omega_0^2 + i0) g \in L_{-\sigma}^2.$$

Since  $\mathbf{p}_1$  is of compact support,  $g \in L_{\sigma'}^2$  for all  $\sigma' \in \mathbb{R}$ . As a result of this,  $\psi$  satisfies a priori estimate (3.60) and radiation condition (3.61) with  $0 < \delta < 1$  (here  $\mu$  in (3.58) is chosen to be 1)

$$\int_{|x| \geq 1} \left| \nabla \psi - i\sqrt{\lambda_0} \frac{x}{|x|} \psi \right|^2 \frac{dx}{(1 + |x|)^{1-\delta}} \leq C\omega_0^4 \int (1 + |x|)^{1+\delta} |g|^2 dx. \quad (3.80)$$

Since  $g \in L_{\sigma'}^2$  for all  $\sigma' \in \mathbb{R}$ , this means  $\psi$  satisfies condition (1.28) of [42] for some  $\delta > 0$ ,

$$\int_{|x| \geq 1} \left| \nabla \psi - i\mathbf{k}_0 \frac{x}{|x|} \psi \right|^2 \frac{dx}{(1 + |x|)^{1-\delta}} < \infty. \quad (3.81)$$

By the second result of [42, Theorem 1.6], solution  $\psi$  satisfies condition (1.27) there,

$$\liminf_{|x|=r} \int \left( |\nabla \psi|^2 + \mathbf{k}_0^2 |\psi|^2 \right) d\sigma(x) \longrightarrow 0, \quad \text{as } |x| \rightarrow \infty. \quad (3.82)$$



– Solution  $\psi$  of (3.79) also satisfies

$$(-\Delta + V_0 - k_0^2) \left( \text{Id} + \omega_0^2 \Re_0(\omega_0^2 + i0) p_1 \right) \psi = 0.$$

After rearrangement, this means  $\psi$  is a solution of the homogeneous equation

$$(-\Delta + V_{\omega_0^2} - k_0^2) \psi = 0. \quad (3.83)$$

By Remark 12, we can then apply the first result of Theorem 1.6 of [42] which gives that  $\psi \equiv 0$  since  $\psi$  is solution of (3.83) and satisfies the radiation condition (3.82).

With these ingredients, for  $\omega_0 > 0$ , we have the convergence

$$\left( \text{Id} + \omega^2 \Re_0(k^2) p_1 \right)^{-1} \longrightarrow \left( \text{Id} + \omega_0^2 \Re_0(k_0^2) p_1 \right)^{-1} \quad \text{in the norm } \mathcal{L}(L_{-\sigma}^2, L_{-\sigma}^2),$$

and we use the Born splitting to define

$$\Re_{\omega_0^2}(k_0^2) := \left( \text{Id} + \omega_0^2 \Re_0(k_0^2) p_1 \right)^{-1} \Re_0(k_0^2), \quad (3.84)$$

as a bounded map in  $\mathcal{L}(L_{\sigma}^2, L_{-\sigma}^2)$  for  $\sigma > 1/2$ .

**Properties of outgoing solution** Using the same argument as above, we can use the left Born splitting to obtain

$$\Re_{\omega_0^2}(k_0^2) := \Re_0(k_0^2) \left( \text{Id} + \omega_0^2 p_1 \Re_0(k_0^2) \right)^{-1}. \quad (3.85)$$

Note that  $\text{Id} + \omega_0^2 p_1 \Re_0(k_0^2)$  is compact and bounded in  $L_{\sigma}^2$ . This allows us to write

$$\Re_{\omega_0^2}(k_0^2) f = \Re_0(k_0^2) g,$$

where

$$g = \left( \text{Id} + \omega_0^2 p_1 \Re_0(k_0^2) \right)^{-1} f,$$

with  $f \in L_{\sigma}^2$ ,  $g \in L_{\sigma}^2$ . From the property of  $\Re_0(k_0^2)$ , the solution  $\Re_0(k_0^2) g$  satisfies radiation condition (3.82), which is of the form of (3.73). As a result, the defined resolvent also defines a solution to (3.72) and satisfies the radiation condition (3.73). The uniqueness of such a solution is guaranteed by [42, Theorem 1.6], employed in Approach 1. In another word, we arrive at the same solution given by (3.71), which is defined uniquely by the radiation condition (3.61) at  $\lambda = k_0^2$ ,

$$\int_{|x| \geq 1} \left| \nabla u - i k_0 \frac{x}{|x|} u \right|^2 \frac{dx}{(1+|x|)^{1-\delta}} < \infty, \quad 0 < \delta < 1. \quad (3.86)$$

In addition, it has the asymptotic expansion, for  $f \in \mathfrak{B}$ ,

$$\begin{aligned} (\Re_{\omega_0^2}(k_0^2) f)(x) &= \pi^{1/2} k_0^{-1/4} \frac{e^{i\phi(x, k_0)}}{|x|} a_+ \left( \frac{x}{|x|} \right) + o(|x|^{-1}); \\ (\partial_r \Re_{\omega_0^2}(k_0^2) f)(x) &= i \pi^{1/2} \lambda_0^{1/4} \frac{e^{i\phi(x, \lambda)}}{|x|} a + \left( \frac{x}{|x|} \right) + o(|x|^{-1}), \end{aligned} \quad (3.87)$$

for some  $a_+, a_- \in L^2(\mathbb{S}^2)$  as  $|x| \rightarrow \infty$ . and the phase  $\phi(x, \lambda)$  is an exact or approximate solution to the the eikonal equation

$$\|\nabla_x \phi(x, \lambda)\|^2 + V_{\omega_0^2}(x) = k_0^2. \quad (3.88)$$

**Remark 16.** In the second approach, the same reasoning still applies if  $p_1$  is a short-range potential. In particular, the compactness of  $\Re_0(k^2) p_1 : L_{-\sigma}^2 \rightarrow L_{-\sigma}^2$  for  $\sigma \in (\frac{1}{2}, \vartheta - \frac{1}{2})$  with  $\vartheta > 2$  still holds true for  $p_1$  short-range.

## 4 The reduced problem in radial symmetry with constant $\alpha$ and constant $c$

In this section, we extend the `Atmo` model to the whole domain and consider Equation (1.1) with the wavespeed  $c$  constant, and density  $\rho$  exponentially decreasing, i.e.

$$\rho(x) = c e^{-\alpha_\infty |x|} \quad \text{with constant } \alpha_\infty > 0. \quad (4.1)$$

This means  $\alpha$  (2.8) is now constant thus  $\partial_r \alpha = 0$  and  $\alpha'_\infty = 0$ . In this case, as shown in Section 2, cf. (2.15), the potential  $q$  (1.5) of the reduced operator simplifies to

$$q(r) = \frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{r}.$$

The *conjugated equation* (1.4) simplifies to

$$\mathcal{L}u = g \quad \text{where} \quad \mathcal{L} = -\Delta + \underbrace{\frac{\alpha_\infty^2}{4} - \frac{\omega^2}{c^2}}_{-k^2} + \frac{\alpha_\infty}{r}, \quad g = \rho^{1/2} f. \quad (4.2)$$

See also Remark 2. The constant  $\frac{\omega^2}{c^2} - \frac{\alpha_\infty^2}{4}$  is called an *energy level*. Here  $k$  is a choice of square root of this value. The choice of square root is discussed in subsection 4.1.

We carry out the following tasks.

1. We introduce the fundamental kernel  $\Phi_k(x, y)$  given by [18] in (4.70) and (4.74) and show that it is indeed a fundamental solution to (4.2), i.e. a distributional solution of

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = \delta(x - y).$$

This is carried out in the proof of Prop 15. We also obtain the asymptotic expansion and radiating property for  $\Phi_k$  and  $\frac{y}{|y|} \cdot \nabla_y \Phi_k(x, y)$  when  $y$  stays in a bounded set and  $|x| \rightarrow \infty$ , cf. Prop 11, Prop 12 and Prop 13.

2. The kernel of the resolvent

$$\mathcal{R}(k^2) := \left( -\Delta - k^2 + \frac{\alpha_\infty}{|x|} \right)^{-1}$$

is given by  $\Phi_k(x, y)$ . This defines outgoing solutions in the presence and absence of absorption, cf. Prop 17. We show that the constructed resolvent and solution satisfy a Sommerfeld-type radiation condition associated with wavenumber  $k$ , cf. Prop 18. This radiation condition and other equivalent variants are shown to characterize the solution uniquely, cf. Prop 19.

3. Additional results are obtained such as a Rellich-type uniqueness theorem, cf. Lemma 20, the expansion of general solutions to the homogeneous equation in spherical harmonics, cf. Prop 21, and the exact outer Dirichlet-to-Neumann map, cf. Prop 22. The last result is used in Section 6 as a reference radiation boundary condition.

**Separation of variables** Decompose the solution  $u$  and right-hand side  $g$  of (4.2) in basis of spherical harmonics,

$$\begin{aligned} u(r, \theta, \phi) &= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_\ell^m(r) Y_\ell^m(\theta, \phi), \\ g(r, \theta, \phi) &= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} g_\ell^m(r) Y_\ell^m(\theta, \phi), \end{aligned}$$

with

$$g_\ell^m = \int_0^\pi \int_0^{2\pi} g(r, \theta, \phi) \overline{Y_\ell^m}(\theta, \phi) \sin \theta \, d\phi \, d\theta.$$

Then  $u_\ell^m$  solves

$$\left( -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) u_\ell^m = g_\ell^m. \quad (4.3)$$

Define unknown  $w$  by

$$u_\ell^m := r^{-1} w. \quad (4.4)$$

Then  $w$  solves

$$\left( -\frac{d^2}{dr^2} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) w = r g_\ell^m. \quad (4.5)$$

We next introduce the change of variable

$$z = 2 e^{i\frac{\pi}{2}} k r. \quad (4.6)$$

The function  $W$  defined by

$$w(r) = W(z := 2 i k r), \quad (4.7)$$

satisfies<sup>13</sup>

$$\left( \frac{d^2}{dz^2} - \frac{1}{4} + \frac{i\alpha_\infty}{z} + \frac{\frac{1}{4} - (\ell + \frac{1}{2})^2}{z^2} \right) W = \frac{z}{2 i k} \frac{1}{4 k^2} g_\ell^m \left( \frac{z}{2 i k} \right), \quad \ell \in \mathbb{Z}. \quad (4.8)$$

When the right-hand-side is zero, equation (4.20) is a special case of the *Whittaker* equation,

$$\partial_z^2 W + \left( -\frac{1}{4} + \frac{\kappa}{z} + \frac{\frac{1}{4} - \mu^2}{z^2} \right) W = 0, \quad \chi \in \mathbb{C}, \mu \in \mathbb{C}, \quad (4.9)$$

studied by Whittaker and Watson, cf. [20, (1.4)]. In our case, the index  $\mu$  is of the form  $\mu = \ell + \frac{1}{2}$  and  $\kappa = \frac{i\alpha_\infty}{2k}$ . We first give a brief description of the solutions to (4.9).

## 4.1 Notations

**Choice of square root branch** We consider the following Argument branches,

$$\text{Arg}_1 : \mathbb{C} \longrightarrow (-\pi, \pi] \quad ; \quad \text{Arg}_2 : \mathbb{C} \longrightarrow [0, 2\pi). \quad (4.10a)$$

The first one is the usual Principal square root branch, cf. [27]. Denote by  $\mathfrak{g}_1$  and  $\mathfrak{g}_2$  the two branches of square root corresponding to the above arguments,

$$\mathfrak{g}_1(z) = |z|^{1/2} e^{\frac{1}{2} i \text{Arg}_1(z)}; \quad (4.11a)$$

$$\mathfrak{g}_2(z) = |z|^{1/2} e^{\frac{1}{2} i \text{Arg}_2(z)}. \quad (4.11b)$$

They have the following properties in terms of the sign of the real and imaginary part,

$$\text{Re } \mathfrak{g}_1(z) \geq 0 \quad \text{while} \quad \text{Im } \mathfrak{g}_2(z) \geq 0. \quad (4.12)$$

---

<sup>13</sup>This can be seen as follows. Under the current assumption,  $c$  and  $\alpha_\infty$  are constant, hence

$$\partial_r w = 2 i k \partial_z W, \quad -\partial_r^2 w = 4 k^2 \partial_z^2 W.$$

We divide by  $4k^2$  the last three terms in (4.5). This gives  $-1/4$  in (4.20). On the other hand,  $\frac{1}{4k^2} \times$  the last two terms in (4.5) gives the corresponding last two terms in (4.20) since

$$\frac{\alpha_\infty}{r} \frac{1}{4k^2} = \frac{i\alpha_\infty}{z} \frac{1}{2k}, \quad \frac{\ell(\ell+1)}{r^2} \frac{1}{4k^2} = -\frac{\ell(\ell+1)}{z^2} = \frac{\frac{1}{4} - (\ell + \frac{1}{2})^2}{z^2}.$$

**The complex frequency** With  $\omega_0 > 0$ , using the square root branch  $\mathfrak{g}_2$ , we define

$$\omega = \mathfrak{g}_2(1 + i\gamma)\omega_0 \quad , \quad \omega_0 \in \mathbb{R}^+, \gamma \in \mathbb{R} . \quad (4.13)$$

With the above convention, we have (see also Remark 17),

$$\text{Im } \omega \geq 0 . \quad (4.14)$$

**The complex wavenumbers and parameters** Using the square root branch  $\mathfrak{g}_2$ , we define  $k$  as the square root,

$$\begin{aligned} k &:= \mathfrak{g}_2\left(\frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4}\right) = \mathfrak{g}_2\left(\frac{\omega_0^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} + i\frac{\gamma_\infty}{c_\infty^2}\omega_0^2\right); \\ \eta &:= \frac{\alpha_\infty}{2k} \quad ; \quad \chi := i\eta . \end{aligned} \quad (4.15)$$

Under the square root branch (4.11b),

$$\text{Im } k \geq 0 . \quad (4.16)$$

To denote the dependency on  $\gamma$ , we will also write

$$k_\gamma , \eta_\gamma , \chi_\gamma .$$

**Remark 17.** We have defined in (4.13) and (4.15)  $\omega$  and  $k$  respectively by using the square root branch  $\mathfrak{g}_2$  (4.11b). However, if  $\gamma \geq 0$ , which is the case in our application,  $\text{Im } \omega^2 \geq 0$ , and  $\text{Im } k^2 \geq 0$ . As a result, from the discussion in Appendix J.1,

$$\begin{aligned} \text{Arg}_1(k^2) &= \text{Arg}_2(k^2) \quad , \quad \text{Arg}_1(\omega^2) = \text{Arg}_2(\omega^2) \quad , \quad \gamma \geq 0 \\ \Rightarrow \quad \mathfrak{g}_1\left(\frac{\omega^2}{c_\infty^2}\right) &= \mathfrak{g}_2\left(\frac{\omega^2}{c_\infty^2}\right) \quad , \quad \mathfrak{g}_1(k^2) = \mathfrak{g}_2(k^2) \quad , \quad \gamma \geq 0 . \end{aligned} \quad (4.17)$$

△

**The real wavenumber and parameters** We will reserve the subscript 0 for the corresponding wavenumber and parameters above at  $\gamma = 0$ ,

$$k_0 = \mathfrak{g}_2\left(\frac{\omega_0^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4}\right) \quad ; \quad \eta_0 = \frac{\alpha_\infty}{2k_0} \quad ; \quad \chi_0 = i\eta_0 . \quad (4.18)$$

However, one has to pay attention to signs when taking the limit of  $k$  and as  $\gamma \rightarrow 0$ , under the current choice of square root branch. We have the following one-sided limits, when  $\frac{\omega_0}{c_\infty} > \frac{\alpha_\infty}{2}$ ,

$$\begin{aligned} k_\gamma &\rightarrow k_0 \quad , \quad \eta_\gamma \rightarrow \eta_0 \quad , \quad \chi_\gamma \rightarrow \chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^+; \\ k_\gamma &\rightarrow -k_0 \quad , \quad \eta_\gamma \rightarrow -\eta_0 \quad , \quad \chi_\gamma \rightarrow -\chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^- . \end{aligned} \quad (4.19)$$

However, for  $\frac{\omega_0}{c_\infty} < \frac{\alpha_\infty}{2}$ , these one-sided limits coincide, i.e.  $\lim_{\gamma \rightarrow 0^+} k_\gamma = \lim_{\gamma \rightarrow 0^-} k_\gamma$ .

## 4.2 Whittaker functions

Here, we introduce the Whittaker functions which are solutions to the Whittaker equation introduced in (4.9),

$$\frac{d^2}{dz^2} W + \left(-\frac{1}{4} + \frac{\kappa}{z} + \frac{\frac{1}{4} - \mu^2}{z^2}\right) W = 0 . \quad (4.20)$$

Solutions to (4.9) are obtained from those of the Kummer's equation

$$z \frac{d^2}{dz^2} u + (b - z) \frac{d}{dz} u - au = 0 . \quad (4.21)$$

In particular, if  $Y(a, b; z)$  is a solution to (4.21), then  $X_{\kappa, \mu}$ , defined as

$$X_{\kappa, \mu}(z) := e^{-\frac{1}{2}z} z^{\frac{1}{2}+\mu} Y\left(\frac{1}{2} + \mu - \kappa, 1 + 2\mu; z\right), \quad (4.22)$$

satisfies (4.9). Below we will give self-contained definitions for the Whittaker functions. However, for completeness of discussion, we also include the full definitions of the Kummer functions in Appendix D.

#### 4.2.1 Definition of Whittaker functions

We will need the following functions.

- Gamma function  $\Gamma$

$$\Gamma(z) := \int_0^\infty e^{-s} s^{z-1} ds, \quad \operatorname{Re} z > 0.$$

For  $\operatorname{Re} z \leq 0$ ,  $\Gamma(z)$  is defined by analytic continuation. It is meromorphic, with no zero, and simple poles of residue  $\frac{(-1)^n}{n!}$  at  $z = -n$ . We note the special values

$$\Gamma(1) = 1, \quad n! = \Gamma(n+1),$$

and recurrence relation

$$\Gamma(z+1) = z\Gamma(z).$$

- The digamma function  $\psi$  is defined as, cf. [32, (13.14.8) p.334],

$$\psi := \frac{\Gamma'(z)}{\Gamma(z)}, \quad z \neq 0, -1, -2, \dots$$

- The Pochhammer's symbol, cf. [32, 5.2(iii)], is

$$\begin{aligned} (a)_0 &= 1; \\ (a)_k &:= a(a+1)(a+2)\dots(a+k-1); \\ (a)_k &= \frac{\Gamma(a+k)}{\Gamma(a)}, \quad a \neq 0, -1, -2, \dots \\ (-a)_k &= (-1)^k (a-k+1)_k. \end{aligned} \quad (4.23)$$

To obtain the expression of the Whittaker functions, we use relation (4.22).

- The **first Whittaker**  $M_{\kappa, \ell + \frac{1}{2}}(z)$ , cf. [32, Eqn 13.14.6] is obtained from the Kummer function (also confluent hypergeometric function)  $M(a, b; z)$  or  ${}_1F_1(a, b; z)$  defined in (D.1) as

$$\begin{aligned} M_{\kappa, \mu}(z) &= e^{-\frac{1}{2}z} z^{\frac{1}{2}+\mu} M\left(\frac{1}{2} + \mu - \kappa, 1 + 2\mu; z\right) \\ &= e^{-\frac{1}{2}z} z^{\frac{1}{2}+\mu} \sum_{k=0}^{\infty} \frac{(\frac{1}{2} + \mu - \kappa)_k}{(1 + 2\mu)_k} \frac{z^k}{k!}, \quad 2\mu \neq -1, -2, -3, \dots \end{aligned} \quad (4.24)$$

$M_{\kappa, \mu}(z)$  is analytic in  $\kappa$ , and meromorphic in  $\mu$  such that  $2\mu \neq -1, -2, -3, \dots$ . Due to the factor  $z^{\frac{1}{2}+\mu}$ , it is a multi-valued function, the principal branch of which uses that for  $\log$ ,  $-\pi < \operatorname{Arg} z \leq \pi$ , i.e.

$$z^{\frac{1+\mu}{2}} := e^{\frac{1+\mu}{2}(\ln|z| + i \operatorname{Arg}(z))}.$$

- For  $\mu = \ell + \frac{1}{2}$ ,  $\ell \in \mathbb{Z}$ , we have to use limiting value (D.5), which gives rise to the **(Buchholtz) Whittaker**  $\mathcal{M}_{-\kappa, \mu}(z)$ . It is defined from the Kummer function  $\mathbf{M}$  (D.4),

$$\mathcal{M}_{\kappa, \mu}(z) := e^{-\frac{1}{2}z} z^{\frac{1}{2}+\mu} \mathbf{M}\left(\frac{1}{2} + \mu - \kappa, 1 + 2\mu; z\right) = \frac{M_{\kappa, \mu}(z)}{\Gamma(1 + 2\mu)}. \quad (4.25)$$

It is defined in particular for all  $\kappa$  and  $\mu$ , in particular, for  $\mu = \ell + \frac{1}{2}$  with  $\ell \in \mathbb{Z}$ . When  $\ell \in \mathbb{Z}$  and  $\ell \geq -1$  then  $2\ell + 2 \geq 0$  thus  $2\ell + 2 \notin \mathbb{Z}^-$ ,

$$\mathcal{M}_{\kappa, \ell + \frac{1}{2}}(z) = z^{\ell+1} e^{-\frac{z}{2}} \frac{M(\ell + 1 - \kappa, 2 + 2\ell; z)}{\Gamma(2 + 2\ell)}, \quad \ell = -1, 0, 1, 2, \dots \quad (4.26)$$

On the other hand, for  $\ell \in \mathbb{Z}$  and  $\ell \leq -2$ , then  $2\ell + 2 \in \mathbb{Z}^-$ , we have to use the limiting value given by (D.5) with  $n = -2\ell - 2$  and  $a = \ell + 1 - \kappa$  in this formula. With some simplification, we obtain<sup>14</sup>

$$\begin{aligned} \mathcal{M}_{\kappa, \ell + \frac{1}{2}}(z) &= \mathcal{M}_{\kappa, -\ell - \frac{1}{2}}(z) \\ &= z^{-\ell} e^{-\frac{z}{2}} M(-\ell - \kappa, -2\ell; z), \quad \ell = -2, -3, \dots \\ &= z^{-\ell} e^{-\frac{z}{2}} \sum_{k=0}^{\infty} \frac{(\ell + 1 - \kappa)_{k-2\ell-1}}{(k - 2\ell - 1)!} \frac{z^k}{k!} = \sum_{k=-2\ell-1}^{\infty} \frac{(\ell + 1 - \kappa)_k}{(k + 2\ell + 1)!} \frac{z^k}{k!}. \end{aligned} \quad (4.29)$$

- The **second Whittaker** function  $W$  is obtained from the Tricomi confluent hypergeometric function  $U$ , cf. (D.7)–(D.10),

$$W_{\kappa, \mu}(z) = e^{-\frac{1}{2}z} z^{\frac{1}{2}+\mu} U\left(\frac{1}{2} + \mu - \kappa, 1 + 2\mu; z\right). \quad (4.30)$$

For  $1 + 2\mu \notin \mathbb{Z}$ , we can use (D.8) to define  $W$ ,

$$W_{\kappa, \mu}(z) = \frac{\Gamma(2\mu)}{\Gamma(\mu + \frac{1}{2} - \kappa)} M_{\kappa, -\mu}(z) + \frac{\Gamma(-2\ell)}{\Gamma(-\mu + \frac{1}{2} - \kappa)} M_{\kappa, \mu}(z), \quad (4.31)$$

,  $-\pi < \text{Arg } z \leq \pi$ ,  $1 + 2\mu \notin \mathbb{Z}$ .

Otherwise, we have to take the limiting value of the above expression<sup>15</sup>. We restrict ourselves to the case where  $\mu = \ell + \frac{1}{2}$ ,  $\ell \in \mathbb{Z}$ . For  $\ell = 0, 1, 2$  then  $1 + 2\mu = 2\ell + 2 \geq 1$ ,  $W$  is defined from the limiting value of  $U$  in (D.9), c.f. [32, 13.14.8],

$$\begin{aligned} W_{\kappa, \ell + \frac{1}{2}}(z) &= -\frac{e^{-\frac{1}{2}z} z^{\ell+1}}{(2\ell + 1)! \Gamma(-\ell - \kappa)} \left( \sum_{k=1}^{2\ell+1} \frac{(2\ell + 1)! (k - 1)!}{(2\ell + 1 - k)! (\kappa - \ell)_k} z^{-k} \right. \\ &\quad \left. - \sum_{k=0}^{\infty} \frac{(\ell + 1 - \kappa)_k}{(2\ell + 2)_k} \frac{z^k}{k!} [\ln z + \psi(\ell + 1 - \kappa + k) - \psi(1 + k) - \psi(2\ell + 2 + k)] \right), \quad (4.32) \\ &\quad \ell \in \mathbb{Z}, \quad \kappa - \ell - 1 \neq 0, 1, 2, \dots \end{aligned}$$

<sup>14</sup>From (D.5), we obtain the limiting value in terms of  $n$  and  $a$ ,

$$\mathcal{M}_{\kappa, \ell + \frac{1}{2}}(z) = z^{\ell+1} e^{-\frac{z}{2}} \lim_{b \rightarrow 2+2\ell} \frac{M(\ell + 1 - \kappa, b; z)}{\Gamma(b)} = z^{\ell+1} e^{-\frac{z}{2}} z^{n+1} M(a + n + 1, n + 2; z) \quad (4.27)$$

$$= z^{\ell+1} e^{-\frac{z}{2}} z^{n+1} \sum_{k=0}^{\infty} \frac{(a)_{n+1+k}}{(n + 1 + k)!} \frac{z^k}{k!} = \sum_{k=n+1}^{\infty} \frac{(a)_k}{(k - n - 1)!} \frac{z^k}{k!}. \quad (4.28)$$

We then express  $a$  and  $n$  in terms of  $\ell, \kappa$  with

$$\begin{aligned} n + 1 &= -2\ell - 1; & n + 2 &= -2\ell; \\ \ell + 1 + n + 1 &= \ell + 1 - 2\ell - 1 = -\ell; & k + n + 1 &= k - 2\ell - 1; \\ a &= \ell + 1 - \kappa = -\frac{1}{2}n - \kappa; & a + n + 1 &= \ell + 1 - \kappa - 2\ell - 1 = -\ell - \kappa. \end{aligned}$$

On the other hand,

$$M_{\kappa, -\ell - \frac{1}{2}}(z) = e^{-\frac{1}{2}z} z^{\frac{1}{2} - \ell - \frac{1}{2}} M\left(\frac{1}{2} - \ell - \frac{1}{2} - \kappa, 1 + 2(-\ell - \frac{1}{2}); z\right) = e^{-\frac{1}{2}z} z^{-\ell} M(-\ell - \kappa, -2\ell; z).$$

<sup>15</sup>In fact, in [8], instead of introducing the value of  $U$  and the limiting value of  $U(a, b; z)$  at  $b \in \mathbb{Z}$ , the Whittaker  $W_{\kappa, \mu}(z)$  and  $W_{-\kappa, \mu}(e^{\pm i\pi} z)$  are defined by relation (4.31) and (4.35) respectively, cf. [8, Eqn 18a–18b]. The value of  $W$  at  $\mu$  such that  $1 + 2\mu \in \mathbb{Z}$  is assigned the limiting value of (4.31), which is calculated (by the Bernoulli-de l'Hospital's rule, cf. [8, Section 2.5 p.20]).

For  $l = -1, -3, \dots$ , then  $2\ell + 2 \leq 0$ , then using (D.10) with  $n = -2\ell - 2$ , and simplification<sup>16</sup>

$$W_{\kappa, \ell + \frac{1}{2}}(z) = e^{-\frac{1}{2}z} z^{-\ell} U(-\ell - \kappa, -2\ell; z) = W_{\kappa, -\ell - \frac{1}{2}}(z). \quad (4.33)$$

**Remark 18** (Analytic continuation). *In the above discussion, we have defined Whittaker functions  $W$  and  $M$  for  $z$  with  $\text{Arg } z \in (-\pi, \pi]$ . We call this the **principal branch of the Whittaker functions**. To extend to  $z$  with argument outside of the principal branch, analytic continuation is used in conjunction with the semi-circuital relations [27, p.297]*

$$\begin{aligned} M_{\kappa, \mu}(ze^{\pm i\pi}) &= e^{\pm i\frac{\pi}{2}(1+2\mu)} M_{-\kappa, \mu}(z); \\ M_{-\kappa, \mu}(ze^{\pm i\pi}) &= e^{\pm i\frac{\pi}{2}(1+2\mu)} M_{\kappa, \mu}(z). \end{aligned} \quad (4.34)$$

Using (D.8), this gives extension for  $W$ ,

$$W_{\kappa, \mu}(ze^{\pm i\pi}) = \frac{\Gamma(2\mu)}{\Gamma(\mu + \frac{1}{2} - \kappa)} e^{\pm i\frac{\pi}{2}(1-2\mu)} M_{-\kappa, -\mu}(z) + \frac{\Gamma(-2\mu)}{\Gamma(-\mu + \frac{1}{2} - \kappa)} e^{\pm i\frac{\pi}{2}(1+2\mu)} M_{-\kappa, \mu}(z). \quad (4.35)$$

△

**Remark 19** (Limiting behavior at  $\alpha = 0$ ). *When  $\alpha = 0$  thus  $\kappa = 0$ , we obtain the Bessel equation, and in this case, the Whittaker functions become the spherical Bessel functions<sup>17</sup>. Following cf. [27, p.20], we have*

$$\begin{aligned} W_{0, \mu}(i\tilde{z}) &= \frac{\sqrt{\pi}}{2} \tilde{z}^{\frac{1}{2}} e^{-i\frac{\pi}{4}(1+2\mu)} H_{\mu}^{(2)}\left(\frac{\tilde{z}}{2}\right); \\ W_{0, \mu}(-i\tilde{z}) &= \frac{\sqrt{\pi}}{2} \tilde{z}^{\frac{1}{2}} e^{i\frac{\pi}{4}(1+2\mu)} H_{\mu}^{(1)}\left(\frac{\tilde{z}}{2}\right). \end{aligned} \quad (4.36)$$

When  $\tilde{z} := 2kr$ , cf. (4.6), and  $\mu = \ell + \frac{1}{2}$ , then  $e^{\pm i\frac{\pi}{4}(1+2\mu)} = e^{\pm i\frac{\pi}{2}(\ell+1)}$

$$\begin{aligned} W_{0, \mu}(i2kr) &= \frac{\sqrt{\pi}}{2} (2kr)^{\frac{1}{2}} i^{-\ell-1} H_{\ell+\frac{1}{2}}^{(2)}(kr) = \frac{i^{-\ell-1}}{2} h_{\ell}^{(2)}(kr); \\ W_{0, \mu}(-i2kr) &= \frac{\sqrt{\pi}}{2} (2kr)^{\frac{1}{2}} i^{\ell+1} H_{\ell+\frac{1}{2}}^{(1)}(kr) = \frac{i^{\ell+1}}{2} h_{\ell}^{(1)}(kr). \end{aligned} \quad (4.37)$$

△

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<sup>16</sup>This is seen as

$$\begin{aligned} W_{\kappa, \ell + \frac{1}{2}}(z) &= e^{-\frac{1}{2}z} z^{1+\ell} U(\ell - \kappa + 1, 2\ell + 2; z) \\ &= e^{-\frac{1}{2}z} z^{1+\ell} z^{-2\ell-2+1} U(\ell - \kappa + 1 - 2\ell - 2 + 1, -2\ell - 2 + 2; z) = e^{-\frac{1}{2}z} z^{-\ell} U(-\ell - \kappa, -2\ell; z). \end{aligned}$$

On the other hand,

$$W_{\kappa, -\ell-1+\frac{1}{2}}(z) = e^{-\frac{1}{2}z} z^{1-\ell-1} U(-\ell-1-\kappa+1, 2(-\ell-1)+2; z) = e^{-\frac{1}{2}z} z^{-\ell} U(-\ell-\kappa, -2\ell; z).$$

<sup>17</sup>The spherical Bessel functions  $y_{\ell}$  are solutions to  $(-\frac{d^2}{dz^2} - \frac{2}{z}\frac{d}{dz} - 1 + \frac{\ell(\ell+1)}{z^2})y_{\ell} = 0$ , while general Bessel functions are  $Y_{\nu}$  are solutions to  $(-\frac{d^2}{dz^2} - \frac{1}{z}\frac{d}{dz} - 1 + \frac{\nu}{z^2})Y_{\nu} = 0$ . The spherical Bessel functions of the first kind are denoted by  $j_{\ell}$ , second  $y_{\ell}$  and third  $h_{\ell}^{(1)}$  and  $h_{\ell}^{(2)}$ , cf. [32, 10.47.3–10.47.6]

$$j_{\ell}(z) = \sqrt{\frac{1}{2}} \frac{\pi}{z} J_{\ell+\frac{1}{2}}(z) = (-1)^{\ell} \sqrt{\frac{1}{2}} \frac{\pi}{z} Y_{-\ell-\frac{1}{2}}(z) \quad ; \quad h_{\ell}^{(1)}(z) = \sqrt{\frac{1}{2}} \frac{\pi}{z} H_{\ell+\frac{1}{2}}^{(1)}(z).$$

They can be defined explicitly, cf. [32, 10.49.1–10.49.7]. In particular, for a specifically defined series  $a_k(\ell + \frac{1}{2})$  cf. [32, 10.49.1],

$$h_{\ell}^{(1)} = e^{iz} \sum_{k=0}^{\ell} i^{k-\ell-1} \frac{a_k(\ell + \frac{1}{2})}{z^{k+1}}.$$

#### 4.2.2 Properties of Whittaker functions near zero

These limiting forms can be found in [32, 13.14.16–13.14.19]

$$\begin{aligned} W_{\kappa, \frac{1}{2}}(z) &= \frac{1}{\Gamma(1-\kappa)} + O(z \ln z); \\ W_{\kappa, 0}(z) &= -\frac{\sqrt{z}}{\Gamma(\frac{1}{2}-\kappa)} \left( \ln z + \psi(\tfrac{1}{2}-\kappa) + 2\gamma \right) + O(z^{3/2} \ln z), \end{aligned} \quad (4.38)$$

where  $\gamma$  is Euler constant. In general,

$$W_{\kappa, \mu}(z) = \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2} + \mu - \kappa)} z^{\frac{1}{2}-\mu} + O(z^{\frac{3}{2}-\operatorname{Re} \mu}) \quad , \quad \operatorname{Re} \mu \geq \frac{1}{2} \quad , \quad \mu \neq \frac{1}{2}. \quad (4.39)$$

For  $\mu = \ell + \frac{1}{2}$ ,  $\ell = 1, 2, \dots$ , then

$$W_{\kappa, \frac{1}{2}+\ell}(z) = \frac{\Gamma(2\ell+1)}{\Gamma(\ell+1-\kappa)} z^{-\ell} + O(z^{1-\ell}) \quad , \quad \operatorname{Re} \mu \geq \frac{1}{2} \quad , \quad \mu \neq \frac{1}{2}. \quad (4.40)$$

The expansion for the derivative is given in Prop. 30 in Appendix C,

$$W'_{\kappa, 1/2}(z) = \frac{\ln z}{\Gamma(-\kappa)} + \frac{\psi(-\kappa) + 2\gamma}{\Gamma(-\kappa)} + \frac{1}{\Gamma(1-\kappa)} + O(z \ln z) \quad , \quad z \rightarrow 0. \quad (4.41)$$

As for the Buchholtz function, we have, as  $z \rightarrow 0$

$$M_{\kappa, 1/2}(0) = 0 \quad ; \quad \lim_{z \rightarrow 0} M'_{\kappa, 1/2}(z) = 1. \quad (4.42)$$

#### 4.2.3 Asymptotic properties of Whittaker functions at infinity

Asymptotic expansion at infinity, [32, 13.19.3] for the Whittaker function  $W$  is given as

$$W_{\kappa, \mu}(z) \sim e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=0}^{\infty} \frac{(\frac{1}{2} + \mu - \kappa)_k (\frac{1}{2} - \mu - \kappa)_k}{s!} (-z)^{-k} \quad , \quad |\operatorname{Arg} z| \leq \frac{3}{2}\pi - \delta. \quad (4.43)$$

Its derivative has the asymptotic expansion,

$$W'_{\kappa, \frac{1}{2}}(z) = e^{-\frac{1}{2}z} z^{\kappa} \left( -\frac{1}{2} + O(|z|^{-1}) \right) \quad , \quad |\operatorname{Arg} z| \leq \frac{3}{2}\pi - \delta \quad , \quad z \rightarrow \infty. \quad (4.44)$$

The radiating property satisfied by  $W_{\kappa, \frac{1}{2}}$  is given as,

$$e^{\frac{1}{2}z} z^{-\kappa} \left( W'_{\kappa, \frac{1}{2}}(z) + \frac{1}{2} W_{\kappa, \frac{1}{2}}(z) \right) = O(|z|^{-1}). \quad (4.45)$$

The proof for these statements is given in Prop. 30 in Appendix C. See also Figure 5–8 for numerical illustrations.

For the Buchholtz Whittaker, cf. Proposition 29, we have,

$$\begin{aligned} M_{\kappa, 1/2}(z) &\sim e^{\frac{1}{2}z} z^{-\kappa} \left( \frac{1}{\Gamma(1-\kappa)} + O(z^{-1}) \right) + e^{-\frac{1}{2}z} z^{\kappa} \left( \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} + O((-z)^{-1}) \right), \\ \operatorname{Arg} z &\in (-\tfrac{1}{2}\pi, \tfrac{3}{2}\pi) \end{aligned} \quad (4.46)$$

and

$$\begin{aligned} M'_{\kappa, \frac{1}{2}}(z) &\sim e^{\frac{1}{2}z} z^{-\kappa} \left( \frac{1}{2\Gamma(1-\kappa)} + O(z^{-1}) \right) + e^{-\frac{1}{2}z} z^{\kappa} \left( -\frac{1}{2} \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} + O((-z)^{-1}) \right) \\ \operatorname{Arg} z &\in (-\tfrac{1}{2}\pi, \tfrac{3}{2}\pi). \end{aligned} \quad (4.47)$$



We write out explicitly the dominant factor describing the oscillatory behavior of  $W$  for the case where  $z = 2i k_0 r$  and  $\kappa = \pm i\eta$ . More details on the following statements are in Appendix C.2. Define

$$\varphi_k(t) := k t - \eta \log(2 k t) + i \frac{\pi}{2} \eta, \quad t \in \mathbb{R}^+, \quad \eta = \frac{\alpha_\infty}{2k}. \quad (4.48)$$

Here  $\log$  uses the Principal Log branch. We also note that  $e^{-\pi i} 2 e^{i \frac{\pi}{2}} k r = 2 e^{-\frac{\pi}{2} i} k r$  has argument  $[-\pi/2, \pi/2]$ .

- For  $\gamma = 0$  and  $\frac{\omega_0}{c_\infty} > \frac{\alpha_\infty}{2}$ . This gives  $k_0^2 > 0$ : By Convention 1, cf. Appendix G,  $W_{i\eta_0, \mu}(2i k_0 r)$  is incoming, while  $W_{-i\eta_0, \mu}(e^{-i\pi} 2i k_0 r)$  is outgoing. The highest order term in their asymptotic expansion at infinity is given by,

$$W_{i\eta_0, \mu}(2i k_0 r) \sim \exp\left(-i\varphi_{k_0}(t)\right) e^{-\pi \eta_0},$$

**Incoming**

$$W_{-i\eta_0, \mu}(e^{-i\pi} 2i k_0 r) \sim \exp\left(i\varphi_{k_0}(t)\right).$$

**Outgoing**

(4.49)

On the other hand,  $M_{-i\eta_0, \mu}(-2i k_0 r)$  has both the incoming and outgoing part,

$$M_{-i\eta_0, \mu}(-2i k_0 r) \sim \exp(-i\varphi_{k_0}(r)) \left( \frac{1}{\Gamma(1-\kappa)} + O((k_0 r)^{-1}) \right) \\ + \exp(i\varphi_{k_0}(r)) \left( \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} + O((k_0 r)^{-1}) \right).$$

(4.50)

Note that the argument of the variable is  $-\pi/2$ , and thus satisfies the argument requirement of (4.46).

- For  $\gamma > 0$ ,

$$W_{i\eta_\gamma, \mu}(2i k_\gamma r) \sim \exp\left(-i\varphi_{k_\gamma}(t)\right) e^{-\pi \eta_\gamma},$$

$\notin L^2([1, \infty))$

(4.51)

$$W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) \sim \exp\left(i\varphi_{k_\gamma}(t)\right).$$

$\in L^2([1, \infty))$

When  $\frac{\omega_0}{c_\infty} > \frac{\alpha_\infty}{2}$ , we have limits,

$$\lim_{\gamma \rightarrow 0^+} W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) = W_{-i\eta_0, \mu}(e^{-i\pi} 2i k_0 r).$$

**Outgoing**

(4.52)

The Buchholtz function  $M_{-i\eta_0, \mu}(-2i k_0 r)$  has both an  $L^2$  bounded and non bounded part,

$$M_{-i\eta, \mu}(-2i k r) \sim \exp(-i\varphi_k(r)) \left( \frac{1}{\Gamma(1-\kappa)} + O((k r)^{-1}) \right) \\ + \exp(i\varphi_k(r)) \left( \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} + O((k r)^{-1}) \right).$$

(4.53)

- For  $\gamma < 0$

$$W_{i\eta_\gamma, \mu}(2i k_\gamma r) \sim \exp\left(-i\varphi_{k_\gamma}(t)\right) e^{-2\pi \eta_\gamma},$$

$\notin L^2([1, \infty))$

$$W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) \sim \exp\left(i\varphi_{k_\gamma}(t)\right).$$

$\in L^2([1, \infty))$

When  $\frac{\omega_0}{c_\infty} > \frac{\alpha_\infty}{2}$ , we have limits,

$$\lim_{\gamma \rightarrow 0^-} W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) = W_{i\eta_0, \mu}(2i k_0 r). \quad (4.54)$$

Incoming

- When  $\gamma = 0$  and  $\frac{\omega_0}{c_\infty} < \frac{\alpha_\infty}{2}$  then  $k_0$  is purely imaginary with positive imaginary part,  $k_0 = ik_0$ . Then  $W_{-i\eta_0, \mu}(-2ik_0 r)$  is exponentially decay, and while  $W_{i\eta_0, \mu}(2ik_0 r)$  is exponentially growing. In this case, the limits from the upper hand plane and lower half, are equal

$$\lim_{\gamma \rightarrow 0^-} W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) = \lim_{\gamma \rightarrow 0^+} W_{-i\eta_\gamma, \mu}(e^{-i\pi} 2i k_\gamma r) \quad (4.55)$$

and give the  $W_{-i\eta_0, \mu}(-2ik_0 r) \in L^2([1, r])$ .

**Remark 20.** We look at the leading term<sup>18</sup> in the phase function, this suffices to select the  $L^2$  function. With  $r > 0$ , we have

$$e^{ik_\gamma r} = e^{-2r \operatorname{Im} k_\gamma} e^{i2r \operatorname{Re} k_\gamma}, \quad e^{-ik_\gamma r} = e^{2r \operatorname{Im} k_\gamma} e^{-i2r \operatorname{Re} k_\gamma}.$$

With the current choice of square root branch,  $\operatorname{Im} k_\gamma > 0$ , which means  $e^{ik_\gamma r} \in L^2$  (and not  $e^{-ik_\gamma r}$ ).  $\triangle$

**Numerical illustrations** In Figures 5–8, we illustrate numerically the asymptotic and radiation behavior of the Whittaker functions  $W_{-i\eta, \frac{1}{2}}(-2ikr)$ , without and with attenuation (i.e. for  $\gamma = 0$  and  $\gamma \neq 0$ ). We use the following parameters

$$c_\infty = 3, \quad \alpha_\infty = 50, \quad \ell = 0, \quad (4.56)$$

and we recall from the notation Subsection 4.1 that,

$$\mu = \ell + 1/2 = 1/2; \quad k^2 = \frac{\omega_0^2}{c_\infty^2} \left( 1 + \frac{2i\gamma}{\omega_0} \right) - \frac{\alpha_\infty^2}{4}; \quad k = \mathfrak{g}_2(k^2); \quad \eta = \frac{\alpha_\infty}{2k}. \quad (4.57)$$

In the first group, Figures 5 and 6, we superpose the plots of the Whittaker function  $W_{-i\eta, \frac{1}{2}}(-2ikr)$  with those of the function,

$$\exp(i\varphi_k(r)) := \exp(ikr - i\eta \log(2kr) - \frac{\pi}{2}\eta). \quad (4.58)$$

We do the same for its derivative which is compared with  $-\frac{1}{2} \exp(i\varphi_k(r))$ . The radiating property is illustrated via the function

$$W'_{-i\eta, \frac{1}{2}}(-2ikr) + \frac{1}{2} W_{-i\eta, \frac{1}{2}}(-2ikr).$$

There is no attenuation ( $\gamma = 0$ ) in Figure 5, while in Figure 6,  $\gamma = 1$ . We have the following observations.

- One expects that the functions portray pure oscillation in absence of attenuation, while with attenuation, the oscillatory behavior is coupled with a decay in magnitude, since they are  $L^2$  in the latter case. In another word, they are oscillating curves with decreasing envelopes. At frequency,  $\omega_0 = 2\pi 20$ , these behaviors are confirmed by Figures 5(a), for  $\gamma = 0$  and 6 for  $\gamma = 1$ , for  $W$  and its derivative, in which there are the oscillations in all figures, but only attenuation of the signal for those with  $\gamma = 1$  (i.e. in Figure 6).

<sup>18</sup>If we expand out the full phase, we obtain the same result,

$$|e^{-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r)}| = e^{2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln r \right)} \left| e^{-\operatorname{Im} k_\gamma \frac{\alpha \ln|2k_\gamma|}{2|k_\gamma|^2} - \eta_\gamma \operatorname{Arg}(k_\gamma)} \right|;$$

$\notin L^2([1, \infty))$

$$|e^{ik_\gamma r - i\eta_\gamma \log(2k_\gamma r)}| = e^{-2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln r \right)} \left| e^{\operatorname{Im} k_\gamma \frac{\alpha \ln|2k_\gamma|}{2|k_\gamma|^2} + \eta_\gamma \operatorname{Arg}(k_\gamma)} \right|.$$

$\in L^2([1, \infty))$

The derivation for this is given in Appendix I.

- On the other hand, at very low frequencies, in particular  $\omega_0 = 2\pi 5$  shown in Figure 5(b) for  $\omega_0 = 2\pi 5$ , even without attenuation i.e.  $\gamma = 0$ , the function simply shows a rapid decay without any oscillation. In fact, it is simply a monotone and rapidly decreasing function to zero. Its derivative also ceases to exhibit oscillatory behavior, and is negative monotone, also with magnitude rapidly decreasing to zero. This is expected for  $\exp(i\varphi_k(r))$ . When  $\gamma = 0$ , with the current values of parameters,  $k = i24.9$ , and the leading term of  $\exp(i\varphi_k(r))$  is  $e^{-24.9r}$ , is thus exponentially decaying. In fact, the whole function in this case is

$$\exp(i\varphi_k(r)) = e^{-24.9r} \times (50r)^{-1.01} \times (\text{a complex constant}).$$

This strong decay will be amplified when  $\gamma = 1$ , making the difference between with and without attenuation indiscernible. For this reason when  $\gamma = 1$ , only the case with higher frequency  $\omega_0 = 2\pi 20$  is plotted.

- The oscillatory phase function (4.58) is expected to give the first term in the asymptotic expansion at infinity for  $W_{-i\eta, \frac{1}{2}}(-2ikr)$ , and  $-\frac{1}{2} \times \exp(i\varphi_k(r))$  for  $W_{-i\eta, \frac{1}{2}}(-2ikr)'$ . The left and middle subfigures of Figure 5– 6 show that the two plots, for  $W_{-i\eta, \frac{1}{2}}(-2ikr)$  and  $\exp(i\varphi_k(r))$ , coincide completely even on the finite interval  $[1, 3]$ . This means that the oscillatory exponential (4.58) gives an excellent representation of the function  $W_{-i\eta, \frac{1}{2}}(-2ikr)$ . What is surprising is that one does not need  $r$  to be very large for this agreement to occur. This is confirmed both for a low frequency  $\omega_0 = 2\pi 5$  and higher one  $\omega_0 = 2\pi 20$ , with and without attenuation. This means that the function  $\exp(i\varphi_k(r))$  also captures the case when  $W_{-i\eta, \frac{1}{2}}(-2ikr)$  ceases to exhibit any oscillatory behavior and only a rapid decay for very small frequencies, cf. Figure 5(b) for  $\omega_0 = 2\pi 5$ . The same conclusion is drawn for  $-\frac{1}{2} \times \exp(i\varphi_k(r))$  and  $W'$ .
- In addition to its oscillatory behavior, for higher frequency  $\omega_0 = 2\pi 20$ , we further note that the function  $(1/2W_{-i\eta, 1/2} + W'_{-i\eta, 1/2})$  is also attenuating, even when  $\gamma = 0$ . This can be explained by the fact that this term is supposed to be an oscillatory term times one decaying like  $r^{-1}$ , i.e.  $\exp(i\varphi_k(r)) \times O(r^{-1})$ . This is explored in more details in the next group of figures.

To further investigate the asymptotics and radiation behavior of  $W$ , we now explore the symbol structure of  $W_{-i\eta, 1/2}(-2ikr)$ , by first factoring out the oscillatory part, and we investigate the decay rate of the remainder term. In particular, we consider the following ratios, which are plotted in Figure 7 and 8.

$$\begin{aligned} \mathbf{r}_1(r) &= \frac{W_{-i\eta, 1/2}(-2ikr)}{\exp(i\varphi_k(r))}; & \mathbf{r}_2(r) &= \frac{W'_{-i\eta, 1/2}(-2ikr)}{\exp(i\varphi_k(r))}; \\ \mathbf{r}_3(r) &= \frac{W'_{-i\eta, 1/2}(-2ikr) + \frac{1}{2}W_{-i\eta, 1/2}(-2ikr)}{\exp(i\varphi_k(r))}. \end{aligned} \quad (4.59)$$

We have the following observations.

- It is expected that ratio  $\mathbf{r}_1$  is  $1 + o(1)$ , and ratio  $\mathbf{r}_2$  is  $-\frac{1}{2} + o(1)$ . This is confirmed in the left subfigures of Figure 7(a) for  $\gamma = 0$  and Figure 7(b) for  $\gamma = 1$ . For second ratio  $\mathbf{r}_2$ , these are the middle subfigures of Figure 7(a) and 7(b). With or without attenuation, the curves of ratio  $\mathbf{r}_1$  decay and level out to the constant 1, i.e. having horizontal asymptotes at 1. For ratio  $\mathbf{r}_2$ , we have similar observations with the horizontal asymptotes at  $-\frac{1}{2}$ .
- The right subfigures of Figure 7(a) for  $\gamma = 0$  and Figure 7(b) for  $\gamma = 1$ , show that Ratio  $\mathbf{r}_3$  is  $0 + o(1)$ , with similar observations as above. The horizontal asymptotes for  $\mathbf{r}_3$  is thus at 0. We will explore further the decay rate of this term in the next figure.
- We expect  $\mathbf{r}_3$  is  $O(r^{-1})$ . In Figure 8, we explore its rate of decay, by testing against powers of  $x = 2|k|r$ . This means, when multiplied  $\mathbf{r}_3$  by  $x$ , the resulting function is expected to stay bounded, which is confirmed by the left subfigures of Figure 8(a) for  $\gamma = 0$  and Figure 8(b) for  $\gamma \neq 1$ , in which the curves not only stay bounded but also decrease to a constant and with a horizontal asymptotes close to zero (well below 0.75). In another word, it behaves like a small constant + a  $o(1)$  term. On the other hand,

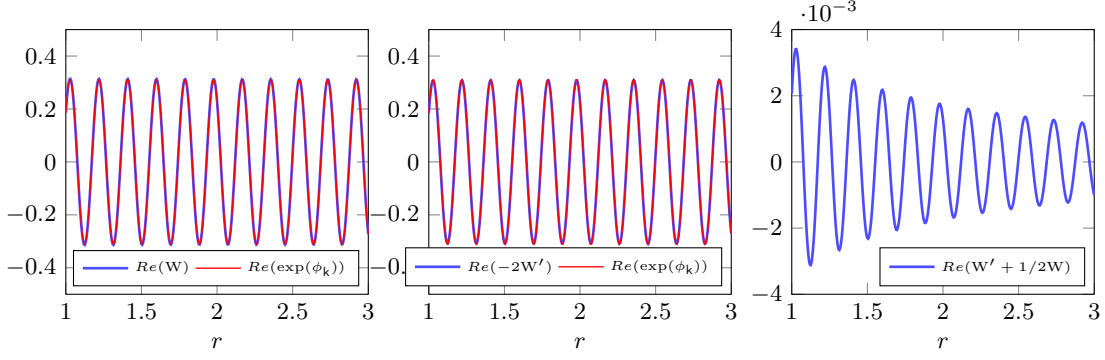
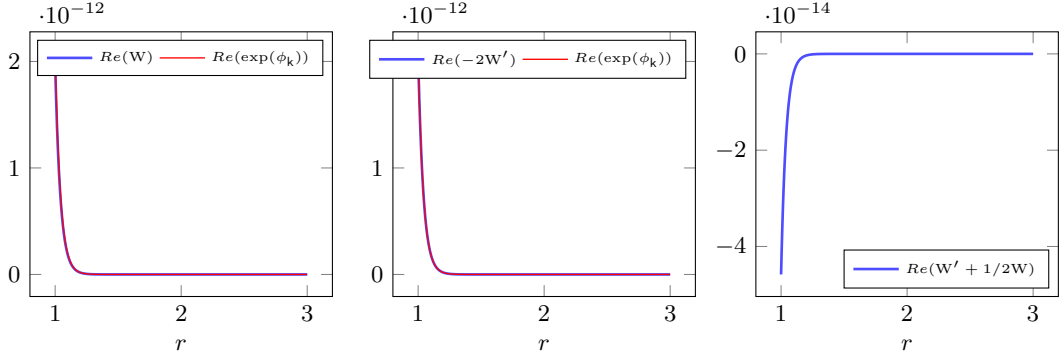

 (a) using  $\omega_0 = 2\pi 20$ ,  $\gamma = 0$ .

 (b) using  $\omega_0 = 2\pi 5$ ,  $\gamma = 0$ . In this case, the first parameter of the Whittaker function is large. The function no longer exhibits oscillatory behavior and is strictly monotone, with a rapid decay towards zero.

Figure 5: Outgoing Whittaker function  $W_{-i\eta, 1/2}(-2ikr)$  in the case without attenuation ( $\gamma = 0$ ). The leading part in the asymptotic is given by  $e^{i\varphi_k(r)}$  where  $\varphi_k(r) := kr - \eta \log(2kr) + i\frac{\pi}{2}\eta$ , and  $\eta = \frac{\alpha}{2k}$  with  $c_\infty = 3$  and  $\alpha_\infty = 50$ , see (4.49) at two frequencies. The figures show that  $\exp(i\varphi_k(r))$  provides an excellent approximation of  $W_{-i\eta, 1/2}(-2ikr)$  and one does not have to wait for  $r$  to be very big. We have similar conclusions for  $-\frac{1}{2}\exp(i\varphi_k(r))$  and  $W'$ .

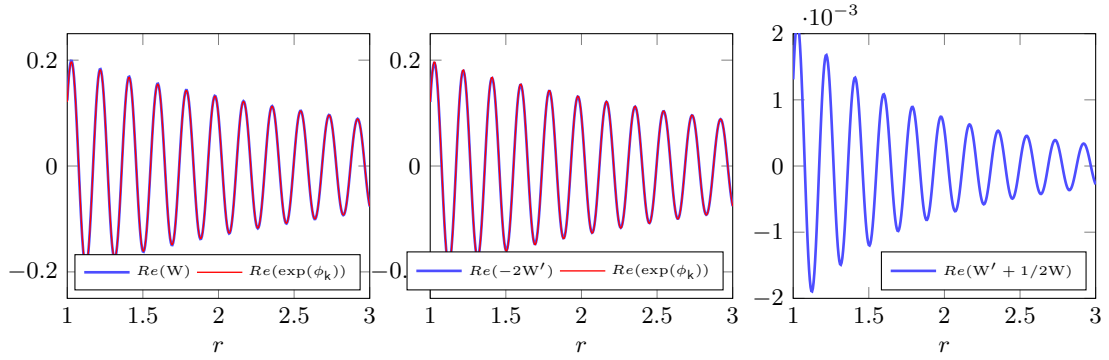


Figure 6: Outgoing Whittaker function  $W_{-i\eta, 1/2}(-2ikr)$  in the case with attenuation ( $\gamma = 1$ ) at frequency  $\omega_0 = 2\pi 20$ . The leading part in the asymptotic is given by  $e^{i\varphi_k(r)}$  where  $\varphi_k(r) := kr - \eta \log(2kr) + i\frac{\pi}{2}\eta$ , and  $\eta = \frac{\alpha}{2k}$  with  $c_\infty = 3$  and  $\alpha_\infty = 50$ , see (4.49). Here, the oscillatory behavior is now coupled with attenuation which translates to a decrease in magnitude of the oscillating curve. The function  $\exp(i\varphi_k(r))$  still represents an excellent approximation as in the case without attenuation.

when multiplied by  $x^2$ , the ratio grows, which is confirmed in the right subfigures of Figure 8(a) for  $\gamma = 0$  and Figure 8(b) for  $\gamma \neq 1$ . In these subfigures, the ratio  $\tau_3$  increases drastically, resulting in a drastic increase in the scale of the value of its function, it increases to order  $10^4$ .

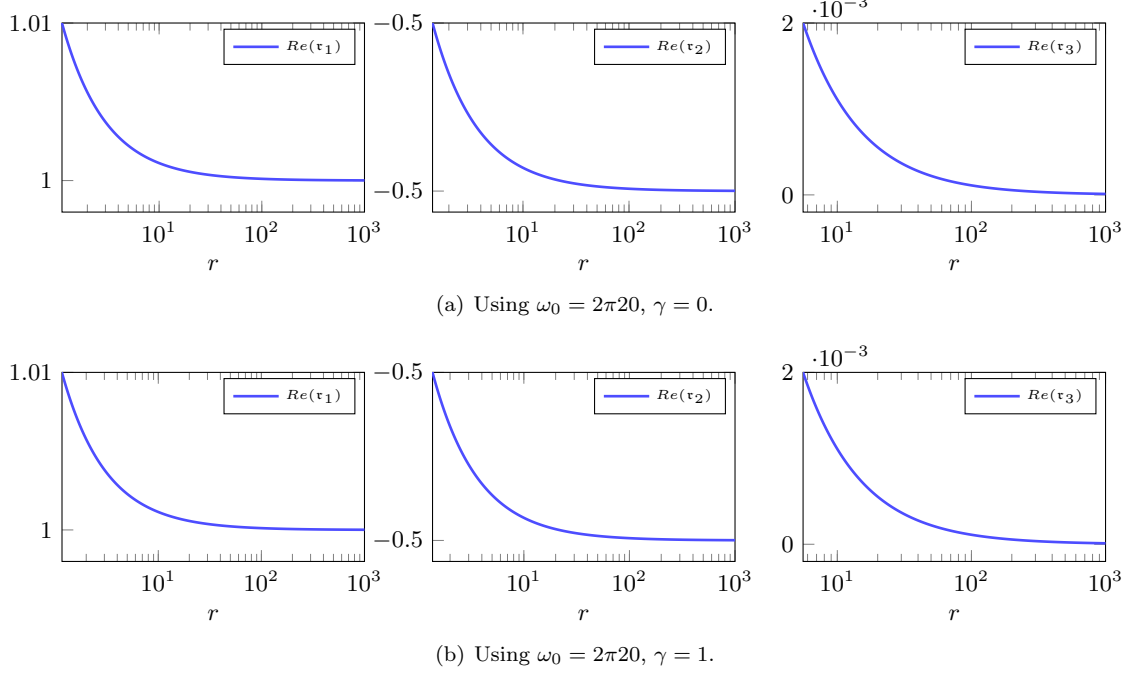


Figure 7: Plots of ratios (4.59) which represent the symbol part of  $W_{-i\eta,1/2}(-2ikr)$ , its derivative and the radiating property. These are the remainder after the oscillatory part  $\exp(i\varphi_k(r))$  defined in (4.58) is factored out from the functions. The curves show that they all have the profile of a constant  $+o(1)$ , thus have horizontal asymptotes given by the leading constants. The horizontal asymptote for  $\tau_1$  is 1, while that for its derivative is  $-1/2$ . As a result, that for  $W_{-i\eta,1/2}(-2ikr)' + \frac{1}{2}W_{-i\eta,1/2}(-2ikr)$  is 0.

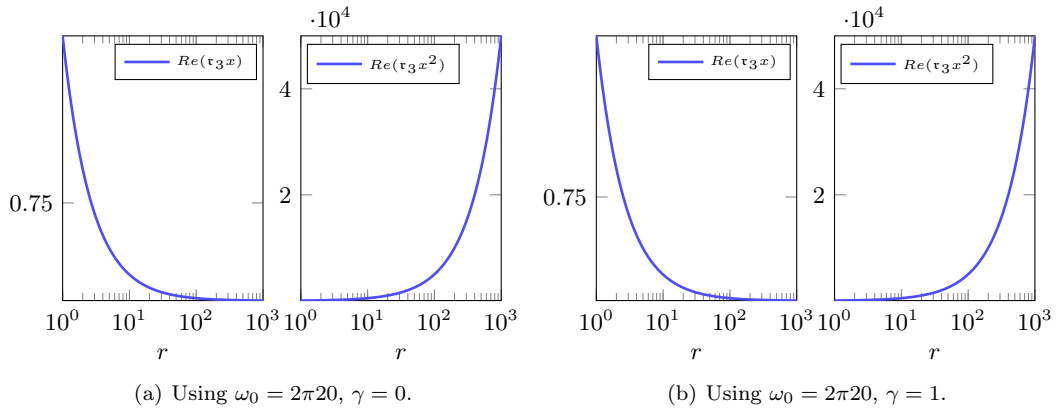


Figure 8: This figure illustrates the radiating asymptotics of  $W_{-i\eta,1/2}(-2ikr)$  by exploring the decay rate of the symbol part  $\tau_3$  of  $W_{-i\eta,1/2}(-2ikr)' + \frac{1}{2}W_{-i\eta,1/2}(-2ikr)$ . This is the remainder after the oscillatory part  $\exp(i\varphi_k(r))$  defined in (4.58) is factored out from the function. The growth/decay rate of  $\tau_3$  is probed by multiplication by powers of  $x = 2|k|r$ . The curves of  $(x\tau_3)$  stay bounded, and in fact decreases rapidly to zero, while the curves of  $(x^2\tau_3)$  increase and explode to  $10^4$ . This shows that  $\tau_3$  decreases as fast as  $r^{-1}$  but not faster than  $r^{-2}$ .

#### 4.2.4 Basis of solutions for Whittaker equation

We restrict to the case where  $\mu = \ell + \frac{1}{2}$ ,  $\ell \in \mathbb{Z}$ . For reference, cf. e.g. [8, Section 2.5 p.23].

- A fundamental pair of solutions to (4.20) in an unbounded domain is given by

$$\begin{aligned} W_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad W_{-\kappa, \ell + \frac{1}{2}}(e^{-\pi i} z) \quad , \quad -\frac{\pi}{2} \leq \text{Arg}(z) < \frac{3\pi}{2} \quad , \\ W_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad W_{-\kappa, \ell + \frac{1}{2}}(e^{\pi i} z) \quad , \quad -\frac{3\pi}{2} \leq \text{Arg}(z) < \frac{1}{2}\pi \quad , \end{aligned} \quad (4.60)$$

with asymptotics

$$W_{\kappa, \ell + \frac{1}{2}}(z) \sim e^{-\frac{z}{2}} z^{\kappa} \quad , \quad |\text{Arg } z| < \frac{3}{2}\pi. \quad (4.61)$$

- On the other hand, a fundamental pair of solutions near origin<sup>19</sup> is given by,

$$\mathcal{M}_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad W_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad |\text{Arg } z| \leq \pi. \quad (4.62)$$

**Remark 21.** Recall that the principal branch of the Whittaker functions is defined for  $z$  with  $\text{Arg } z \in (-\pi, \pi]$ , cf. Remark 18. Consider complex wavenumber  $\mathbf{k}$  defined in (4.15). Write  $\mathbf{k} = |\mathbf{k}| e^{i \text{Arg}(\mathbf{k})}$  then  $2e^{i\frac{\pi}{2}} r \mathbf{k} = 2|\mathbf{k}| r e^{i \text{Arg}(\mathbf{k}) + i\frac{\pi}{2}}$ . By the choice of square root (4.11b) and with  $\gamma > 0$ ,

$$0 \leq \text{Arg}(\mathbf{k}) \leq \frac{\pi}{2} \quad \Rightarrow \quad \frac{\pi}{2} \leq \text{Arg}(2e^{i\frac{\pi}{2}} r \mathbf{k}) \leq \pi.$$

This is in the range  $(-\pi, \pi)$  of the principal branch of the pair of linearly independent solutions around the origin given in (4.62),

$$\mathcal{M}_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad W_{\kappa, \ell + \frac{1}{2}}(z) \quad , \quad |\text{Arg } z| \leq \pi.$$

Similarly,

$$\frac{\pi}{2} \leq \text{Arg}(2e^{i\frac{\pi}{2}} r \mathbf{k}) \leq \pi \quad , \quad -\frac{\pi}{2} < \text{Arg}(e^{-i\pi} 2e^{i\frac{\pi}{2}} r \mathbf{k}) < 0. \quad (4.63)$$

This is in the definition range  $(-\frac{\pi}{2}, \frac{3\pi}{2})$  for the first pair of fundamental solution in (4.60), i.e.

$$W_{\kappa, \mu}(z) \quad , \quad W_{-\kappa, \mu}(e^{-\pi i} z) \quad , \quad -\frac{\pi}{2} < \text{Arg}(z) < \frac{3\pi}{2}.$$

In fact, when  $\gamma > 0$ , for  $z := 2e^{i\frac{\pi}{2}} r \mathbf{k}$ , cf. (4.6), both  $z$  and  $e^{-\pi i} z$  are in the range  $(-\pi, \pi]$  of the principal branch of the Whittaker function. In another word, we do not have to use analytic extension by formula (4.35) in Remark 18.  $\triangle$

### 4.3 Outgoing fundamental solutions

We look for the Green's function  $\Phi_{\mathbf{k}}(x, y)$ ,  $x, y \in \mathbb{R}^3$ , solution to

$$\left(-\Delta_x - \mathbf{k}^2 + \frac{\alpha_{\infty}}{|x|}\right) \Phi_{\mathbf{k}}(x, y) = \delta(x - y), \quad (4.64)$$

such that

$$\text{when } \mathbf{k}^2 \in \mathbb{C} \setminus [0, \infty) \quad , \quad \text{for } y \text{ in compact subset} \quad , \quad \Phi_{\mathbf{k}}(x, y) \in L^2(\mathbb{R}_x^3). \quad (4.65)$$

Note that  $\text{Im } \mathbf{k} \neq 0$  is equivalent to  $\gamma \neq 0$ , this is from their definition in (4.15),

$$\mathbf{k} := \sqrt{\frac{\omega^2}{c^2} - \frac{\alpha_{\infty}^2}{4}} = \sqrt{\frac{\omega_0^2}{c^2} - \frac{\alpha_{\infty}^2}{4} + i \frac{\gamma}{c^2} \omega_0^2}.$$

We also recall the definition of  $\chi$ :

$$\chi = i \frac{\alpha_{\infty}}{2\mathbf{k}}.$$

<sup>19</sup>Note that when  $2\mu + 1 \notin \mathbb{Z} \Leftrightarrow 2\mu \notin \mathbb{Z}$ , a fundamental pair of solutions near origin to (4.20) is given by,

$$\mathcal{M}_{\kappa, \mu}(z) \quad , \quad \mathcal{M}_{\kappa, -\mu}(z) \quad , \quad 2\mu \notin \mathbb{Z} \quad , \quad |\text{Arg } z| \leq \pi,$$

cf. [8, Eqn (3a),(4),(7)]. However, they fail to be linearly independent when  $2\mu + 1 \in \mathbb{Z}$ .

### 4.3.1 Definitions

**Case 1a :**  $y = 0$  and  $k^2 \in \mathbb{C} \setminus [0, \infty)$  In this case, (4.64) reduces to

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = \delta(x). \quad (4.66)$$

We look for a solution that is radially symmetric in  $x$ , i.e.

$$\Phi_k(x, 0) = g(|x|).$$

On  $x \neq 0$ ,  $g(r)$  solves

$$\left( -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} - k^2 + \frac{\alpha_\infty}{r} \right) g = 0 \quad \text{in } \mathbb{R} \setminus \{0\}.$$

With the change of variable (4.6)  $z = 2e^{i\frac{\pi}{2}} k r$ , and consider the function  $g(z)$  defined by  $h(r) = r^{-1}g(z)$  solves

$$\left( \frac{d^2}{dz^2} - \frac{1}{4} + \frac{\chi}{z} \right) g = 0 \quad \text{in } \mathbb{R} \setminus \{0\}. \quad (4.67)$$

This equation is a special case of the Whittaker equation (4.20) with  $\mu = \frac{1}{2}$ . In subsubsection 4.2.4, the two linearly independent solutions in the neighborhood of infinity are given by  $W_{\chi, \frac{1}{2}}(z)$  and  $W_{-\chi, \frac{1}{2}}(e^{-i\pi} z)$ .

We recall the definition of the Whittaker function with the current parameters from (4.32),

$$\begin{aligned} W_{\chi, \frac{1}{2}}(z) = & -\frac{e^{-\frac{1}{2}z}}{\Gamma(-\chi)} \\ & + \frac{e^{-\frac{1}{2}z}}{\Gamma(-\chi)} \sum_{k=0}^{\infty} \frac{(1-\chi)_k}{(2)_k k!} z^k [\ln z + \psi(1-\chi+k) - \psi(1+k) - \psi(2+k)]. \end{aligned} \quad (4.68)$$

Only the latter solution given by  $W_{-\chi, \frac{1}{2}}(e^{-i\pi} z)$  satisfies condition (4.65), cf. Remark 20. As a result, when the source is at the origin, the fundamental solution is given as,

$$\Phi_k(x, 0) := \mathfrak{c} \frac{W_{-\chi, 1/2}(e^{-i\pi} e^{i\frac{\pi}{2}} 2k|x|)}{|x|}, \quad \text{for some constant } \mathfrak{c}.$$

The constant  $\mathfrak{c}$  can be determined in the process of showing that the candidate is indeed a fundamental solution. This is done specifically for the case  $y = 0$  in Appendix H, or for general  $y \neq 0$  in Prop. 15 and gives,

$$\boxed{\Phi_k(x, 0) := \frac{\Gamma(1+\chi)}{4\pi} \frac{W_{-\chi, 1/2}(e^{-i\pi} e^{i\frac{\pi}{2}} 2k|x|)}{|x|}.} \quad (4.69)$$

**Case 1b :**  $y \neq 0$  and  $k^2 \in \mathbb{C} \setminus [0, \infty)$  We will start with the kernel obtained from [18] by Hostler and Pratt, cf. [18, Eqn 8] in the closed form (see also Remark 22),

$$\begin{aligned} \Phi_k(x, y) &:= \frac{\Gamma(1+\chi)}{4\pi|x-y|} \frac{1}{ik} \left( \frac{\partial}{\partial_s} - \frac{\partial}{\partial_t} \right) \left( W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) \right) \\ &:= \frac{\Gamma(1+\chi)}{4\pi|x-y|} \begin{vmatrix} W_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix}. \end{aligned} \quad (4.70)$$

Here, the auxiliary variable is defined as,

$$s := |x| + |y| + |x-y| \quad ; \quad t := |x| + |y| - |x-y|. \quad (4.71)$$

We recall

$$M_{\chi, \frac{1}{2}}(z) = e^{-\frac{1}{2}z} z M(1 - \chi, 2; z) = e^{-\frac{1}{2}z} z \sum_{k=0}^{\infty} \frac{(1 - \chi)_k}{(2)_k} \frac{z^k}{k!}. \quad (4.72)$$

Note that  $(2)_k = \frac{\Gamma(2+k)}{\Gamma(2)} = (k+1)!$  since  $\Gamma(2) = 1$ . We will assume the fact that

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = 0 \quad , \quad x \in \mathbb{R}^3 \setminus \{y\}. \quad (4.73)$$

**Remark 22.** In [18], the definition is given in terms of the Whittaker function defined by Buchholtz [8, Eqn. 7 p.12], cf. (4.26)

$$\mathcal{M}_{\chi, \frac{1}{2}}(z) = z e^{-\frac{z}{2}} \frac{M(1 - \chi, 2; z)}{\Gamma(2)}.$$

However, when  $\mu = \frac{1}{2}$ ,  $\Gamma(2) = (2-1)! = 1$ , thus these two functions are the same,

$$\mathcal{M}_{-\chi, \frac{1}{2}}(z) = M_{-\chi, \frac{1}{2}}(z). \quad \triangle$$

**Case 2 :**  $k = k_0 > 0$  Using the limits (4.19),

$$\begin{aligned} k_\gamma &\rightarrow k_0 \quad , \quad \eta_\gamma \rightarrow \eta_0 \quad , \quad \chi_\gamma \rightarrow \chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^+; \\ k_\gamma &\rightarrow -k_0 \quad , \quad \eta_\gamma \rightarrow -\eta_0 \quad , \quad \chi_\gamma \rightarrow -\chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^- , \end{aligned}$$

we define limiting fundamental kernel as limits of the fundamental kernel,

$$\begin{aligned} \text{outgoing} \quad \Phi_{k_0}^+(x, y) &:= \lim_{\gamma \rightarrow 0^+} \Phi_k(x, y) \quad , \quad k_0 > 0; \\ \text{incoming} \quad \Phi_{k_0}^-(x, y) &:= \lim_{\gamma \rightarrow 0^-} \Phi_k(x, y) \quad , \quad k_0 > 0. \end{aligned} \quad (4.74)$$

Here the incoming and outgoing labeling follows Convention 1 discussed in Appendix, see also subsubsection 4.2.3. In particular, the  $k_0$ -outgoing kernel is defined as,

$$\Phi_{k_0}^+(x, y) := \frac{\Gamma(1 + \chi_0)}{4\pi |x - y|} \frac{1}{i k_0} \left( \frac{\partial}{\partial_s} - \frac{\partial}{\partial_t} \right) \left( W_{-\chi_0, 1/2}(-i k_0 s) M_{-\chi, 1/2}(-i k_0 t) \right), \quad (4.75)$$

while the incoming one,

$$\Phi_{k_0}^-(x, y) := \frac{\Gamma(1 - \chi_0)}{4\pi |x - y|} \frac{1}{i k_0} \left( \frac{\partial}{\partial_t} - \frac{\partial}{\partial_s} \right) \left( W_{\chi_0, 1/2}(i k_0 s) M_{\chi, 1/2}(i k_0 t) \right). \quad (4.76)$$

### 4.3.2 Basic properties of the fundamental kernels

Here, we work with an equivalent form of  $\Phi_k(x, y)$

$$\Phi_k(x, y) = \mathfrak{c} \frac{G(x, y)}{|x - y|} \quad ; \quad \mathfrak{c} := \frac{\Gamma(1 + \chi)}{4\pi}. \quad (4.77)$$

We have introduced the reduced Green function  $G(x, y)$ .

$$\begin{aligned} G(x, y) &:= H(s, t) := \frac{1}{i k} \left( \frac{\partial}{\partial_s} - \frac{\partial}{\partial_t} \right) \left( W_{-\chi, 1/2}(-i k s) M_{-\chi, 1/2}(-i k t) \right) \\ &= -W'_{-\chi, 1/2}(-i k s) M_{-\chi, 1/2}(-i k t) + W_{-\chi, 1/2}(-i k s) M'_{-\chi, 1/2}(-i k t) \\ &= \begin{vmatrix} W_{-\chi, 1/2}(-i k s) & M_{-\chi, 1/2}(-i k t) \\ W'_{-\chi, 1/2}(-i k s) & M'_{-\chi, 1/2}(-i k t) \end{vmatrix}. \end{aligned} \quad (4.78)$$



**Property 1** – (symmetry) While  $\Phi_k(x, y)$  are not functions of  $|x - y|$  as in the case of the Helmholtz equation, these fundamental solutions are still symmetric in  $x$  and  $y$ , i.e.  $\Phi_k(x, y) = \Phi_k(y, x)$ .

**Property 2** – (Limiting form when  $y = 0$ ) In this case,  $s = 2|x|$ , and  $t = 0$ . To find the limiting form, we need the limit of  $M_{-\chi, 1/2}(z)$  and its derivative  $M'_{-\chi, 1/2}(z)$  when  $z \rightarrow 0$ . By Prop 29 in Appendix C.1, we have

$$M_{-\chi, 1/2}(0) = 0 \quad , \quad \lim_{z \rightarrow 0} M'_{-\chi, 1/2}(z) = 1. \quad (4.79)$$

As a result of this, we obtain the value of the reduced Green kernel  $\Phi_k(x, y)$  defined in (4.70) for  $y = 0$ ,

$$\Phi_k(x, 0) = \frac{\Gamma(1 + \chi)}{4\pi|x|} W_{-\chi, 1/2}(-2ik|x|). \quad (4.80)$$

This is confirmed in [18, Eqn. 9]. This current form of the fundamental solution when the source position  $y = 0$  is also obtained by Meixner, see further discussion of literature and history in [18].

By (C.11) in Prop 30 in Appendix C.1,

$$W_{\kappa, \frac{1}{2}}(0) = \frac{1}{\Gamma(1 - \kappa)}.$$

The reduced kernel thus satisfies,

$$\lim_{x \rightarrow 0} G(x, 0) = \lim_{x \rightarrow 0} W_{-\chi, 1/2}(-2ik|x|) = \frac{1}{\Gamma(1 + \chi)}. \quad (4.81)$$

**Property 3** – (Behavior at  $x = y$ ) These properties will be needed for the consideration of local integrability of the fundamental kernel. In the current investigation, we keep  $y$  fixed and vary  $x$ .

**Proposition 9.** 1. For each fixed  $y \in \mathbb{R}^3$ , we have

$$\lim_{x \rightarrow y} G(x, y) = \frac{1}{\Gamma(1 + \chi)} \quad , \quad \forall y \in \mathbb{R}^3. \quad (4.82)$$

As a result of this,

$$\lim_{x \rightarrow y} |x - y| \Phi_k(x, y) = \frac{1}{4\pi} \quad , \quad \forall y \in \mathbb{R}^3; \quad (4.83a)$$

$$\lim_{x \rightarrow y} |x - y|^2 \Phi_k(x, y) = 0 \quad , \quad \forall y \in \mathbb{R}^3. \quad (4.83b)$$

2. For each fixed  $y \in \mathbb{R}^3$ , we have

$$\lim_{x \rightarrow y} |x - y|^2 \frac{x - y}{|x - y|} \cdot \nabla_x \Phi_k(x, y) = -\frac{1}{4\pi} \quad , \quad \forall y \in \mathbb{R}^3. \quad (4.84)$$

*Proof. Statement 1* We first obtain the limiting form of the reduced kernel  $G$  at  $x = y$  with  $y \neq 0$ . When  $x = y$ , we have

$$s = t = 2|x| = 2|y|. \quad (4.85)$$

Thus straight from the definition (4.70) of the reduced fundamental solution  $G$ , and using the value (4.79) of  $M_{-\chi, 1/2}$  and its derivative at  $z = 0$ , we obtain

$$\begin{aligned} \lim_{\substack{x \rightarrow y, \\ y \neq 0}} G(x, y) &= \mathcal{W} \left\{ W_{-\chi, 1/2}(-2ik|y|) , M_{-\chi, 1/2}(-2ik|y|) \right\} \\ &= \frac{\Gamma(2)}{\Gamma(1 + \chi)} = \frac{1}{\Gamma(1 + \chi)}. \end{aligned} \quad (4.86)$$

Here,  $\mathcal{W}\{\cdot, \cdot\}$  is the Wronskian, cf. [32, (13.14.26) p.335]. Note  $\Gamma(n) = (n-1)!$  hence  $\Gamma(2) = 1$ . Together with (4.81) (which gives the result for  $y = 0$ ), we obtain (4.82).

**Statement 2** We next obtain the result for  $\nabla_x \Phi_k(x, y)$ . For the normal gradient we consider separately the case when  $y = 0$  and  $y \neq 0$ .

$y = 0$  Using identity (F.31), we have

$$\begin{aligned} \frac{x}{|x|} \cdot \nabla_x \frac{1}{\mathfrak{c}} \Phi_k(x, 0) &= G(x, 0) \frac{x}{|x|} \cdot \nabla_x |x|^{-1} + \frac{1}{|x|} \frac{x}{|x|} \cdot \nabla_x G(x, 0); \\ &= -G(x, 0) \frac{1}{|x|^2} - 2ik \mathcal{W}'_{-\chi, 1/2}(-2ik|x|) \frac{1}{|x|}. \end{aligned}$$

From here we obtain

$$|x|^2 \frac{x}{|x|} \cdot \nabla_x \Phi_k(x, 0) = -\mathfrak{c} G(x, 0) - 2ik \mathfrak{c} \mathcal{W}'_{-\chi, 1/2}(-2ik|x|) |x|.$$

Next, to obtain the limit of the second term as  $|x| \rightarrow 0$ , we use Prop 30 in Appendix C.1 which gives,

$$\mathcal{W}'_{\chi, \frac{1}{2}}(z) = \frac{2 \ln z}{\Gamma(-\chi)} + 2 \frac{\psi(-\chi) + 2\gamma}{\Gamma(-\chi)} + \frac{1}{\Gamma(1-\chi)} + \mathcal{O}(z \ln z) \quad , \quad z \rightarrow 0.$$

At the end, we arrive at (4.84) for  $y = 0$ ,

$$\lim_{x \rightarrow 0} |x|^2 \frac{x}{|x|} \cdot \nabla_x \Phi_k(x, 0) = -\mathfrak{c} \lim_{x \rightarrow 0} G(x, 0) \stackrel{(4.82)}{=} -\frac{\Gamma(1+\chi)}{4\pi} \frac{1}{\Gamma(1+\chi)} = -\frac{1}{4\pi}.$$

$y \neq 0$  Using identity (F.32), we have

$$\begin{aligned} &\frac{x-y}{|x-y|} \cdot \nabla_x \Phi_k(x, y) \\ &= -\mathfrak{c} G(x, y) \frac{x-y}{|x-y|} \cdot \frac{(x-y)}{|x-y|^3} + \frac{\mathfrak{c}}{|x-y|} \left( \frac{x-y}{|x-y|} \cdot \frac{x}{|x|} (\partial_s + \partial_t) H + |x-y| (\partial_s - \partial_t) H \right). \end{aligned}$$

This gives

$$|x-y|^2 \frac{x-y}{|x-y|} \cdot \nabla_x \frac{1}{\mathfrak{c}} \Phi_k(x, y) = -G(x, y) + \underbrace{\frac{(x-y) \cdot x}{|x|} (\partial_s + \partial_t) H + |x-y|^2 (\partial_s - \partial_t) H}_{:= \mathbb{I}}.$$

We next consider the limit of the right-hand side (RHS) as  $x \rightarrow y$  for fixed  $y \neq 0$ . By Remark 33 in Appendix F.5, we have

$$\lim_{\substack{x \rightarrow y, \\ y \neq 0}} \partial_s H \quad \text{and} \quad \lim_{\substack{x \rightarrow y, \\ y \neq 0}} \partial_t H \quad \text{are finite and continuous functions of } y.$$

As a result of this,

$$\lim_{\substack{x \rightarrow y, \\ y \neq 0}} \mathbb{I} = 0,$$

and we obtain (4.84) for  $y \neq 0$ . In particular,

$$\lim_{\substack{x \rightarrow y, \\ y \neq 0}} |x-y|^2 \frac{x-y}{|x-y|} \cdot \nabla_x \Phi_k(x, y) = -\mathfrak{c} \lim_{\substack{x \rightarrow y, \\ y \neq 0}} G(x, y) \stackrel{(4.82)}{=} -\frac{\Gamma(1+\chi)}{4\pi} \frac{1}{\Gamma(1+\chi)} = -\frac{1}{4\pi}.$$

□

**Property 4** – (Asymptotic expansion when one variable goes to infinity and the other stays in a compact set) For  $t \in \mathbb{R}$ , define the phase function

$$\varphi_k(t) := \frac{1}{2} i k t - i \eta \log(k t) - \frac{\pi}{2} \eta. \quad (4.87)$$

This gives <sup>20</sup>

$$\exp(\varphi_k(t)) = e^{\frac{1}{2} i k t} (e^{-i \pi i k t})^{-i \eta} = \exp\left(\frac{1}{2} i k t - i \eta \log(k t) - \frac{\pi}{2} \eta\right).$$

Also define the phase  $\tilde{\varphi}_{k,y}(x)$  by

$$\begin{aligned} \tilde{\varphi}_{k,y}(x) := & -\frac{\pi}{2} \eta + i k |x| + \frac{1}{2} i k |y| \left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right) \\ & - i \eta \log\left(2k|x| + k|y| \left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right). \end{aligned} \quad (4.88)$$

This in turn gives,

$$\begin{aligned} \exp(\tilde{\varphi}_{k,y}(x)) := & e^{-\frac{\pi}{2} \eta} \exp\left[i k |x| + \frac{1}{2} i k |y| \left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right] \\ & \times \exp\left[-i \eta \log\left(2k|x| + k|y| \left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right)\right]. \end{aligned} \quad (4.89)$$

With auxiliary variable  $s$  defined in (4.71), the leading factor in the asymptotic of  $\Phi_k$ , cf. (C.17) is given by  $e^{\varphi_k(s)}$ . Here, we investigate the approximation of  $e^{\phi(s)}$  by  $e^{\varphi_k(2|x|)}$  or  $e^{\tilde{\varphi}_{k,y}(x)}$  for  $y$  belonging in compact set and  $|x| \rightarrow \infty$ . See below in Figure 9 and 10 for its numerical illustration.

**Proposition 10.** *The leading factor in the asymptotic of  $\Phi_k$ , cf. (C.17)*

$$\exp(\varphi_k(s)) = e^{\frac{1}{2} i k s} (e^{-i \pi i k s})^{-i \eta} = \exp\left(\frac{1}{2} i k s - i \eta \log(k s) - \frac{\pi}{2} \eta\right)$$

can be approximated by

$$\exp(\varphi_k(s)) = \underbrace{\exp\left(i k |x| - i \eta \log(2k|x|) - \frac{\pi}{2} \eta\right)}_{\exp(\varphi_k(2|x|))} \exp\left(i k \times O(1)\right), \quad (4.90)$$

or

$$\exp(\varphi_k(s)) = \exp(\tilde{\varphi}_{k,y}(x)) \exp\left(i k \times O(|x|^{-1})\right). \quad (4.91)$$

*Proof. Zero-th order approximation*, we first write the auxiliary variable  $s$  defined in (4.71) as,

$$s = 2|x| + \varepsilon, \quad \varepsilon = O(1).$$

We have

$$\begin{aligned} e^{\frac{1}{2} i k s} (e^{-i \pi i k s})^{-i \eta} &= \exp\left(i k (|x| + \varepsilon) - i \eta \log(2k|x| + 2k\varepsilon) - \frac{\pi}{2} \eta\right) \\ &= \exp\left(i k |x| - i \eta \log(2k|x|) - \frac{\pi}{2} \eta\right) \times \exp\left(\frac{1}{2} i k \varepsilon - i \eta \varepsilon'\right), \end{aligned} \quad (4.92)$$

<sup>20</sup>This is verified as follows. With  $\gamma > 0$ ,  $0 \leq \text{Arg}(k\gamma) \leq \frac{\pi}{2}$ , then  $-\frac{\pi}{2} \leq \text{Arg}(e^{-i \frac{\pi}{2} k}) \leq 0$ . With  $\log$  denoting the principal branch for the log, i.e.  $-\pi < \text{Im}(\log z) \leq \pi$ , we have

$$\log(e^{-i \pi i k s}) = \log(e^{-i \frac{\pi}{2} k s}) = \log(k s) - i \frac{\pi}{2}.$$

Use this to rewrite,

$$\begin{aligned} e^{\frac{1}{2} i k s} (e^{-i \pi i k s})^{-i \eta} &= \exp\left(\frac{1}{2} i k s - i \eta \log(e^{-i \pi i k s})\right) = \exp\left(\frac{1}{2} i k s - i \eta \log(k s) - i \eta (-\frac{\pi}{2})\right) \\ &= \exp\left(\frac{1}{2} i k s - i \eta \log(k s) - \frac{\pi}{2} \eta\right). \end{aligned}$$

where

$$\epsilon' := \log(ks) - \log(2k|x|) = \log(|k|s) - \log(2|k||x|) = \log(s) - \log(2|x|).$$

The second equality is due to the two terms having the same argument. We next bound this by using, for  $w > 0$  and  $w + \delta > 0$ ,

$$|\log(w + \delta) - \log w| = \left| \int_w^{w+\delta} \frac{1}{z} dz \right| \leq \frac{|\delta|}{\min(w, w + \delta)}. \quad (4.93)$$

Since  $s = O(|x|)$ , cf. (F.7a),

$$|\epsilon'| \leq \frac{|\epsilon|}{\min\{s, 2|x|\}} \Rightarrow \epsilon' = O(|x|^{-1}).$$

The last factor of the RHS of (4.92) is

$$\exp\left(\frac{1}{2}ik\epsilon - i\eta\epsilon'\right) = \exp(ikO(1)).$$

**Second order approximation** If we use a higher order expansion,

$$s = 2|x| + |y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right) + \tilde{\epsilon}, \quad \tilde{\epsilon} = O(|x|^{-1}).$$

Using this, we obtain

$$\begin{aligned} & \exp\left(\frac{1}{2}iks - i\eta \log(ks) - \frac{\pi}{2}\eta\right) \\ &= \exp\left(ik\left(|x| + \frac{1}{2}|y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right) + \frac{1}{2}\tilde{\epsilon}\right) - i\eta \log(ks) - \frac{\pi}{2}\eta\right). \end{aligned}$$

This thus gives

$$\begin{aligned} \exp\left(\frac{1}{2}iks - i\eta \log(ks) - \frac{\pi}{2}\eta\right) &= e^{-\frac{\pi}{2}\eta} \exp\left[ik|x| + \frac{1}{2}ik|y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right] \\ &\times \exp\left[-i\eta \log\left(2k|x| + k|y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right)\right] \exp\left(\frac{1}{2}ik\tilde{\epsilon} - i\eta\tilde{\epsilon}\right), \end{aligned} \quad (4.94)$$

where

$$\begin{aligned} \tilde{\epsilon} &:= \log(ks) - \log\left(2k|x| + k|y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right) \\ &= \log(|k|s) - \log\left(2|k||x| + |k||y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right) \\ &= \log(s) - \log\left(2|x| + |y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\right). \end{aligned}$$

As before, the second equality is due to the two terms having the same argument. We next bound this remainder term by using (4.93),

$$|\tilde{\epsilon}| \leq \frac{|\tilde{\epsilon}|}{\min\{s, 2|x| + |y|\left(1 - \frac{y}{|y|} \cdot \frac{x}{|x|}\right)\}} \Rightarrow \tilde{\epsilon} = O(|x|^{-2}).$$

Since  $\tilde{\epsilon} = O(|x|^{-1})$  and  $\tilde{\epsilon} = O(|x|^{-2})$ , the last factor of the RHS of (4.94) can be bounded as follow,

$$\exp\left(\frac{1}{2}ik\tilde{\epsilon} - i\eta\tilde{\epsilon}\right) = \exp\left(\frac{1}{2}ik \times O(|x|^{-1}) - i\eta \times O(|x|^{-2})\right) = \exp(ik \times O(|x|^{-1})).$$

□

**Numerical illustration for Prop 10** We fix a source position at  $y_0 = (0, 0, 1)$ , and investigate the oscillatory behavior of the phase functions considered in Prop 10 along different directions of approaching infinity. The results are shown in Figure 9 and 10. We consider a source in  $y_0$  and the functions

$$\operatorname{Re} \exp(\varphi_k(s)), \quad s := |x| + |y_0| + |x - y_0|,$$

and the real part of the ratios between the oscillatory phases  $\varphi_k(2|x|)$  and  $\tilde{\varphi}_{k,y}(x)$ , labeled as,

$$\tilde{\tau}_1 = \frac{\exp(\varphi_k(s))}{\exp(\varphi_k(2|x|))}; \quad \tilde{\tau}_2 = \frac{\exp(\varphi_k(s))}{\exp(\tilde{\varphi}_{k,y}(x))}. \quad (4.95)$$

We consider  $x$  in the  $(y, z)$ -plane along two directions with polar angles  $\theta_x = \frac{\pi}{6}$  and  $\frac{3\pi}{4}$ , while keeping the azimuthal angle  $\phi_x = \frac{\pi}{2}$ . For each of these polar angles, the phase functions and ratios are evaluated at  $y_0 = (0, 0, 1)$  and  $x = (0, r \sin(\theta_x), r \cos(\theta_x))$ , and are thus plotted as functions of  $r$ .

We use the following parameters

$$c = 3; \quad \alpha_\infty = 50; \quad \omega_0 = 2\pi 20; \quad (4.96)$$

and experiment with attenuation in Figure 10 and without in Figure 9.

We have the following observations

- As expected, in the left of Figure 9, for  $\gamma = 0$ , the function  $\exp(\varphi_k(s))$  exhibits pure oscillation, while in the left one of Figure 10,  $\gamma = 1$ , the oscillatory behavior is coupled with attenuation, i.e. with the decreasing magnitude of the envelope of the oscillation. The same conclusion holds for both directions.
- The subfigures on the right, cf. subfigure 9(b) for  $\gamma = 0$  and 10(b) for  $\gamma = 1$ , show that the ratios  $\tilde{\tau}_i$  are now polynomial decay or bounded. The computation expects that  $\tilde{\tau}_2$  is  $\exp(O(r^{-1}))$ , cf. (4.91), thus its curve will level out at the constant 1. This is confirmed in the graphs of  $\tilde{\tau}_1$  for both directions, cf. the upper subfigures of subfigure 9(b) and 10(b). On the other hand, it is expected that  $\tilde{\tau}_1$  is  $\exp(O(1))$  and is simply bounded, cf. (4.90). In the lower subfigures of subfigure 9(b) and 10(b), we still see the pattern of the curves having horizontal asymptotes with different values for each direction, yet this is not as clear as with ratio  $\tilde{\tau}_1$ . This shows that while both phase functions  $\varphi_k(2|x|)$  and  $\tilde{\varphi}_{k,y}(x)$  approximate well  $\varphi_k(s)$ , the result is more uniform in all directions with the latter (i.e.  $\tilde{\varphi}_{k,y}(x)$ ).

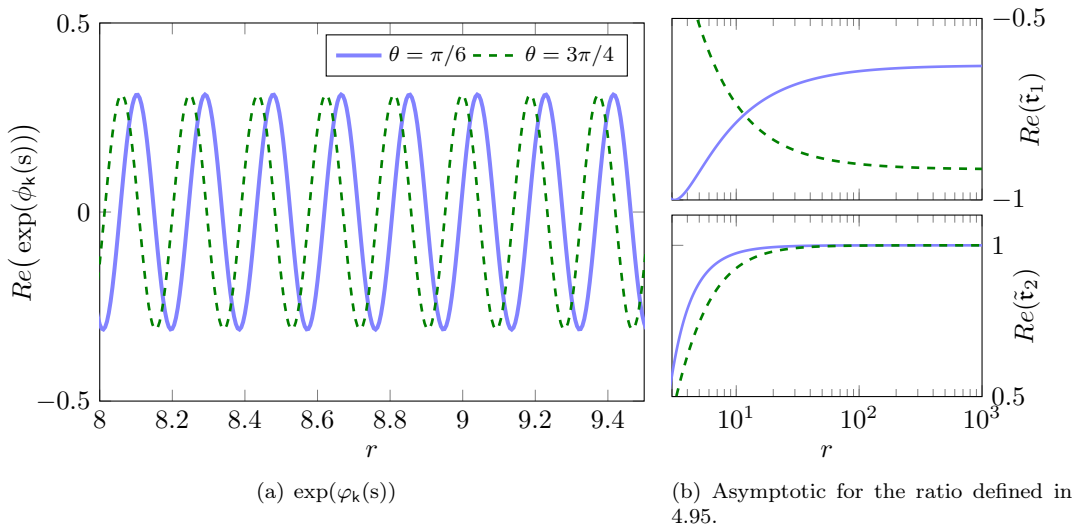


Figure 9: Numerical illustration for Prop 10 for  $\gamma = 0$ . The right subfigures 9(b) show the asymptotics for the ratios comparing  $\varphi_k(s)$  with  $\tilde{\varphi}_{k,y}(x)$  represented by  $\tilde{\tau}_2$ , and with  $\varphi_k(2|x|)$  represented by  $\tilde{\tau}_1$ .

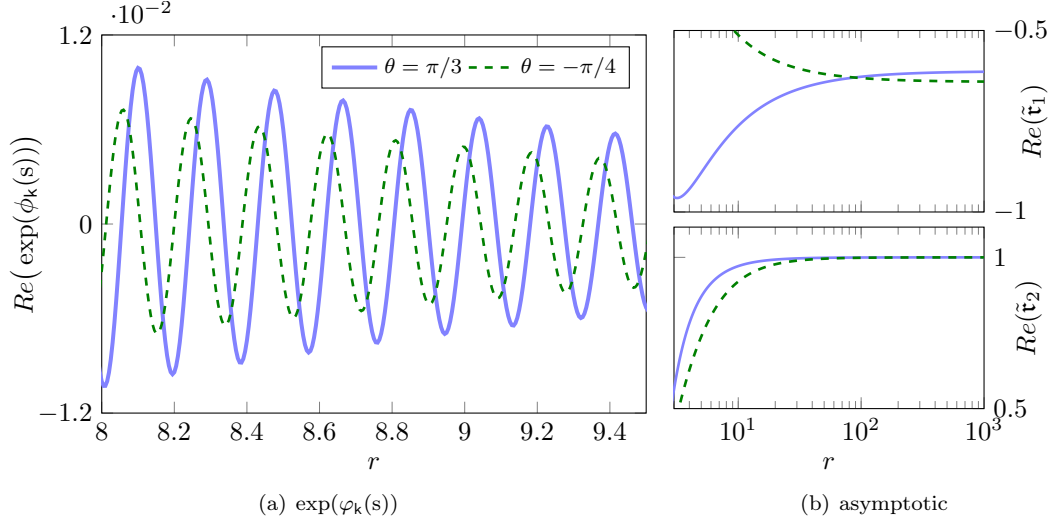


Figure 10: Numerical illustration for Prop 10 for  $\gamma = 1$ . The right subfigures 10(b) show the asymptotics for the ratios comparing  $\varphi_k(s)$  with  $\tilde{\varphi}_{k,y}(x)$  represented by  $\tilde{\tau}_2$ , and with  $\varphi_k(2|x|)$  represented by  $\tilde{\tau}_1$ .

Having analyzed the oscillatory part of  $\Phi_k(x, y)$ , which can be described either by

$$\exp(\varphi_k(s)) \quad \text{or} \quad \exp(\tilde{\varphi}_{k,y}(x)),$$

we now describe the full structure of  $\Phi_k(y, x)$  including its symbol part, with explicit description of the leading constant. See Figures 9 and 10 for its numerical illustration.

**Proposition 11.** • With  $e^{\tilde{\varphi}_y(k,x)}$  given in (4.89) and  $e^{\varphi_k(s)}$  in (4.87) the asymptotics at infinity of  $\Phi_k$ , for  $y$  in compact set, when  $|x| \rightarrow \infty$ , is given by

$$\begin{aligned} \Phi_k(x, y) &= \frac{\exp(\varphi_k(s))}{|x - y|} \left( \mathfrak{C}(y, \hat{x}) + O(|x|^{-1}) \right) \\ &= \frac{\exp(\tilde{\varphi}_k(y, x))}{|x|} \left( \mathfrak{C}(y, \hat{x}) + O(|x|^{-1}) \right), \end{aligned} \quad (4.97)$$

where for a point  $y \in \mathbb{R}^3$  and direction  $\hat{x} \in \mathbb{S}^2$ , the constant  $\mathfrak{C}(y, \hat{x})$  is defined as,

$$\mathfrak{C}(y, \hat{x}) := \frac{\Gamma(1 + \chi)}{4\pi} \left( \frac{1}{2} M_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) + M'_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) \right). \quad (4.98)$$

The remainder  $O(|x|^{-1})$  is uniformly bounded for all  $y$  in a bounded set and all directions of  $\hat{x}$ .

When the attenuation  $\gamma = 0$ , for  $y$  in compact set, and  $|x| \rightarrow \infty$ , we simply have

$$\Phi_{k_0}(x, y) = \mathfrak{C}(y, \hat{x}) \frac{\exp(\tilde{\varphi}_{k_0}(y, x))}{|x|^{-1}} + O(|x|^{-2}). \quad (4.99)$$

As a result of this, when  $\gamma \neq 0$ , for fixed  $y$ , the function  $x \mapsto \Phi(x, y)$  is exponentially decaying, and thus  $L^2(\mathbb{R}^3)$ .

- For  $y$  in compact set and  $x$  tending to infinity, one obtains similar results for  $\frac{y}{|y|} \cdot \nabla_y \Phi_k(x, y)$  with constant  $\mathfrak{D}(y, \hat{x})$  defined in (4.109)

*Proof. Part 1* We first recall the definition of the fundamental kernel,

$$\Phi_k(x, y) = \frac{\mathfrak{c}}{|x - y|} G,$$

where

$$G(x, y) = H(s, t) = -W'_{-\chi, 1/2}(-i k s) M_{-\chi, 1/2}(-i k t) + W_{-\chi, 1/2}(-i k s) M'_{-\chi, 1/2}(-i k t).$$

For directions  $\hat{x} = \frac{x}{|x|}$  and  $\hat{y} = \frac{y}{|y|}$ , i.e.

$$\hat{x} = (\sin \theta_x \cos \phi_x, \sin \theta_x \sin \phi_x, \cos \theta_x) \quad , \quad \hat{y} = (\sin \theta_y \cos \phi_y, \sin \theta_y \sin \phi_y, \cos \theta_y).$$

Here,  $(|x|, \theta_x, \phi_x)$  is the spherical coordinates of  $x$  with  $0 \leq \theta_x \leq \pi$  and  $0 \leq \phi_x \leq 2\pi$ , we have defined in (F.2) the bounded quantity

$$\mathfrak{d}_{\hat{x}, \hat{y}} = \cos \theta_x \cos \theta_y + \sin \theta_x \sin \theta_y \cos(\phi_x - \phi_y).$$

From the expansion (F.7a) and (F.7b) of  $s$  and  $t$ , for a fixed  $y$  and as  $x$  goes to infinity, we have

$$\lim_{|x| \rightarrow \infty} \frac{s}{2|x|} = 1 \quad \text{and} \quad \frac{s}{2|x|} = 1 + O(|x|^{-1}), \quad (4.100)$$

and for  $x$  goes to infinity along a fixed angle  $(\theta_x, \phi_x)$ ,

$$\lim_{|x| \rightarrow \infty} t = |y| \mathfrak{d}_{\hat{x}, \hat{y}} \quad \text{and} \quad t = |y| \left(1 + \mathfrak{d}_{x, y}\right) + O(|x|^{-1}). \quad (4.101)$$

Using the asymptotic property of  $W$  given (4.43), for  $y$  fixed and as  $x$  goes to infinity, we have

$$\lim_{|x| \rightarrow \infty} \frac{W_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} = 1 \quad \text{and} \quad \frac{W_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} = 1 + O(|s|^{-1}) = 1 + O(|x|^{-1}). \quad (4.102)$$

Similarly, for its derivative in (4.44), with  $y$  fixed and as  $x$  goes to infinity,

$$\lim_{|x| \rightarrow \infty} \frac{W'_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} = -\frac{1}{2} \quad \text{and} \quad \frac{W'_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} = -\frac{1}{2} + O(|x|^{-1}). \quad (4.103)$$

For fixed  $y$  and for  $x$  goes to infinity along a fixed angle  $(\theta_x, \phi_x)$ , using the limit of  $t$ ,

$$\begin{aligned} \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} \frac{G}{\exp(\varphi_k(s))} &= - \lim_{|x| \rightarrow \infty} \frac{W'_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M_{-\chi, 1/2}(-i k t) \\ &\quad + \lim_{|x| \rightarrow \infty} \frac{W_{-\chi, 1/2}(-i k s)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M'_{-\chi, 1/2}(-i k t) \\ &= \frac{1}{2} M_{-\chi, 1/2}(-i k |y| \mathfrak{d}_{\hat{x}, \hat{y}}) + M'_{-\chi, 1/2}(-i k |y| \mathfrak{d}_{\hat{x}, \hat{y}}). \end{aligned}$$

The stronger result is obtained by using the asymptotic expansions,

$$\begin{aligned} \frac{G}{\exp(\varphi_k(s))} &= -\left(\frac{1}{2} + O(|x|^{-1})\right) \left(M_{-\chi, 1/2}(-i k |y| \mathfrak{d}_{\hat{x}, \hat{y}}) + O(|x|^{-1})\right) \\ &\quad + \left(1 + O(|x|^{-1})\right) \left(M'_{-\chi, 1/2}(-i k |y| \mathfrak{d}_{\hat{x}, \hat{y}}) + O(|x|^{-1})\right). \end{aligned} \quad (4.104)$$

Note that the constant bound for each direction  $\hat{x}$  and  $y$  depends on  $|y|$ ,  $\hat{y}$ , and  $|x|$ . Since  $y$  stays in a bounded set, and direction  $\hat{y}$ ,  $\hat{x}$  are both in compact set  $\mathbb{S}^2$  (the unit sphere), they have a uniform bound for all  $y$  in a bounded set and all direction of  $\hat{x}$ . The original phase  $\varphi_k(|s|)$  can be replaced by  $\tilde{\varphi}_{k, y}(x)$  without changing the asymptotes of the remainder, cf. Prop 10. In particular,

$$\frac{\exp(\varphi_k(s))}{\exp(\tilde{\varphi}_{k, y}(x))} = 1 + O(|x|^{-1}) \quad , \quad \frac{|x|}{|x - y|} = 1 + O(|x|^{-1}).$$

Thus

$$\begin{aligned}
\Phi_k(x, y) &= \frac{\exp(\varphi_k(s))}{|x - y|} \left( \mathfrak{C}(y, \hat{x}) + \mathcal{O}(|x|^{-1}) \right) \\
&= \frac{\exp(\tilde{\varphi}_k(y, x))}{|x|} \times \frac{\exp(\varphi_k(s))}{\exp(\tilde{\varphi}_{k,y}(x))} \times \frac{|x|}{|x - y|} \times \left( \mathfrak{C}(y, \hat{x}) + \mathcal{O}(|x|^{-1}) \right) \\
&= \frac{\exp(\tilde{\varphi}_k(y, x))}{|x|} \times (1 + \mathcal{O}(|x|^{-1})) \times (1 + \mathcal{O}(|x|^{-1})) \times \left( \mathfrak{C}(y, \hat{x}) + \mathcal{O}(|x|^{-1}) \right) \\
&= \frac{\exp(\tilde{\varphi}_k(y, x))}{|x|} \left( \mathfrak{C}(y, \hat{x}) + \mathcal{O}(|x|^{-1}) \right).
\end{aligned}$$

**Part 2** We first expand out radial derivative of  $\Phi$  in the  $y$  variable. Here we introduce the notation

$$\partial_{r(y)} := \frac{y}{|y|} \cdot \nabla_y.$$

We have

$$\partial_{r(y)} \frac{1}{\mathfrak{c}} \Phi_k = G \underbrace{\partial_{r(y)} |x - y|^{-1}}_{\mathcal{O}(|x|^{-2})} + \underbrace{\frac{\partial_{r(y)} s}{|x - y|}}_{\mathcal{O}(|x|^{-1})} \partial_s H + \underbrace{\frac{\partial_{r(y)} \mathfrak{t}}{|x - y|}}_{\mathcal{O}(|x|^{-1})} \partial_t H.$$

The indicated orders of decay use the calculation in (F.12), (F.15b) and (F.16b),

$$\begin{aligned}
\partial_{r(y)} s &= 1 + \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1); \\
\partial_{r(y)} \mathfrak{t} &= 1 - \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1).
\end{aligned} \tag{4.105}$$

We recall from (F.22) and (F.23), the partial derivatives of  $H$ ,

$$\begin{aligned}
\partial_s H &= -ik \left( W'_{-\chi, 1/2}(-ik s) M'_{-\chi, 1/2}(-ik t) - \frac{1}{4} W_{-\chi, 1/2}(-ik s) M_{-\chi, 1/2}(-ik t) \right) \\
&\quad + \frac{\chi}{s} W_{-\chi, 1/2}(-ik s) M_{-\chi, 1/2}(-ik t); \\
\partial_t H &= -ik \left( \frac{1}{4} W_{-\chi, 1/2}(-ik s) M_{-\chi, 1/2}(-ik t) - W'_{-\chi, 1/2}(-ik s) M'_{-\chi, 1/2}(-ik t) \right) \\
&\quad - \frac{\chi}{t} W_{-\chi, 1/2}(-ik s) M_{-\chi, 1/2}(-ik t).
\end{aligned} \tag{4.106}$$

Thus

$$\begin{aligned}
\lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} \frac{\partial_s H}{\exp(\varphi_k(s))} &= -ik \lim_{|x| \rightarrow \infty} \frac{W'_{-\chi, 1/2}(-ik s)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M'_{-\chi, 1/2}(-ik t) \\
&\quad - \frac{ik}{4} \lim_{|x| \rightarrow \infty} \frac{W_{-\chi, 1/2}(-ik s)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M_{-\chi, 1/2}(-ik t)
\end{aligned} \tag{4.107}$$

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$$= \frac{ik}{2} M'_{-\chi, 1/2}(-ik |y| \mathfrak{d}_{\hat{x}, \hat{y}}) - \frac{ik}{4} M_{-\chi, 1/2}(-ik |y| \mathfrak{d}_{\hat{x}, \hat{y}}).$$



In a similar manner, we obtain

$$\begin{aligned}
\lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} \partial_t H &= -\frac{ik}{4} \lim_{|x| \rightarrow \infty} \frac{W_{-\chi, 1/2}(-iks)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M_{-\chi, 1/2}(-ikt) \\
&+ ik \lim_{|x| \rightarrow \infty} \frac{W'_{-\chi, 1/2}(-iks)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} M'_{-\chi, 1/2}(-ikt) \\
&- \chi \lim_{|x| \rightarrow \infty} \frac{W_{-\chi, 1/2}(-iks)}{\exp(\varphi_k(s))} \times \lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} \frac{M_{-\chi, 1/2}(-ikt)}{t} \\
&= -\frac{ik}{4} M_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) - \frac{ik}{2} M'_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) - \chi \frac{M_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}})}{|y| \mathfrak{d}_{\hat{x}, \hat{y}}}.
\end{aligned} \tag{4.108}$$

Putting together results (4.100)–(4.103) and (4.105)–(4.108), we obtain

$$\lim_{\substack{|x| \rightarrow \infty \\ \hat{x} \text{ fixed}}} \frac{|x-y|}{c} \partial_{r(y)} \Phi_k = \mathfrak{D}(y, \hat{x}),$$

where the value of the limit is a function depending continuously on  $y$  and direction  $\hat{x}$ ,

$$\begin{aligned}
\mathfrak{D}(y, \hat{x}) &:= (1 + \mathfrak{d}_{x,y}) \left( \frac{ik}{2} M'_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) - \frac{ik}{4} M_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) \right) \\
&+ (\mathfrak{d}_{x,y} - 1) \left( \left( \frac{ik}{4} + \frac{\chi}{|y| \mathfrak{d}_{\hat{x}, \hat{y}}} \right) M_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) + \frac{ik}{2} M'_{-\chi, 1/2}(-ik|y| \mathfrak{d}_{\hat{x}, \hat{y}}) \right).
\end{aligned} \tag{4.109}$$

The asymptotic expansion version is obtained in a similar manner as in Part 1, cf. (4.104), by using the expansion version of each component (instead of just limits).  $\square$

**Numerical illustration for Prop 11** As in the illustration of the phase (in Figure 9 and 10), to illustrate the uniformness of the asymptotic expansion 4.97 for  $\Phi_k(x, y)$ , we take a fixed source  $y_0 = (0, 0, 1)$ , and investigate the oscillatory behavior of  $\Phi_k(x, y)$  along different directions of approaching infinity. To illustrate the symbol structure of  $\Phi_k(x, y)$ , it suffices to work with  $G$ . We recall the definition of  $\Phi_k(x, y)$ , cf. (4.77),

$$\Phi_k(x, y) = c \frac{G(x, y)}{|x-y|} \quad ; \quad c := \frac{\Gamma(1+\chi)}{4\pi},$$

with the reduced Green function  $G(x, y)$  introduced in (4.78),

$$G(x, y) := H(s, t) := \frac{1}{ik} \left( \frac{\partial}{\partial_s} - \frac{\partial}{\partial_t} \right) \left( W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) \right).$$

The leading oscillatory phase of  $G$  is given by  $\exp(\varphi_k(s))$ . We factor this out of  $G$  and plot the ratio to investigate structure of the symbol part. We will also do with the oscillatory phase function  $\varphi_k(2|x|)$  and  $\tilde{\varphi}_{k,y}(x)$ . For the leading factor, we define the following ratios:

$$\hat{\mathfrak{t}}_1 = \frac{G_{k_0}(x, y_0)}{\exp(\varphi_k(s))}; \quad \hat{\mathfrak{t}}_2 = \frac{G_{k_0}(x, y_0)}{\exp(\varphi_k(2|x|))}; \quad \hat{\mathfrak{t}}_3 = \frac{G_{k_0}(x, y_0)}{\exp(\tilde{\varphi}_{k,y}(x))}. \tag{4.110}$$

We consider two directions of approaching infinity along polar angle of  $x$  with  $\theta_x = \frac{\pi}{6}$  and  $\frac{3\pi}{2}$ , keeping the azimuthal angle  $\phi_x = \frac{\pi}{2}$ . Thus we are working in the  $(y, z)$ -plane. This means for each of these two polar angles, the phase functions and ratios are evaluated at fixed  $y_0 = (0, 0, 1)$ , and  $x = (0, r \sin(\theta_x), r \cos(\theta_x))$ . They are thus plotted as functions of  $r$ . The results are shown in Figure 11 for no attenuation ( $\gamma = 0$ ) and Figure 12 for constant attenuation  $\gamma = 1$ .

We have the following observations.

- As  $\exp(\varphi_k(s))$  dominates the behavior of the fundamental kernel, we have the same observations for the Figures 11(a) and 12(a) as those for the phase (in Figures 9 and 10). That is in the left of Figure 11,  $\gamma = 0$ , thus the phase exhibits pure oscillation, while in the left of Figure 12,  $\gamma = 1$ , the oscillatory behavior is coupled with attenuation, i.e. with the decreasing magnitude of the envelope of the oscillation. Same conclusion for both directions.
- Regarding the symbol structure illustrated by the right of Figures 11(b) and 12(b), we see that  $\varphi_k(s)$  and  $\tilde{\varphi}_{k,y}(x)$  give better representation of the dominant behavior of the fundamental kernel. They are represented by the curves for ratio  $\hat{\mathbf{t}}_1$  and  $\hat{\mathbf{t}}_3$ . With and without attenuation, the convergence to the horizontal asymptotes is much earlier than what is exhibited in the curve for  $\hat{\mathbf{t}}_2$  which represents  $\varphi_k(2|x|)$ . The plots also show the uniformity of the asymptotic expansion, with the ratio curves of the two directions of infinity staying close together and behaving in the same manner. They are much closer for  $\gamma = 0$  than for  $\gamma = 1$ . These curves also have the profile of a constant  $+ o(1)$ .

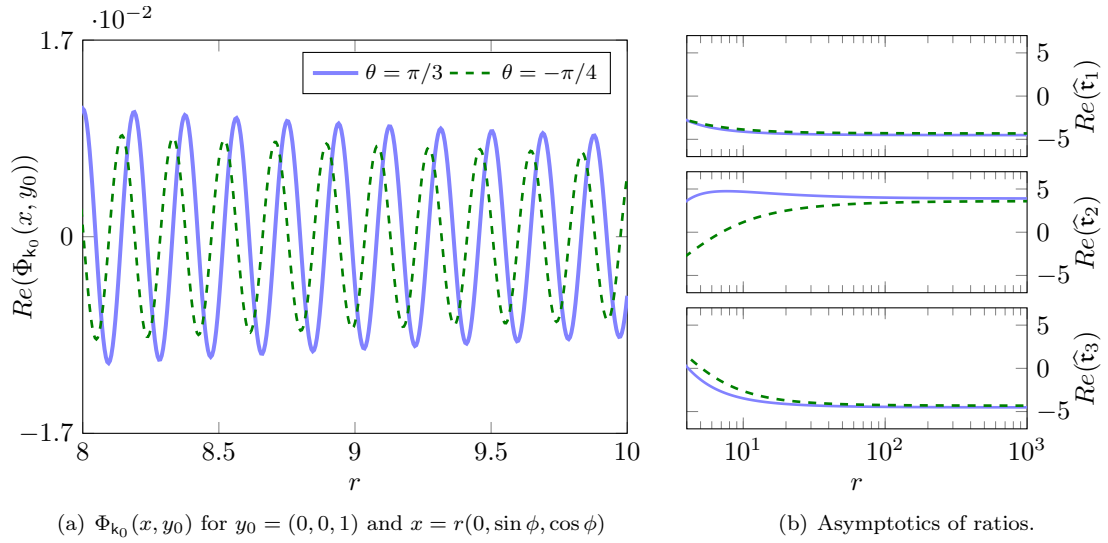


Figure 11: Numerical illustration for Prop 11 of asymptotic expansion of  $\Phi_k(x, y_0)$  for  $\gamma = 0$ . Here, for fixed source  $y_0 = (0, 0, 1)$  and  $x = r(0, \sin \theta, \cos \theta)$  going to infinity along two different directions represented by polar angle  $\theta = \frac{\pi}{6}$  and  $\frac{3\pi}{2}$ . In Figure (b), we factor out the oscillatory part from the reduced Green kernel, and consider  $G(x, y_0)e^{-\phi}$  with  $\phi = \phi_{k_0}(s)$  for  $\hat{\mathbf{t}}_1$ ,  $\phi = \phi_{k_0}(2|x|)$  for  $\hat{\mathbf{t}}_2$ , and  $\phi = \tilde{\varphi}_{k_0, y_0}(x)$  for  $\hat{\mathbf{t}}_3$ . The plots also show the uniformity of the asymptotic expansion, it also shows that the three expansions represent well the leading behavior of  $\Phi_k(x, y)$  with  $\varphi_k(s)$  and  $\phi_{k,y}(x)$  giving small error and faster convergence. All three remainders have the profile of a constant  $+ o(1)$ .

**Property 5** – (Radiating asymptotics) In the next two propositions, Prop 12 and 13, we will show the radiating property of the fundamental solution  $\Phi_{k_0}^+(x, y)$ , as  $|x| \rightarrow \infty$  and  $y$  in compact set. We will make heavily use of the radiating property,

$$e^{\frac{1}{2}z} z^{-\chi} \left( W'_{\chi, \frac{1}{2}}(z) + \frac{1}{2} W_{\chi, \frac{1}{2}}(z) \right) = O(|z|^{-1}).$$

of  $W_{\chi, \frac{1}{2}}$  (cf. Prop 30 in App C.1), and the gradient calculation in Appendix F.

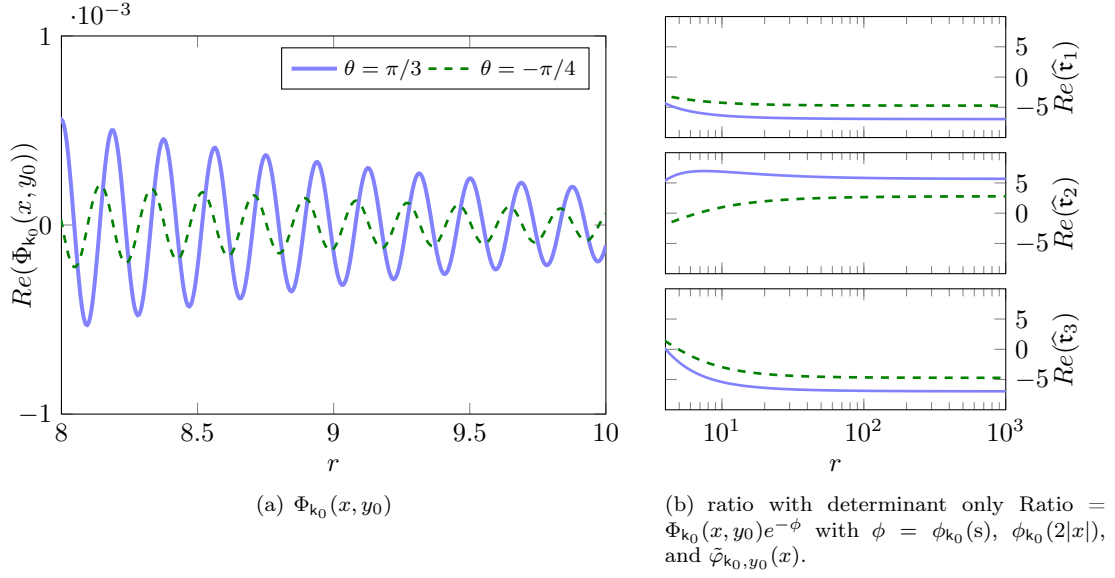


Figure 12: Numerical illustration for Prop 11 of asymptotic expansion of  $\Phi_{k_0}(x, y_0)$  for  $\gamma = 1$ . Here, for fixed source  $y_0 = (0, 0, 1)$  and  $x = r(0, \sin \theta, \cos \theta)$  going to infinity along two different directions represented by polar angle  $\theta = \frac{\pi}{6}$  and  $\frac{3\pi}{2}$ . The ratios are defined in (4.110). We have the same conclusion as in the case without attenuation shown in Figure 11.

**Proposition 12.** For  $y$  in compact set, when  $|x| \rightarrow \infty$ .

$$\left( \frac{x}{|x|} \cdot \nabla_x - i k_0 \right) \Phi_k(x, y) = e^{\varphi_k(2|x|)} O(|x|^{-2}), \quad (4.111)$$

with  $\varphi_k(\cdot)$  defined in (4.87),

$$\varphi_k(2|x|) = i k |x| - i \eta \log(2k|x|) - \frac{\pi}{2} \eta.$$

When the attenuation  $\gamma = 0$ , we simply have

$$\left( \frac{x}{|x|} \cdot \nabla_x - i k_0 \right) \Phi_{k_0}^+(x, y) = O(|x|^{-2}), \quad (4.112)$$

uniformly for  $y$  in compact set, when  $|x| \rightarrow \infty$ .

*Proof.* We have

$$\begin{aligned} \partial_{r(x)} \frac{1}{c} \Phi_k &= G \partial_{r(x)} |x - y|^{-1} + \frac{\partial_{r(x)} G}{|x - y|}; \\ &= G \partial_{r(x)} |x - y|^{-1} + \frac{\partial_{r(x)} s}{|x - y|} \partial_s H + \frac{\partial_{r(x)} t}{|x - y|} \partial_t H. \end{aligned} \quad (4.113a)$$

From (F.5b) and (F.11a), we have

$$\begin{aligned} |x - y|^{-1} &= |x|^{-1} (1 + O(|x|^{-1})); \\ \partial_{r(x)} |x - y|^{-1} &= -\frac{x}{|x|} \cdot \frac{x - y}{|x - y|^3} = O(|x|^{-2}); \end{aligned}$$

and from (F.14),

$$\begin{aligned}\partial_{r(x)} s &= 1 + \frac{x}{|x|} \cdot \frac{x-y}{|x-y|} = 2 + O(|x|^{-1}) = O(1); \\ \partial_{r(x)} t &= 1 - \frac{x}{|x|} \cdot \frac{x-y}{|x-y|} = 1 - (1 + O(|x|^{-1})) = O(|x|^{-1}).\end{aligned}$$

As a result, the first and the third terms in (4.113a) are already of order  $|x|^{-2}$ . Also from the above expansion for  $\partial_{r(x)} s$ , we have

$$\frac{1}{|x-y|} (\partial_{r(x)} s - 2) = \frac{1}{|x-y|} \frac{x}{|x|} \cdot \frac{x-y}{|x-y|} = O(|x|^{-2}).$$

This allows us to write

$$\begin{aligned}\frac{1}{c} (\partial_{r(x)} \Phi_k - ik \Phi_k) &= \frac{1}{c} \partial_{r(x)} \Phi_k - \frac{2}{|x-y|} \partial_s H + \frac{2}{|x-y|} \partial_s H - \frac{1}{c} ik \Phi_k; \\ \Rightarrow \frac{e^{-\phi_{\text{out}}(s)}}{c} (\partial_{r(x)} \Phi_k - ik \Phi_k) &= \frac{e^{-\phi_{\text{out}}(s)}}{|x-y|} (2 \partial_s H - ik H) + O(|x|^{-2}).\end{aligned}$$

Here, we have denoted by  $\phi_{\text{out}}$  the oscillatory phase

$$\phi_{\text{out}}(s) := \frac{1}{2} ik s - i \eta \log(2ks) - \frac{\pi}{2} \eta. \quad (4.114)$$

The lower order terms (of order  $|x|^{-2}$ ) on the RHS comprise of

$$e^{-\phi_{\text{out}}(s)} \left( ik H \frac{\partial_{r(x)} s - 2}{|x-y|} + \partial_{r(x)} |x-y|^{-1} + \frac{\partial_{r(x)} s}{|x-y|} \partial_s H + \frac{\partial_{r(x)} t}{|x-y|} \partial_t H \right).$$

**Step 2 :** The proof is finished if we can show that  $e^{-\phi_{\text{out}}(s)} (\partial_s H - ik H) = O(|x|^{-1})$ . To do this, we expand this out by using (F.14),

$$\begin{aligned}2 \partial_s H - ik H &= -ik \left( 2W'_{-\chi, 1/2}(-iks) M'_{-\chi, 1/2}(-ikt) - \frac{1}{2} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) \right) \\ &\quad - ik \left( W_{-\chi, 1/2}(-iks) M'_{-\chi, 1/2}(-ikt) - W'_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) \right) \\ &\quad + 2 \frac{\chi}{s} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt).\end{aligned}$$

- From (F.7a), the last term is of order  $|x|^{-1}$  due to the factor  $s^{-1}$ , since

$$s = 2|x| + O(1) \Rightarrow s^{-1} = O(|x|^{-1}).$$

- On the other hand, the first two lines can be combined as

$$-ik \left( W'_{-\chi, 1/2}(-iks) + \frac{1}{2} W_{-\chi, 1/2}(-iks) \right) \left( 2M'_{-\chi, 1/2}(-ikt) - M_{-\chi, 1/2}(-ikt) \right).$$

By (F.7b), for  $y$  in compact set,  $t = O(|x|^{-1})$  as  $|x| \rightarrow \infty$ , the factor

$$\left( 2M'_{-\chi, 1/2}(-ikt) - M_{-\chi, 1/2}(-ikt) \right) = O(1),$$

while from (4.45) in Prop 30 in Appendix C.1, we have

$$\begin{aligned}e^{\frac{1}{2}z} z^{-\chi} \left( W'_{\chi, \frac{1}{2}}(z) + \frac{1}{2} W_{\chi, \frac{1}{2}}(z) \right) &= O(|z|^{-1}); \\ \Rightarrow e^{-\phi_{\text{out}}(s)} \left( W'_{-\chi, 1/2}(-iks) + \frac{1}{2} W_{-\chi, 1/2}(-iks) \right) &= O(|x|^{-1}).\end{aligned}$$

As a result, we obtain

$$e^{-\phi_{\text{out}}(s)} \left( \partial_s H - i k H \right) = O(|x|^{-1}). \quad (4.115)$$

and thus (4.111). For the statement (4.112), when the attenuation  $\gamma = 0$ , we just note that

$$|e^{\phi_{\text{out}}(s)}| = e^{-\frac{\pi}{2} \eta_0}.$$

□

**Proposition 13.** *The quantity  $\frac{y}{|y|} \cdot \nabla_y \Phi_{k_0}^+(x, y)$  satisfies radiating property, i.e.*

$$\left( \frac{x}{|x|} \cdot \nabla_x - i k_0 \right) \partial_{r(y)} \Phi_{k_0}^+(x, y) = O(|x|^{-2}), \quad (4.116)$$

for  $y$  in compact set and as  $|x| \rightarrow \infty$ .

*Proof.* We first expand out  $\partial_{r(y)} \mathfrak{c}^{-1} \Phi_k$  and  $\partial_{r(x)} \partial_{r(y)} \mathfrak{c}^{-1} \Phi_k$  in terms of the partial derivatives of  $H$  with respect to  $s$  and  $t$ , together with the order of their coefficients. We have

$$\partial_{r(y)} \frac{1}{\mathfrak{c}} \Phi_k = G \underbrace{\partial_{r(y)} |x - y|^{-1}}_{O(|x|^{-2})} + \underbrace{\frac{\partial_{r(y)} s}{|x - y|}}_{O(|x|^{-1})} \partial_s H + \underbrace{\frac{\partial_{r(y)} t}{|x - y|}}_{O(|x|^{-1})} \partial_t H.$$

And,

$$\begin{aligned} & \partial_{r(x)} \partial_{r(y)} \frac{\Phi_k}{\mathfrak{c}} \\ &= \underbrace{\left( \partial_{r(x)} \partial_{r(y)} |x - y|^{-1} \right)}_{O(|x|^{-3})} G + \underbrace{\left( \partial_{r(y)} |x - y|^{-1} \right) \partial_{r(x)} s}_{O(|x|^{-2})} \partial_s H + \underbrace{\left( \partial_{r(y)} |x - y|^{-1} \right) \partial_{r(x)} t}_{O(|x|^{-3})} \partial_t H \\ &+ \underbrace{\left( \partial_{r(x)} \frac{\partial_{r(y)} s}{|x - y|} \right)}_{O(|x|^{-2})} \partial_s H + \underbrace{\left( \frac{\partial_{r(y)} s}{|x - y|} \partial_{r(x)} s \right)}_{O(|x|^{-1})} \partial_s^2 H + \underbrace{\left( \frac{\partial_{r(y)} s}{|x - y|} \partial_{r(x)} t \right)}_{O(|x|^{-2})} \partial_{ts} H \\ &+ \underbrace{\left( \partial_{r(x)} \frac{\partial_{r(y)} t}{|x - y|} \right)}_{O(|x|^{-2})} \partial_t H + \underbrace{\left( \frac{\partial_{r(y)} t}{|x - y|} \partial_{r(x)} s \right)}_{O(|x|^{-1})} \partial_{st} H + \underbrace{\left( \frac{\partial_{r(y)} t}{|x - y|} \partial_{r(x)} t \right)}_{O(|x|^{-2})} \partial_t^2 H. \end{aligned} \quad (4.117)$$

The orders of the coefficients come from the calculation in Appendix F. In particular,

$$\begin{aligned} & \partial_{r(y)} |x - y|^{-1} \stackrel{(F.12)}{=} O(|x - y|^{-2}) \quad ; \quad \partial_{r(x)} \partial_{r(y)} |x - y|^{-1} \stackrel{(F.12)}{=} O(|x - y|^{-3}); \\ & \partial_{r(x)} s \stackrel{(F.15)}{=} 2 + O(|x|^{-1}) = O(1) \quad ; \quad \partial_{r(y)} s \stackrel{(F.16)}{=} 1 + \cos(\theta_y - \theta_x) + O(|x|^{-1}) = O(1); \\ & \partial_{r(x)} t \stackrel{(F.15)}{=} O(|x|^{-1}) \quad ; \quad \partial_{r(y)} t \stackrel{(F.16)}{=} 1 - \cos(\theta_y - \theta_x) + O(|x|^{-1}) = O(1). \end{aligned}$$

This leads to

$$\begin{aligned} \partial_{r(x)} \frac{\partial_{r(y)} s}{|x - y|} &= \frac{\partial_{r(x)} \partial_{r(y)} s}{|x - y|} + \left( \partial_{r(y)} s \right) \partial_{r(x)} |x - y|^{-1} = O(|x|^{-2}) + O(|x|^{-2}) = O(|x|^{-2}); \\ \partial_{r(x)} \frac{\partial_{r(y)} t}{|x - y|} &= \frac{\partial_{r(x)} \partial_{r(y)} t}{|x - y|} + \left( \partial_{r(y)} t \right) \partial_{r(x)} |x - y|^{-1} = O(|x|^{-2}) + O(|x|^{-2}) = O(|x|^{-2}); \\ \frac{\partial_{r(y)} s}{|x - y|} &= O(|x|^{-1}) \quad ; \quad \frac{\partial_{r(y)} t}{|x - y|} = O(|x|^{-1}). \end{aligned}$$

We will gather all terms with lower order coefficients on the RHS of (4.117) into one denoted by  $\mathfrak{L}$ . With  $\phi_{\text{out}}$  defined in (4.114), to say that a quantity  $A$  is of lower orders, we mean

$$e^{-\phi_{\text{out}}(s)} A = \mathcal{O}(|x|^{-1}).$$

Using this notation, we write

$$\begin{aligned} & (\partial_{r(x)} - i\mathbf{k})\partial_{r(y)}\Phi_{\mathbf{k}} \\ &= -i\mathbf{k} \frac{\partial_{r(y)s}}{|x-y|} \partial_s H - i\mathbf{k} \frac{\partial_{r(y)t}}{|x-y|} \partial_t H + \left( \frac{\partial_{r(y)s}}{|x-y|} \partial_{r(x)s} \right) \partial_s^2 H + \left( \frac{\partial_{r(y)t}}{|x-y|} \partial_{r(x)s} \right) \partial_{st} H + \mathfrak{L} \\ &= \frac{\partial_{r(y)s}}{|x-y|} (-i\mathbf{k} \partial_s H + 2 \partial_s^2 H) + \frac{\partial_{r(y)t}}{|x-y|} (-i\mathbf{k} \partial_t H + 2 \partial_{st} H) + \mathfrak{L} \\ &\quad + \frac{\partial_{r(y)s}}{|x-y|} \underbrace{(\partial_{r(x)s} - 2)}_{\mathcal{O}(|x|^{-2})} \partial_s^2 H + \frac{\partial_{r(y)t}}{|x-y|} \underbrace{(\partial_{r(x)s} - 2)}_{\mathcal{O}(|x|^{-2})} \partial_{st} H. \end{aligned}$$

In the last equality, we have used the same trick as in Prop. 12 to replace  $\partial_{r(x)s}$  by 2 modulo lower order terms,

$$\partial_{r(x)s} - 2 \stackrel{\text{(F.15)}}{=} \mathcal{O}(|x|^{-1}).$$

The resulting lower order terms can be absorbed in to  $\mathfrak{L}$  to give  $\tilde{\mathfrak{L}}$ . In short, at the end of step 1, we have written

$$(\partial_{r(x)} - i\mathbf{k})\partial_{r(y)}\Phi_{\mathbf{k}} = \frac{\partial_{r(y)s}}{|x-y|} (-i\mathbf{k} \partial_s H + 2 \partial_s^2 H) + \frac{\partial_{r(y)t}}{|x-y|} (-i\mathbf{k} \partial_t H + 2 \partial_{st}^2 H) + \tilde{\mathfrak{L}}.$$

**Step 2:** The proof for the radiating property of  $\partial_{r(y)}\Phi_{\mathbf{k}}$  is finished by showing that

$$\underbrace{e^{-\phi_{\text{out}}(s)} (-i\mathbf{k} \partial_s H + 2 \partial_s^2 H)}_{:=\mathbb{I}_1} = \mathcal{O}(|x|^{-1}) \quad \text{and} \quad \underbrace{e^{-\phi_{\text{out}}(s)} (-i\mathbf{k} \partial_t H + 2 \partial_{st}^2 H)}_{:=\mathbb{I}_2} = \mathcal{O}(|x|^{-1}).$$

From the calculation in (F.24) and (F.25) in Appendix F,

$$\begin{aligned} \partial_s^2 H &= -k^2 \left( \frac{1}{4} + \frac{\chi}{i\mathbf{k}s} \right) H - \frac{\chi}{s^2} M_{-\chi,1/2}(-i\mathbf{k}t) W'_{-\chi,1/2}(-i\mathbf{k}s); \\ \partial_{st}^2 H &= \frac{1}{4} k^2 H + i\mathbf{k}\chi \begin{vmatrix} W'_{-\chi,1/2}(-i\mathbf{k}s) & M'_{-\chi,1/2}(-i\mathbf{k}t) \\ s^{-1}W_{-\chi,1/2}(-i\mathbf{k}s) & t^{-1}M_{-\chi,1/2}(-i\mathbf{k}t) \end{vmatrix}. \end{aligned}$$

We can thus rewrite these factors as,

$$\begin{aligned} 2\partial_s^2 H - i\mathbf{k}\partial_s H &= -2k^2 \left( \frac{1}{4} + \frac{\chi}{i\mathbf{k}s} \right) H - \frac{\chi}{s^2} M_{-\chi,1/2}(-i\mathbf{k}t) W'_{-\chi,1/2}(-i\mathbf{k}s) - i\mathbf{k}\partial_s H \\ &= -i\mathbf{k}\frac{1}{2} \left( -i\mathbf{k}H + 2\partial_s H \right) + \mathcal{O}(|x|^{-1}) + \mathcal{O}(|x|^{-2}), \end{aligned}$$

and

$$\begin{aligned} 2\partial_{st}^2 H - i\mathbf{k}\partial_t H &= \frac{1}{2} k^2 H - k^2 \left( \frac{1}{4} W_{-\chi,1/2}(-i\mathbf{k}s) M_{-\chi,1/2}(-i\mathbf{k}t) \right. \\ &\quad \left. - W'_{-\chi,1/2}(-i\mathbf{k}s) M'_{-\chi,1/2}(-i\mathbf{k}t) \right) \end{aligned} \tag{4.118a}$$

$$+ 2 \frac{i\mathbf{k}\chi}{t} W' M + i\mathbf{k} \frac{\chi}{t} W_{-\chi,1/2}(-i\mathbf{k}s) M_{-\chi,1/2}(-i\mathbf{k}t). \tag{4.118b}$$

That  $\mathbb{I}_1$  is  $O(|x|^{-1})$  is due to (4.115), which was shown in Step 2 of Part 2 of Prop. 12 (which shows the radiation property of  $\Phi_k$ ). Each factor in  $\mathbb{I}_2$  can be shown to be  $O(|x|^{-1})$  as follows.

$$\begin{aligned}
 (4.118b) &= \frac{ik\chi}{t} M_{-\chi,1/2}(-ikt) \underbrace{\left( 2W'_{-\chi,1/2}(-iks) + W_{-\chi,1/2}(-iks) \right)}_{O(|x|^{-1}) \text{ cf. (4.45)}}; \\
 (4.118a) &= k^2 \underbrace{\left( \frac{1}{2}W_{-\chi,1/2}(-iks) + W'_{-\chi,1/2}(-iks) \right)}_{O(|x|^{-1}) \text{ cf. (4.45)}} \underbrace{\left( M'_{-\chi,1/2}(-ikt) - \frac{1}{2}M_{-\chi,1/2}(-ikt) \right)}_{O(1) \text{ since } t=O(|x|^{-1}) \text{ cf. (F.7b)}}.
 \end{aligned}$$

□

**Property 6** - When  $k^2 \in \mathbb{C} \setminus [0, \infty)$ , we verify that the  $\Phi_k(x, y)$  satisfies the hypothesis of Schur's test<sup>21</sup> which will be used to show that  $\Phi_k$  gives rise to an  $L^2(\mathbb{R}^3)$  bounded operator.

**Proposition 14.** *When  $k^2 \in \mathbb{C} \setminus [0, \infty)$ , then  $\Phi_k(x, y)$  defined in (4.71) satisfies the requirement of Schur's test, i.e. there exists  $C$  independent of  $x$  and  $y$  such that*

$$\sup_{x \in \mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\Phi_k|}{|x-y|} dy < C \quad ; \quad \sup_{y \in \mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\Phi_k|}{|x-y|} dx < C.$$

*Proof.* Due to the symmetry in  $x$  and  $y$  of  $\Phi_k$ , it suffices to show the first statement. For convenience, we work with the reduced kernel  $G_k$ .

**Step 1 :** Choose  $\delta > 0$ , such that for all  $r > \delta$ , there exists  $c(\delta) > 0$  such that,

$$r - \frac{\alpha_\infty \operatorname{Im} k}{2k^2} \ln(\tfrac{1}{2}r) > cr. \quad (4.120)$$

Case 1: We consider first the case where  $t \leq \delta$ . Define  $C = C(\delta, \alpha_\infty, k)$  the max of the following bounds,

$$\begin{aligned}
 C := \max \Big\{ & \max_{t \in [0, \delta]} M_{-\chi,1/2}(-ikt), \max_{t \in [0, \delta]} M'_{-\chi,1/2}(-ikt), \max_{t \in [0, \delta]} \frac{M_{-\chi,1/2}(-ikt)}{t}, \\
 & \max_{s \in [0, \delta]} W_{-\chi,1/2}(-iks), \max_{s \in [0, \delta]} s W'_{-\chi,1/2}(-iks) \Big\}.
 \end{aligned} \quad (4.121)$$

Here, we have used the fact that  $W'_{-\chi,1/2}(\cdot)$  blows up as  $\ln z$  for  $z \sim 0$ , and  $M_{-\chi,1/2}(\cdot)$  vanishes at the origin, given in (4.41) and (4.42). For  $t \leq \delta$  and  $s \leq \delta$ , we then have

$$G_k \leq |W_{-\chi,1/2}(-iks)| |M'_{-\chi,1/2}(-ikt)| + |s W'_{-\chi,1/2}(-iks)| \frac{t}{s} \left| \frac{M'_{-\chi,1/2}(-iks)}{t} \right|.$$

With  $t < s$ , we obtain,

$$G_k \leq 2C^2 \quad , \quad t \leq \delta \quad , \quad s \leq \delta. \quad (4.122)$$

<sup>21</sup>See eg. [25, Lemma 3.7.4 p.75]. Let  $(X, \mu)$  and  $(Y, \nu)$  be measurable spaces and let  $K : X \times Y \rightarrow \mathbb{C}$  satisfy

$$\int |K(x, y)| d\mu(x) \leq C \quad , \quad \int |K(x, y)| d\nu(y) \leq C' \quad (4.119)$$

where  $C$  and  $C'$  are independent of  $y$  and  $x$  respectively. Then

$$f \mapsto \int_Y K(x, y) f(y) dy$$

maps  $L^2(Y, \nu)$  to  $L^2(X, \mu)$ .

On the other hand, when  $t \leq \delta$  and  $s > \delta$ ,

$$|G_k| \leq C(|W_{-\chi, 1/2}(-iks)| + |W'_{-\chi, 1/2}(-iks)|) \leq \check{C} \exp(i\varphi_k(\tfrac{1}{2}s)).$$

Here we have used

$$\begin{aligned} W_{-\chi, \frac{1}{2}}(-iks) &= \exp(i\varphi_k(\tfrac{1}{2}s))(1 + O(s)^{-1}); \\ W'_{-i\eta, \frac{1}{2}}(-iks) &= \exp(i\varphi_k(\tfrac{1}{2}s))(-\tfrac{1}{2} + O(s)^{-1}) \end{aligned} \quad (4.123)$$

Note that factors in the parentheses are bounded uniformly for  $s > \delta$ , thus the constant  $\check{C}$  depends only on  $\delta, \alpha_\infty$  and  $k$ . Using the choice of  $\delta$  determined by (4.120), we can bound  $|G_k|$  further by

$$|G_k| \leq \check{C} \exp(-ic \operatorname{Im} k s) \leq \exp(-ic \operatorname{Im} k |x - y|) \quad , \quad t \leq \delta, \quad s > \delta. \quad (4.124)$$

Case 2: We next consider  $t > \delta$ . Since  $s \geq t$ , we automatically have  $s > \delta$ . Using (4.53), we have

$$\begin{aligned} M_{-\chi, \frac{1}{2}}(-ikt) &\sim \exp(-i\varphi_k(\tfrac{1}{2}t))(\mathfrak{a} + O(t^{-1})) + \exp(i\varphi_k(\tfrac{1}{2}t))(\mathfrak{b} + O(t^{-1})); \\ M'_{-\chi, \frac{1}{2}}(-ikt) &\sim \exp(-i\varphi_k(\tfrac{1}{2}t))(\check{\mathfrak{a}} + O(t^{-1})) + \exp(i\varphi_k(\tfrac{1}{2}t))(\check{\mathfrak{b}} + O(t^{-1})). \end{aligned} \quad (4.125)$$

As before, the factors in the parentheses are also bounded uniformly for  $s > \delta$ .

We write  $G = G_1 - G_2$ , with

$$G_1 = W_{-\chi, \frac{1}{2}}(-iks) M'_{-\chi, \frac{1}{2}}(-ikt) \quad ; \quad G_2 = W'_{-\chi, \frac{1}{2}}(-iks) M_{-\chi, \frac{1}{2}}(-ikt).$$

To treat separately the two components in the asymptotics of  $M'$ , we further decompose  $G_1$  into  $G_1 = G_{1a} + G_{1b}$ , with

$$\begin{aligned} G_{1a} &= \exp(i\varphi_k(\tfrac{1}{2}s) - i\varphi_k(\tfrac{1}{2}t))(1 + O(s^{-1}))(\check{\mathfrak{a}} + O(t^{-1})); \\ G_{1b} &= \exp(i\varphi_k(\tfrac{1}{2}s) + i\varphi_k(\tfrac{1}{2}t))(1 + O(s^{-1}))(\check{\mathfrak{b}} + O(t^{-1})). \end{aligned}$$

A similar decomposition is obtained for  $G_2 = G_{2a} + G_{2b}$ , now working with the two components in the asymptotic of  $M$ . We can define a constant  $D$  that only depends on  $\delta, \alpha_\infty$  and  $k$  so that

$$|G_{2a}|, |G_{1a}| \leq D \exp(i\varphi_k(\tfrac{1}{2}s) - i\varphi_k(\tfrac{1}{2}t)) \quad ; \quad |G_{2b}|, |G_{1b}| \leq D \exp(i\varphi_k(\tfrac{1}{2}s) + i\varphi_k(\tfrac{1}{2}t)).$$

It remains to bound the exponentials. For this, we use Appendix I, which gives

$$\begin{aligned} |\exp(-i\varphi_k(\tfrac{1}{2}ks))| &= \left| \exp(-ik\tfrac{1}{2}s + i\eta \log(ks) + \tfrac{\pi}{2}\eta) \right| = \exp\left(\operatorname{Im} k \left(s - \frac{\alpha}{2|k|^2} \ln(\tfrac{1}{2}s)\right)\right) |e^{-\mathfrak{d}}|; \\ |\exp(i\varphi_k(\tfrac{1}{2}ks))| &= \exp\left(-\operatorname{Im} k \left(s - \frac{\alpha}{2|k|^2} \ln(\tfrac{1}{2}s)\right)\right) |e^{\mathfrak{d}}|. \end{aligned}$$

Here the constant  $\mathfrak{d}$  depends only on  $k$  and  $\alpha_\infty$ ,

$$\mathfrak{d} = \mathfrak{d}(k, \alpha_\infty) = \operatorname{Im} k \frac{\alpha \ln|2k|}{2|k|^2} + \eta \operatorname{Arg} k + i\frac{\pi}{2}\eta.$$

The exponential in  $G_{1a}$  is rewritten as,

$$\begin{aligned} \exp(i\varphi_k(\tfrac{1}{2}ks)) \exp(-i\varphi_k(\tfrac{1}{2}kt)) &= \exp(-\operatorname{Im} k (s - t)) \exp\left(\frac{\alpha \operatorname{Im} k}{2|k|^2} \ln \frac{s}{t}\right) \\ &= \exp(-\operatorname{Im} k 2|x - y|) \left(1 + \frac{2|x - y|}{|x| + |y| - |x - y|}\right)^{\frac{\alpha \operatorname{Im} k}{2|k|^2}}. \end{aligned}$$

And using  $t > \delta$ , we have

$$\exp(i\varphi_k(\tfrac{1}{2}ks)) \exp(-i\varphi_k(\tfrac{1}{2}kt)) < \exp(-2\operatorname{Im} k |x - y|) \left(1 + \frac{2}{\delta} |x - y|\right)^{\frac{\alpha \operatorname{Im} k}{2|k|^2}}. \quad (4.126)$$



For the exponential of  $G_{1b}$ , both exponentials are decay, using the choice of  $\delta$  (4.120), we can bound them as

$$\exp(i\varphi_k(\tfrac{1}{2}ks)) \exp(i\varphi_k(\tfrac{1}{2}ks)) \leq \exp(-ick(s+t)) = \exp(-i2ck(|x| + |y|))$$

thus

$$\exp(i\varphi_k(\tfrac{1}{2}ks)) \exp(i\varphi_k(\tfrac{1}{2}ks)) \leq \exp(-2ick|x-y|). \quad (4.127)$$

We have used in the last inequality  $|x| + |y| \geq |x-y|$ . Thus combining with (4.126), we obtain

$$|G_k| \leq 2 \exp(-2ick|x-y|) + \exp(-2\operatorname{Im} k|x-y|) \left(1 + \tfrac{2}{\delta}|x-y|\right)^{\frac{\alpha \operatorname{Im} k}{2|k|^2}}. \quad (4.128)$$

**Step 2:** We denote by  $\chi_S(x, y)$  the indicator of the set  $S$ . We have

$$G_k = \chi_{t>\delta} G_k + \chi_{t\leq\delta} \chi_{s>\delta} G_k + \chi_{t\leq\delta} \chi_{s\leq\delta} G_k. \quad (4.129)$$

Thus

$$|G_k| \leq \chi_{t>\delta} |G_k| + \chi_{t\leq\delta} \chi_{s>\delta} |G_k| + \chi_{t\leq\delta} \chi_{s\leq\delta} |G_k|.$$

And

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|G_k|}{|x-y|} dy &\leq 2 \int_{\mathbb{R}^3} \chi_{t\leq\delta}(y) \chi_{s\leq\delta}(y) \frac{C^2}{|x-y|} dy + 2 \int_{\mathbb{R}^3} \chi_{t\leq\delta}(y) \chi_{s>\delta}(y) \frac{\exp(-ick|x-y|)}{|x-y|} dy \\ &\quad + \int_{\mathbb{R}^3} \chi_{t>\delta}(y) \frac{\exp(-2\operatorname{Im} k|x-y|)}{|x-y|} \left(1 + \tfrac{2}{\delta}|x-y|\right)^{\frac{\alpha \operatorname{Im} k}{2|k|^2}} dy \\ &\quad + \int_{\mathbb{R}^3} \chi_{t>\delta}(y) \frac{\exp(-i2ck(|x|+|y|))}{|x-y|} dy. \end{aligned}$$

We can bound the last three integrals by an integration over  $\mathbb{R}^3$ ,

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|G_k|}{|x-y|} dy &\leq 2 \int_{\mathbb{R}^3} \chi_{t\leq\delta}(y) \chi_{s\leq\delta}(y) \frac{C^2}{|x-y|} dy + 2 \int_{\mathbb{R}^3} \frac{\exp(-ick|x-y|)}{|x-y|} dy \\ &\quad + \int_{\mathbb{R}^3} \frac{\exp(-2\operatorname{Im} k|x-y|)}{|x-y|} \left(1 + \tfrac{2}{\delta}|x-y|\right)^{\frac{\alpha \operatorname{Im} k}{2|k|^2}} dy \\ &\quad + \int_{\mathbb{R}^3} \frac{\exp(-i2ck(|x|+|y|))}{|x-y|} dy. \end{aligned}$$

These integrals are finite and are bounded by a constant independent of  $x$ . They are directly computed by using spherical coordinates centered at  $x$ . Denote them respectively by  $\mathbb{I}_1$ ,  $\mathbb{I}_2$ ,  $\mathbb{I}_3$  and  $\mathbb{I}_4$ . Since  $s, t \leq \delta$  implies that  $|x|, |y| \leq \delta$ , we have

$$\mathbb{I}_1 \leq \int_{|x|\leq\delta, |y|\leq\delta} dy \leq 4\pi \int_0^\delta r dr = 2\pi\delta^2.$$

For  $\mathbb{I}_2, \dots, \mathbb{I}_3$ , due to the exponential decay factor, they are all bounded by, for some constant  $d$ , independent of  $x$  and  $y$ ,

$$\mathbb{I}_2, \mathbb{I}_3, \mathbb{I}_4 \leq 4\pi \int_0^\infty \exp(-i2d\operatorname{Im} k r) dr.$$

This finishes the verification. □

### 4.3.3 Verification of fundamental solution properties

The proof is adapted from [38, Prop. 4.9] for the Laplacian and from [35, Prop. 2.1] for the Helmholtz operator. We will use the second Green's formula: for a bounded region  $\mathcal{R}$  and  $w, v \in \mathcal{C}^2(\mathcal{R})$ ,

$$\int_{\mathcal{R}} \left( (\Delta_x w) v - w (\Delta_x v) \right) dx = \int_{\partial \mathcal{R}} \left( v \frac{\partial}{\partial \nu(x)} w - w \frac{\partial}{\partial \nu(x)} v \right) d\sigma(x), \quad (4.130)$$

where  $\nu(x)$  is the normal vector along  $\partial \mathcal{R}$  and points outward of  $\mathcal{R}$ . By a fundamental solution to

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = \delta(x - y) \quad , \quad \text{in } \mathcal{D}'(\mathbb{R}^3), \quad (4.131)$$

we mean

$$\lim_{\epsilon \rightarrow 0^+} \int_{\Omega_{(y, \epsilon)}} \left[ (-\Delta_x - k^2 + \frac{\alpha_\infty}{|x|}) \phi(x) \right] \Phi_k(x, y) dx = \phi(y) \quad , \quad \forall \phi \in \mathcal{C}_c^\infty(\mathbb{R}^3).$$

**Proposition 15.** *When  $\gamma \neq 0$  (i.e. in the presence of attenuation), the function  $\Phi_k(x, y)$  defined in (4.70)*

$$\Phi_k(x, y) := \frac{\Gamma(1 + \chi)}{4\pi |x - y|} \frac{1}{i k} \left( \frac{\partial}{\partial_s} - \frac{\partial}{\partial_t} \right) \left( W_{-\chi, 1/2}(-i k s) M_{-\chi, 1/2}(-i k t) \right); \quad (4.132)$$

$$\text{with} \quad s := |x| + |y| + |x - y| \quad ; \quad t := |x| + |y| - |x - y|$$

*is a fundamental solution to (4.131). In this case ( $\gamma \neq 0$ ),  $\Phi_k(x, y) \in L^2(\mathbb{R}_x^3)$  for  $y$  in compact subset of  $\mathbb{R}^3$  and vice versa (due to the symmetry in  $x$  and  $y$ ).*

*When  $\gamma = 0$ , the kernel  $\Phi_{k_0}^\pm(x, y)$ , defined in (4.74) and (4.76) respectively, is a fundamental solution to*

$$\left( -\Delta_x - k_0^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_{k_0}^\pm(x, y) = \delta(x - y) \quad , \quad \text{in } \mathcal{D}'(\mathbb{R}^3). \quad (4.133)$$

*Proof.* Let us first define

$$\begin{aligned} \Omega_{(y, \epsilon)} &:= \mathbb{R}^3 \setminus \mathbb{B}_{(y, \epsilon)} \quad \text{with} \quad \mathbb{B}_{(y, \epsilon)} := \{x \in \mathbb{R}^3 \mid |x - y| \leq \epsilon\}; \\ \mathbb{S}_{(0, \epsilon)} &:= \partial \mathbb{B}_{(y, \epsilon)} := \{x \in \mathbb{R}^3 \mid |x - y| = \epsilon\}. \end{aligned} \quad (4.134)$$

To show that  $\Phi_k$  as defined in (4.70) is a fundamental solution (or equivalently that  $\Phi_\omega$  is a distributional solution to (4.131)) means, for arbitrary  $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^3)$ , we have to show

$$\left\langle \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) \quad , \quad \phi(x) \right\rangle = \phi(y);$$

$$\text{or equivalently} \quad \left\langle \Phi_k(x, y) \quad , \quad \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \phi \right\rangle = \phi(y);$$

$$\text{or equivalently} \quad \lim_{\epsilon \rightarrow 0} \int_{\Omega_{y, \epsilon}} \phi \frac{G(x, y)}{|x - y|} \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \phi(x) dx = \phi(y).$$

Here  $\langle \cdot, \cdot \rangle$  is the distributional pairing  $\mathcal{D}'(\mathbb{R}^3) \times \mathcal{D}(\mathbb{R}^3)$ .

Using the fact that  $\Phi_k$  satisfies

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = 0 \quad , \quad \text{on } \Omega_{(y, \epsilon)} \quad , \quad \epsilon > 0, \quad (4.135)$$

we can write

$$\begin{aligned}
& \int_{\Omega_{(y,\epsilon)}} \left[ (-\Delta_x - k^2 + \frac{\alpha_\infty}{|x|}) \phi(x) \right] \Phi_k(x, y) dx \\
&= \int_{\Omega_{(y,\epsilon)}} \left[ \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \phi(x) \right] \Phi_k(x, y) dx - \int_{\Omega_{(y,\epsilon)}} \phi(x) \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) dx \\
&= \int_{\Omega_{(y,\epsilon)}} (-\Delta_x \phi) \Phi_k(x, y) dx - \int_{\Omega_{(y,\epsilon)}} \phi(x) (-\Delta_x \Phi_k(x, y)) dx \\
&\stackrel{(4.130)}{=} - \int_{\partial\Omega_{(y,\epsilon)}} \left( \Phi_k(x, y) (\partial_{\nu(x)} \phi)(x) - \phi(x) (\partial_{\nu(x)} \Phi_k)(x, y) \right) d\sigma(x) \quad , \\
&= \mathbb{I}_1 - \mathbb{I}_2 \quad ,
\end{aligned}$$

with  $\nu(x)$  the normal vector pointing outside of  $\Omega_{(y,\epsilon)}$ . Here, we have defined (a spherical change of variable centered at  $y$ , i.e.  $x = y + \epsilon\varpi$  with  $\epsilon = |x|$ )

$$\begin{aligned}
\mathbb{I}_1 &:= \int_{\mathbb{S}_{(0,1)}} \Phi_k(y + \epsilon\varpi, y) \left( \frac{(x-y)}{|x-y|} \cdot \nabla_x \phi \right) \Big|_{x=y+\epsilon\omega} \epsilon^2 d\varpi \quad ; \\
\mathbb{I}_2 &:= \int_{\mathbb{S}_{(0,1)}} \left( \frac{(x-y)}{|x-y|} \cdot \nabla_x \Phi_k(x, y) \right) \Big|_{x=y+\epsilon\omega, y} \phi(y + \epsilon\omega) \epsilon^2 d\varpi \quad .
\end{aligned}$$

We next consider the limits of each integral as  $\epsilon \rightarrow 0^+$ . Use (4.83b) to obtain that

$$\lim_{\epsilon \rightarrow 0} \mathbb{I}_1 = 0 \quad ,$$

while use (4.84), to obtain that

$$\lim_{\epsilon \rightarrow 0} \mathbb{I}_2 = -\frac{1}{4\pi} \int_{\mathbb{S}_{(0,1)}} \phi(y) d\sigma(\varpi) = -\phi(y) \quad .$$

Putting together these two limits, we have

$$\lim_{\epsilon \rightarrow 0^+} \int_{\Omega_{(y,\epsilon)}} \left[ (-\Delta_x - k^2 + \frac{\alpha_\infty}{|x|}) \phi(x) \right] \Phi_k(x, y) dx = \lim_{\epsilon \rightarrow 0^+} (\mathbb{I}_1 - \mathbb{I}_2) = \phi(y) \quad .$$

□

#### 4.4 Green representation in bounded domain

The following proposition generalizes Helmholtz representation. The proof is similar to that for Prop. 15.

**Proposition 16** (Green representation in bounded domain). *Consider  $\Omega$  bounded,  $u \in H^2(\Omega)$ ,  $n(x)$  normal vector points outward. We have the following three representations. The first one uses  $\Phi_k$  with  $\text{Im } k \neq 0$  (i.e. with attenuation).*

$$\begin{aligned}
u(x) &= \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_k(x, y) - u(y) (\partial_{n(y)} \Phi_k)(x, y) \right) d\sigma(y) \\
&\quad - \int_{\Omega} \Phi_k(x, y) \left( \Delta + k^2 - \frac{\alpha_\infty}{|y|} \right) u(y) dy \quad .
\end{aligned} \tag{4.136}$$

At real  $k_0 > 0$  (i.e. without attenuation), we have

$$\begin{aligned} u(x) = & \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_{k_0}^\pm(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^\pm)(x, y) \right) d\sigma(y) \\ & - \int_{\Omega} \Phi_{k_0}^\pm(x, y) \left( \Delta + k_0^2 - \frac{\alpha_\infty}{|y|} \right) u(y) dy. \end{aligned} \quad (4.137)$$

*Proof.* Define the bounded subregion  $\Omega_{(y, \epsilon)}$  of  $\Omega$ ,

$$\Omega_{(y, \epsilon)} := \Omega \setminus \mathbb{B}(y, \epsilon).$$

As before, using the fact that  $\Phi_k(x, y)$  satisfies

$$\left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) = 0 \quad , \quad \text{on } \Omega_{(y, \epsilon)} \quad , \quad \epsilon > 0,$$

we can write

$$\begin{aligned} & \int_{\Omega_{(y, \epsilon)}} \left[ (-\Delta_x - k^2 + \frac{\alpha_\infty}{|x|}) u(x) \right] \Phi_k(x, y) dx \\ &= \int_{\Omega_{(y, \epsilon)}} \left[ \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) u(x) \right] \Phi_k(x, y) dx - \int_{\Omega_{(y, \epsilon)}} u(x) \left( -\Delta_x - k^2 + \frac{\alpha_\infty}{|x|} \right) \Phi_k(x, y) dx \\ &= \int_{\Omega_{(y, \epsilon)}} (-\Delta_x u) \Phi_k(x, y) dx - \int_{\Omega_{(y, \epsilon)}} u(x) (-\Delta_x \Phi_k(x, y)) dx \\ &\stackrel{(4.130)}{=} - \int_{\partial\Omega \cup \mathbb{S}_{y, \epsilon}} \left( \Phi_k(x, y) (\partial_{\nu(x)} u)(x) - u(x) (\partial_{\nu(x)} \Phi_k)(x, y) \right) d\sigma(x) \quad , \quad \nu \text{ points outward of } \Omega_{(y, \epsilon)} \\ &= - \int_{\partial\Omega} \left( \Phi_k(x, y) (\partial_{n(x)} u)(x) - u(x) (\partial_{n(x)} \Phi_k)(x, y) \right) d\sigma(x) \\ &\quad + \int_{\mathbb{S}_{(y, \epsilon)}} \left( \Phi_k(x, y) \left( \frac{x-y}{|x-y|} \cdot \nabla_x u \right)(x) - u(x) \left( \frac{x-y}{|x-y|} \cdot \nabla_x \Phi_k \right)(x, y) \right) d\sigma(x). \end{aligned}$$

We thus have

$$\begin{aligned} & \int_{\Omega_{(y, \epsilon)}} \left[ (-\Delta_x - k^2 + \frac{\alpha_\infty}{|x|}) u(x) \right] \Phi_k(x, y) dx \\ &= - \int_{\partial\Omega} \left( \Phi_k(x, y) (\partial_{n(x)} u)(x) - u(x) (\partial_{n(x)} \Phi_k)(x, y) \right) d\sigma(x) \quad + \quad \mathbb{I}_1 - \mathbb{I}_2. \end{aligned} \quad (4.138)$$

Here, we have used a change of variable  $x = \epsilon\varpi$  and introduce the integrals,

$$\begin{aligned} \mathbb{I}_1 &:= \int_{\mathbb{S}_{(0,1)}} \Phi_k(y + \epsilon\varpi, x) \left( \frac{x-y}{|x-y|} \cdot \nabla_x u \right) \Big|_{x=y+\epsilon\varpi} \epsilon^2 d\varpi; \\ \mathbb{I}_2 &:= \int_{\mathbb{S}_{(0,1)}} \left( \frac{x-y}{|x-y|} \cdot \nabla_x \Phi_k \right) \Big|_{x=y+\epsilon\varpi, y} u(y + \epsilon\varpi) \epsilon^2 d\varpi. \end{aligned}$$

As in the proof for Prop 15, we use (4.83b) and (4.84) to obtain that

$$\lim_{\epsilon \rightarrow 0} \mathbb{I}_1 = 0 \quad ; \quad \lim_{\epsilon \rightarrow 0} \mathbb{I}_2 = -\frac{1}{4\pi} \int_{\mathbb{S}_{(0,1)}} u(y) d\sigma(\varpi) = -u(y).$$

Letting  $\epsilon \rightarrow 0$  on both sides of (4.138), we obtain (4.136). The proof for the representation with  $\Phi_{k_0}^\pm$  follows in the exact same manner.  $\square$

#### 4.5 Construction of solutions to the inhomogeneous equation

Under the choice of square root  $\mathfrak{g}_2$  (4.11a), working with  $\mathbf{k}^2 \in \mathbb{C}$  is equivalent to working with  $\mathbf{k}$  in the upper hand plane and the positive real axis. For  $\mathbf{k}^2$ , we distinguish  $\mathbf{k}^2 \in \mathbb{C} \setminus [0, \infty)$  and  $\mathbf{k}^2 > 0$ , the first case is equivalent to working with  $\text{Im } \mathbf{k} > 0$  and the second one  $\mathbf{k} = \mathbf{k}_0 > 0$ . Consider the inhomogeneous equation (i.e. with a non-zero right-hand side)

$$\left( -\Delta - \mathbf{k}^2 + \frac{\alpha_\infty}{|x|} \right) u(x) = f(x). \quad (4.139)$$

Define the following integrals,

$$\text{Re } \mathbf{k}^2 > 0, \text{ Im } \mathbf{k}^2 \neq 0 : \quad \mathcal{R}(\mathbf{k})f := \tilde{\mathcal{R}}(\mathbf{k}^2)f := \int_{\mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) f(y) dy, \quad f \in L^2(\mathbb{R}^3), \quad (4.140)$$

and

$$\mathbf{k}_0 > 0 : \quad \mathcal{R}^\pm(\mathbf{k}_0)f := \tilde{\mathcal{R}}^\pm(\mathbf{k}_0^2)f := \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^\pm(x, y) f(y) dy, \quad f \in L_c^2(\mathbb{R}^3). \quad (4.141)$$

**Proposition 17.** • For  $f \in L^2(\mathbb{R}^3)$  and  $\mathbf{k}$  with  $\text{Im } \mathbf{k} \neq 0$ ,  $\mathcal{R}(\mathbf{k})f$  in (4.140) defines the unique  $L^2$  solution to (4.139).

- For  $f \in L_c^2(\mathbb{R}^3)$ ,  $\mathcal{R}^\pm(\mathbf{k}_0)f$  in (4.141) defines a solution for (4.139) with the property,

$$\left( \partial_{r(x)} \mp i \mathbf{k}_0 \right) \mathcal{R}^\pm(\mathbf{k}_0)f = O(|x|^{-2}), \quad |x| \rightarrow \infty. \quad (4.142)$$

- For  $f \in L_c^2(\mathbb{R}^3)$ , we have pointwise convergence as follows: for each  $x \in \mathbb{R}^3$ ,

$$\lim_{\gamma \rightarrow 0^\pm} (\mathcal{R}(\mathbf{k})f)(x) = (\mathcal{R}^\pm(\mathbf{k}_0)f)(x).$$

There is also the convergence in  $L_{loc}^2(\mathbb{R}^3)$ , i.e. for  $\phi \in C_c^\infty(\mathbb{R}^3)$  with  $\text{Supp } \phi = \Omega$ ,

$$\lim_{\gamma \rightarrow 0^\pm} \left\| \phi \left( \mathcal{R}(\mathbf{k}) - \mathcal{R}^\pm(\mathbf{k}_0) \right) f \right\|_{L^2(\Omega)} = 0.$$

*Proof. Part 1a* For fixed  $x \in \mathbb{R}^3$ , we show that the integrals of the form

$$\begin{aligned} \mathbb{I}_\gamma &= \int_{\mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) f(y) dy, \quad \text{with } \text{Im } \mathbf{k} \neq 0, \quad f \in L^2(\mathbb{R}^3), \\ \text{and } \mathbb{I}_0^\pm &= \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^\pm(x, y) f(y) dy, \quad \text{with } f \in L_c^2(\mathbb{R}^3). \end{aligned}$$

are well-defined. We break them up into a sum of an integration on  $\mathbb{B}_{(x, \epsilon)} := \{y | |x - y| \leq \epsilon\}$  and one on the complement,

$$\begin{aligned} \mathbb{I} &= \int_{\mathbb{B}_{(x, \epsilon)}} \Phi_{\mathbf{k}}(x, y) f(y) dy + \int_{\mathbb{R}^3 \setminus \mathbb{B}_{(x, \epsilon)}} \Phi_{\mathbf{k}}(x, y) f(y) dy; \\ \mathbb{I}_0^\pm &= \int_{\mathbb{B}_{(x, \epsilon)}} \Phi_{\mathbf{k}_0}^\pm(x, y) f(y) dy + \int_{\mathbb{R}^3 \setminus \mathbb{B}_{(x, \epsilon)}} \Phi_{\mathbf{k}_0}^\pm(x, y) f(y) dy. \end{aligned} \quad (4.143)$$

For all three cases, the integrals on  $\mathbb{B}_{(x, \epsilon)}$  are well-defined due to (4.83b) of Prop 9. On the other hand, cf. subsection 4.2.3,  $W_{-\chi, 1/2}(-2iks)$  and  $W'_{-\chi, 1/2}(-2iks)$  decay for  $\mathbf{k} \in \mathbb{C}$  with  $\text{Im } \mathbf{k} \neq 0$ , and oscillates but stay bounded for  $\mathbf{k}_0 > 0$ . As a result, the integrals on  $\mathbb{R}^3 \setminus \mathbb{B}_{(x, \epsilon)}$  are well-defined for  $\text{Im } \mathbf{k} \neq 0$  and  $f \in L^2(\mathbb{R}^3)$ . For  $\mathbf{k}_0 > 0$  (i.e.  $\text{Im } \mathbf{k} = 0$ ), they are only well-defined for  $f \in L_c^2(\mathbb{R}^3)$ .

**Part 1b** We show that it defines a (distributional) solution. For  $\phi \in C_c^\infty(\mathbb{R}^3)$ , we show that

$$\int_{\mathbb{R}^3} (\mathcal{R}(\mathbf{k})f)(x) \left( -\Delta_x - \mathbf{k} + \frac{\alpha_\infty}{|x|} \right) \phi(x) dx = \int_{\mathbb{R}^3} f(x) \phi(x) dx \quad , \quad \text{Im } \mathbf{k} \neq 0 \quad , \quad f \in L^2(\mathbb{R}^3) ,$$

and

$$\int_{\mathbb{R}^3} (\mathcal{R}^\pm(\mathbf{k}_0)f)(x) \left( -\Delta_x - \mathbf{k}_0 + \frac{\alpha_\infty}{|x|} \right) \phi(x) dx = \int_{\mathbb{R}^3} f(x) \phi(x) dx \quad , \quad f \in L_c^2(\mathbb{R}^3) .$$

We first note that the order of integration in the above expressions can be reversed, i.e.

$$\begin{aligned} \int_{\mathbb{R}^3} (\mathcal{R}(\mathbf{k})f)(x) \phi(x) dx &= \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) f(y) dy \right) \left( -\Delta_x - \mathbf{k} + \frac{\alpha_\infty}{|x|} \right) \phi(x) dx \\ &= \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) \left( -\Delta_x - \mathbf{k} + \frac{\alpha_\infty}{|x|} \right) \phi(x) dx \right) f(y) dy \end{aligned} \quad (4.144)$$

This is justified by Tonelli's theorem, cf. [11, Prop. 5.2.1], since

$$\begin{aligned} &\Phi_{\mathbf{k}}(x, y) f(y) \phi(x) \quad , \quad \text{with } \text{Im } \mathbf{k} \neq 0 \quad , \quad f \in L^2(\mathbb{R}^3) , \\ \text{and } &\Phi_{\mathbf{k}_0}^\pm(x, y) f(y) \phi(x) \quad , \quad \text{with } f \in L_c^2(\mathbb{R}^3) , \end{aligned}$$

are almost everywhere continuous in  $\mathbb{R}_x^3 \times \mathbb{R}_y^3$  (continuous except at  $x = y$ ). They are thus measurable. Next, using the fact that  $\Phi$  is a fundamental solution given in Prop 15 to rewrite the second expression on the right-hand-side of (4.144), we obtain

$$\int_{\mathbb{R}^3} (\mathcal{R}(\mathbf{k})f)(x) \phi(x) dx = \int_{\mathbb{R}^3} \phi(y) f(y) dy .$$

The proof for  $\Phi_{\mathbf{k}_0}^\pm$  and  $f \in L_c^2(\mathbb{R}^3)$  is verbatim.

**Part 2a :** That  $\mathcal{R}(\mathbf{k})f \in L^2$  when  $\mathbf{k}^2 \in \mathbb{C} \setminus [0, \infty)$  follows from Proposition 14. The uniqueness of the  $L^2$  solution when  $\text{Im } \mathbf{k} \neq 0$  is given by Proposition 1 of Section 3.

**Part 2b :** We show the radiation condition in the case of no attenuation for  $\mathbf{k}_0$ . It is justified in Appendix E, for

$$y \in \Omega \text{ bounded} \quad , \quad f \in L_c^2(\mathbb{R}^3) \quad , \quad \text{Supp } f \subset \Omega ,$$

and

$$0 \in \Omega \quad , \quad x \in \mathbb{R}^3 \setminus \Omega ,$$

to pass the differentiation across the integral sign and obtain

$$\partial_{r(x)} \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy = \int_{\mathbb{R}^3} \partial_{r(x)} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy .$$

In another word, we have

$$\left( \frac{x}{|x|} \cdot \nabla_x \mp i \mathbf{k}_0 \right) \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy = \int_{\mathbb{R}^3} f(y) \left( \frac{x}{|x|} \cdot \nabla_x \mp i \mathbf{k}_0 \right) \Phi_{\mathbf{k}_0}^+(x, y) dy .$$

Next, we use the radiating property of  $\Phi_{\mathbf{k}_0}^\pm$  given in (4.112) of Prop 12,

$$\left( \frac{x}{|x|} \cdot \nabla_x \mp i \mathbf{k}_0 \right) \Phi_{\mathbf{k}_0}^\pm(x, y) = O(|x|^{-2}) ,$$

uniformly for  $y$  in compact set, when  $|x| \rightarrow \infty$ . We thus obtain the uniform Sommerfeld radiation for  $\mathcal{R}^+(\mathbf{k}_0)f$ .

$$\left( \frac{x}{|x|} \cdot \nabla_x \mp i \mathbf{k}_0 \right) \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy = \int_{\text{Supp } f} O(|x|^{-2}) f(y) dy = O(|x|^{-2}) .$$

**Part 3** This uses dominated convergence theorem and the limits (4.19)

$$\begin{aligned} \mathbf{k}_\gamma &\rightarrow \mathbf{k}_0 \quad , \quad \eta_\gamma \rightarrow \eta_0 \quad , \quad \chi_\gamma \rightarrow \chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^+; \\ \mathbf{k}_\gamma &\rightarrow -\mathbf{k}_0 \quad , \quad \eta_\gamma \rightarrow -\eta_0 \quad , \quad \chi_\gamma \rightarrow -\chi_0 \quad , \quad \text{as } \gamma \rightarrow 0^- . \end{aligned}$$

Denote the following regions in  $\mathbb{C}$ , with  $a, b, c > 0$

$$\begin{aligned} \mathfrak{R}^+ &:= \{z \in \mathbb{C} \mid \operatorname{Re} z \in [a, b] , \operatorname{Im} z \in [0, c]\} ; \\ \mathfrak{R}^- &:= \{z \in \mathbb{C} \mid \operatorname{Re} z \in [a, b] , \operatorname{Im} z \in [-c, 0]\} . \end{aligned}$$

Using the branch of square root defined in (4.11b), the following maps

$$\begin{aligned} \mathfrak{R}^+ &\longrightarrow \mathcal{C}(\mathbb{R}^3 \times \mathbb{R}^3, \mathbb{C}) \quad ; \quad \mathbf{z} \mapsto \Phi_{\sqrt{\mathbf{z}}}(x, y) , \\ \mathfrak{R}^- &\longrightarrow \mathcal{C}(\mathbb{R}^3 \times \mathbb{R}^3, \mathbb{C}) \quad ; \quad \mathbf{z} \mapsto \Phi_{\sqrt{\mathbf{z}}}(x, y) , \end{aligned}$$

are uniformly continuous. □

**Remark 23.** Here, we have considered  $H := -\Delta + \frac{\beta}{|x|}$  with constant  $\beta \in \mathbb{R}$  and  $\beta \geq 0$ . This is called a repulsive potential, which is the case for application in helioseismology. The above results can be rephrased from the perspective of spectral theory as

$$\sigma(H) = \sigma_{\text{cont}}(H) = \sigma_{\text{ac}}(H) = [0, \infty) ,$$

see also [16]. However, for  $\beta < 0$ , there are point spectrum on the negative axis<sup>22</sup>. Note that in both cases (either  $\beta > 0$  or  $\beta \leq 0$ ), there is no embedded positive eigenvalue into the spectrum (equivalently the spectrum is absolutely continuous).

## 4.6 Uniqueness under radiation condition at $\mathbf{k}_0$

In previous section, we have constructed a solution to

$$(-\Delta - \mathbf{k}_0^2 + \frac{\alpha_\infty}{|x|})u = f \quad , \quad \text{with } f \in L_c^2(\mathbb{R}^3) , \quad (4.146)$$

which satisfies the uniform Sommerfeld radiation condition

$$\partial_r u(x) - i\mathbf{k}_0 u(x) = o(r^{-1}) \quad , \quad \text{as } r = |x| \rightarrow \infty \text{ uniformly in } \frac{x}{|x|} \in \mathbb{S}(0, 1) .$$

We will show that this is a defining property, i.e. such a solution (with this property) is unique. We first discuss several equivalent forms of radiation conditions. Recall the second Green's formula (4.130), for a bounded domain  $\Omega$ ,

$$\int_{\Omega} \left( w(\Delta_x u) - u(\Delta_x w) \right) dx = \int_{\partial\Omega} w \partial_{n(x)} u - u \partial_{n(x)} w ,$$

where  $n(x)$  is the normal vector along  $\partial\Omega$  and points outward (from the interior of  $\mathfrak{R}$ ). On the other hand,

$$\int_{\Omega} \left( (\Delta_x u) w - u(\Delta_x w) \right) dx = \int_{\Omega} w \left( (\Delta_x + \mathbf{k}_0^2 - \frac{\alpha_\infty}{|x|})u - u(\Delta_x + \mathbf{k}_0^2 - \frac{\alpha_\infty}{|x|})w \right) dx .$$

<sup>22</sup>For the attractive Coulomb potential i.e.  $\beta < 0$

$$\sigma(H) = [0, \infty) \cup \sigma_{\text{point}}(H) \quad , \text{ with } \sigma_{\text{cont}}(H) = \sigma_{\text{ac}}(H) = [0, \infty) ,$$

and the point spectrum consisting of an infinite discrete set of negative eigenvalues with finite multiplicity with zero accumulation point,

$$\sigma_{\text{dis}}(H) = \left\{ -\frac{\beta^2}{4n^2} \in [-\beta^2, 0) , n = 1, 2, \dots \right\} . \quad (4.145)$$

For computation see [26, Chapter 10 p.191].

As a result, we have

$$\int_{\Omega} w \left( (\Delta_x + k_0^2 - \frac{\alpha_{\infty}}{|x|}) u - u (\Delta_x + k_0^2 - \frac{\alpha_{\infty}}{|x|}) w \right) dx = \int_{\partial\Omega} w \partial_{n(x)} u - u \partial_{n(x)} w. \quad (4.147)$$

In particular, we can apply (4.147) to the pair  $(u, \bar{u})$  to obtain

$$\int_{\Omega} \left( \bar{u} \left( \Delta_x + k_0^2 - \frac{\alpha_{\infty}}{|x|} \right) u - u \left( \Delta_x + k_0^2 - \frac{\alpha_{\infty}}{|x|} \right) \bar{u} \right) dx = - \int_{\partial\Omega} 2i \operatorname{Im} \left( u \partial_{n(x)} \bar{u} \right) d\sigma(x), \quad (4.148)$$

since

$$\bar{u} \partial_{n(x)} u - u \partial_{n(x)} \bar{u} = -2i \operatorname{Im} (u \partial_{n(x)} \bar{u}) = 2i \operatorname{Im} (\bar{u} \partial_{n(x)} u).$$

In the same spirit of the proof for Helmholtz equation, cf. e.g. [35, Thm 2.3], we obtain the results with additional presence of a positive Coulomb potential.

**Proposition 18** (Equivalent forms of radiation conditions). *For  $u$  a solution to*

$$\left( -\Delta - k_0^2 + \frac{\alpha_{\infty}}{|x|} \right) u = 0, \quad (4.149)$$

*in the exterior domain  $k_0 > 0$  of  $\Omega^{\complement} := \mathbb{R}^3 \setminus \bar{\Omega}$ , with  $\Omega$  bounded, the following statements are equivalent.*

1. *Uniform Sommerfeld radiation condition*

$$\partial_r u(x) - ik_0 u(x) = o(r^{-1}) \quad , \quad \text{as } r = |x| \rightarrow \infty \text{ uniformly in } \frac{x}{|x|} \in \mathbb{S}(0, 1). \quad (4.150)$$

2.  *$L^2$ -radiation condition*

$$\lim_{R \rightarrow \infty} \int_{\mathbb{S}(0, R)} |(\partial_r u)(x) - ik_0 u(x)|^2 d\sigma(x) = 0. \quad (4.151)$$

*This can be written as*

$$\lim_{r \rightarrow \infty} \int_{\mathbb{S}(0, r)} |(\partial_r u)(x)|^2 + k_0^2 |u(x)|^2 d\sigma(x) = -2k_0 \int_{\partial\Omega} \operatorname{Im} (u(x) \partial_r \bar{u}(x)) d\sigma(x). \quad (4.152)$$

3. *Exterior representation formula*

$$u(x) = \int_{\partial\Omega} \left( (\partial_n u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y). \quad (4.153)$$

*Proof.* **Part 1** : (1)  $\Rightarrow$  (2) Assuming the uniform radiation condition (4.150), we show that

$$\int_{\mathbb{S}(0, r)} |\partial_r u - ik_0 u|^2 dS_r = o(1) \quad , \quad \text{as } r \rightarrow \infty.$$

This is because

$$\int_{\mathbb{S}(0, r)} |\partial_r u - ik_0 u|^2 dS_r = \int_{\mathbb{S}(0, 1)} |\partial_r u(\varpi) - ik_0 u(r\varpi)|^2 r^2 d\varpi = \int_{\mathbb{S}(0, 1)} o(r^2) r^2 d\varpi = o(1).$$

**Part 2** : (2)  $\Rightarrow$  (3) **Step 0** Consider  $r$  so that

$$\Omega \subset \mathbb{B}_{(0, r)}.$$



Denote by

$$\mathfrak{R}_r := \Omega^c \cap \mathbb{B}_{(0,r)}, \quad (4.154)$$

where  $\Omega^c$  denotes the complement,  $\Omega^c = \mathbb{R}^3 \setminus \Omega$ . Since  $u$  is a solution of  $(-\Delta - k_0^2 + \frac{\alpha_\infty}{|x|})u = 0$  in  $\mathfrak{R}_r$ , apply Proposition 16 which gives the integral representation in  $\mathfrak{R}_r$ ,

$$u(x) = \int_{\partial\Omega} \left( (\partial_n u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_n \Phi_{k_0}^+)(x, y) \right) d\sigma(y).$$

Note that

$$\partial\mathfrak{R}_r = \partial\Omega \cup \mathbb{S}_{(0,r)}.$$

Denote by  $\mathbb{I}$  this integral along  $\mathbb{S}_{(0,r)}$ , i.e.

$$\mathbb{I} := \int_{\mathbb{S}_{(0,r)}} \left( (\partial_n u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_n \Phi_{k_0}^+)(x, y) \right) d\sigma(y).$$

We need to show that

$$\lim_{r \rightarrow \infty} \mathbb{I} = 0.$$

**Step 1** We first obtain the second form (4.152) of the  $L^2$ -radiation condition using (4.148). Since both  $\alpha_\infty$  and  $k_0$  are real, both  $u$  and  $\bar{u}$  satisfy the homogeneous equation in  $\mathfrak{R}_r$

$$\left( \Delta_x + k_0^2 - \frac{\alpha_\infty}{|x|} \right) \bar{u} = 0 \quad ; \quad \left( \Delta_x + k_0^2 - \frac{\alpha_\infty}{|x|} \right) u = 0.$$

Using this fact and applying the modified Green's formula (4.148) to  $(u, \bar{u})$  in region  $\mathfrak{R}_r$ , we have

$$\int_{\partial\mathfrak{R}_r} \text{Im} (u(x) \partial_{\nu(x)} \bar{u}(x)) d\sigma(x) = 0 \quad , \quad \nu(x) \text{ normal vector pointing outward of } \mathfrak{R}_r.$$

Since  $\partial\mathfrak{R}_r = \partial\Omega \cup \mathbb{S}_{(0,r)}$ , with  $n(x)$  denoting the normal vector along  $\partial\Omega$  and  $\mathbb{S}_{(0,r)}$  but now points outward (towards infinity), we have

$$\int_{\partial\Omega} \text{Im} (u(x) \partial_{n(x)} \bar{u}(x)) d\sigma(x) = \int_{\mathbb{S}_{(0,r)}} \text{Im} (u(x) \partial_{n(x)} \bar{u}(x)) d\sigma(x). \quad (4.155)$$

On the other hand, since

$$|(\partial_r u)(x) - ik_0 u(x)|^2 = |(\partial_r u)(x)|^2 + k_0^2 |u(x)|^2 + 2 \text{Im} (u(x) \partial_r \bar{u}(x)),$$

we have

$$\begin{aligned} & \int_{\mathbb{S}_{(0,r)}} |(\partial_r u)(x) - ik_0 u(x)|^2 d\sigma(x) \\ &= \int_{\mathbb{S}_{(0,r)}} (|(\partial_r u)(x)|^2 + k_0^2 |u(x)|^2) d\sigma(x) + \int_{\mathbb{S}_{(0,r)}} 2 \text{Im} (u(x) \partial_r \bar{u}(x)) d\sigma(x) \\ &\stackrel{(4.155)}{=} \int_{\mathbb{S}_{(0,r)}} (|(\partial_r u)(x)|^2 + k_0^2 |u(x)|^2) d\sigma(x) + \int_{\partial\Omega} 2 \text{Im} (u(x) \partial_r \bar{u}(x)) d\sigma(x). \end{aligned}$$

Hence we obtain the second form of (4.151)

$$\lim_{r \rightarrow \infty} \int_{\mathbb{S}_{(0,r)}} (|(\partial_r u)(x)|^2 + k_0^2 |u(x)|^2) d\sigma(x) = -2k_0 \int_{\partial\Omega} \text{Im} (u(x) \partial_r \bar{u}(x)) d\sigma(x).$$

**Step 2** To make use of the  $L^2$ -radiation condition (4.151) and (4.152), we next rewrite  $\mathbb{I}$  as

$$\mathbb{I} = \mathbb{I}_1 + \mathbb{I}_2,$$

where

$$\begin{aligned}\mathbb{I}_1 &:= \int_{\mathbb{S}_{(0,r)}} \left( (\partial_n u)(y) - i k_0 u(y) \right) \Phi_{k_0}^+(x, y) d\sigma(y); \\ \mathbb{I}_2 &:= \int_{\mathbb{S}_{(0,r)}} u(y) \left( i k_0 \Phi_{k_0}^+(x, y) - (\partial_n u) \Phi_{k_0}^+(x, y) \right) d\sigma(y).\end{aligned}$$

Here, we have added and subtracted the term  $i k_0 \Phi_{k_0}^+ u$ . From (4.152), we have that

$$\int_{\mathbb{S}_{(0,r)}} |(\partial_r u)(x)|^2 d\sigma(x) = O(1) \quad , \quad \int_{\mathbb{S}_{(0,r)}} |u(x)|^2 d\sigma(x) = O(1) \quad , \quad \text{as } r \rightarrow \infty.$$

We first consider  $\mathbb{I}_2$ . With  $x$  in a compact set and considered as a parameter,  $y \mapsto \Phi_{k_0}^+(x, y)$  solves (4.149) in  $\mathbb{R}^3 \setminus \{x\}$  and satisfies

$$\left( \frac{y}{|y|} \cdot \nabla_y - i k \right) \Phi_k^+ = O(|y|^{-2}).$$

Result of Part 1 (now applied in variable  $y$ ) then gives

$$\int_{\mathbb{S}_{(0,r)}} \left| \frac{y}{|y|} \cdot \nabla_y \Phi_k^+ - i k \Phi_k^+ \right|^2 d\sigma(y) = o(1) \quad , \quad \text{as } r \rightarrow \infty.$$

By Cauchy-Schwarz, we obtain

$$|\mathbb{I}_2| \leq \left( \int_{\mathbb{S}_{(0,r)}} |u(y)|^2 d\sigma(y) \right)^{1/2} \left( \int_{\mathbb{S}_{(0,r)}} \left| \frac{y}{|y|} \cdot \nabla_y \Phi_k^+ - i k \Phi_k^+ \right|^2 d\sigma(y) \right)^{1/2} = O(1) o(1),$$

as  $r \rightarrow \infty$ .

Thus

$$\mathbb{I}_2 = o(1) \quad , \quad \text{as } r \rightarrow \infty.$$

We next consider  $\mathbb{I}_1$ . For  $x$  in a compact set,

$$\begin{aligned}\Phi_{k_0}^+(x, y) &= e^{\frac{1}{2} i k_0 |y|} (e^{-i \pi i k_0 |y|})^{\chi_0} (1 + O(|y|^{-2})) \frac{1}{y} (1 + O(|y|^{-1})) \\ \Rightarrow \Phi_{k_0}^+(x, y) &= e^{\frac{1}{2} i k_0 |y|} (e^{-i \pi i k_0 |y|})^{\chi_0} \frac{1}{|y|} (1 + O(|y|^{-1})).\end{aligned}$$

Since

$$\int_{\mathbb{S}_{(0,r)}} |\Phi_{k_0}^+(x, y)|^2 d\sigma(y) = \int_{\mathbb{S}_{(0,1)}} |\Phi_{k_0}^+(x, y)|^2 |y|^2 d\sigma(y),$$

we thus have, for  $x$  in a compact set

$$\int_{\mathbb{S}_{(0,r)}} |\Phi_{k_0}^+(x, y)|^2 d\sigma(y) = O(1) \quad , \quad \text{as } r \rightarrow \infty.$$

Note that we are currently assuming (4.151), i.e.

$$\int_{\mathbb{S}_{(0,r)}} |(\partial_r u)(y) - i k_0 u(y)|^2 d\sigma(y) = o(1) \quad \text{as } r \rightarrow \infty.$$

As before, we now use Cauchy-Schwarz to bound

$$|\mathbb{I}_1| \leq \left( \int_{\mathbb{S}_{(0,r)}} |\Phi_{k_0}^+(x, y)|^2 d\sigma(y) \right)^{1/2} \left( \int_{\mathbb{S}_{(0,r)}} \left| \frac{y}{|y|} \cdot \nabla_y \Phi_{k_0}^+ - i k \Phi_{k_0}^+ \right|^2 d\sigma(y) \right)^{1/2} = O(1) o(1), \quad \text{as } r \rightarrow \infty.$$

As a result of this,

$$\mathbb{I}_1 = o(1) \quad , \quad \text{as } r \rightarrow \infty .$$

Together with the result for  $\mathbb{I}_2$ , we obtain the conclusion for  $\mathbb{I}$ , i.e.  $\mathbb{I} = o(1)$  as  $r \rightarrow \infty$ , and hence (4.153).

**Part 3** (3)  $\Rightarrow$  (1) Now we assume that  $u$  is a solution to (4.149) in  $\Omega^{\mathbb{C}}$  and that  $u$  can be given by (4.153).

$$u(x) = \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) , \quad (4.156)$$

with the normal vector  $n$  points outward of  $\partial\Omega$ . In fact, we can obtain a representation on  $\mathbb{S}_{(0, \tau)}$  for  $\tau > 0$  large enough so that

$$\Omega \subset \mathbb{B}_{(0, \tau)} .$$

As done in the proof for Part 2, we apply Proposition 16 which gives the integral representation in  $\mathfrak{R}_r$ ,

$$u(x) = \int_{\partial\Omega \cup \mathbb{S}_{(0, \tau)}} \left( (\partial_{\nu(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{\nu(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) ,$$

where  $\nu$  points outward from  $(\mathbb{R}^3 \setminus \Omega) \cap \mathbb{B}_{(0, \tau)}$ . Combining with the representation (4.156)

$$\begin{aligned} & \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) \\ &= - \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) \\ &+ \int_{\mathbb{S}_{(0, \tau)}} \left( (\partial_{r(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{r(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) . \end{aligned}$$

This leads to

$$\begin{aligned} & \int_{\partial\Omega} \left( (\partial_{n(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{n(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) \\ &= \frac{1}{2} \int_{\mathbb{S}_{(0, \tau)}} \left( (\partial_{r(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{r(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) . \end{aligned}$$

As a result of this,  $u$  can be written as

$$u = \frac{1}{2} \int_{\mathbb{S}_{(0, \tau)}} \left( (\partial_{r(y)} u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_{r(y)} \Phi_{k_0}^+)(x, y) \right) d\sigma(y) .$$

We will work with this representation.

With differentiation under the integral sign justified in Appendix E, we can write

$$(\partial_{r(x)} - i k_0) 2u = \mathbb{A}_1 + \mathbb{A}_2 ,$$

where

$$\begin{aligned} \mathbb{A}_1 &:= \int_{\mathbb{S}_{(0, \tau)}} (\partial_n u)(y) \left( \frac{x}{|x|} \nabla_x - i k_0 \right) \Phi_{k_0}^+(x, y) , \\ \mathbb{A}_2 &:= \int_{\mathbb{S}_{(0, \tau)}} u(y) \left( \frac{x}{|x|} \nabla_x - i k_0 \right) \partial_{n(y)} \Phi_{k_0}^+(x, y) d\sigma(y) . \end{aligned}$$

Note that we are integrating with respect to  $y \in \partial\Omega$ , the boundary of bounded domain  $\Omega$ , thus  $y$  is indeed in a bounded set and we can apply the radiating property of  $\Phi_{k_0}^+(x, y)$ . Prop 11 and 13 give the asymptotic properties of  $\Phi_{k_0}^+(x, y)$  and  $\partial_{r(y)} \Phi_{k_0}^+(x, y)$ ,

$$\begin{aligned} (\partial_{r(x)} - i k_0) \Phi_{k_0}^+(x, y) &= O(|x|^{-2}) , \\ (\partial_{r(x)} - i k_0) \partial_{r(y)} \Phi_{k_0}^+(x, y) &= O(|x|^{-2}) , \end{aligned}$$

as  $|x| \rightarrow \infty$  and  $y$  in a bounded set. As a result of this

$$\mathbb{A}_1 = \int_{\partial\Omega} \mathcal{O}(1) \mathcal{O}(|x|^{-2}) d\sigma(y) = \mathcal{O}(|x|^{-2}).$$

Similarly, we obtain  $\mathbb{A}_2 = \mathcal{O}(|x|^{-2})$ . And thus

$$(\partial_{r(x)} - ik_0)u = \mathcal{O}(|x|^{-1}),$$

which implies (4.150). □

**Definition 3.** For  $k_0 > 0$ , a function  $u \in L^2_{loc}(\mathbb{R}^3)$  is a outgoing solution for

$$(-\Delta - k_0^2 + \frac{\alpha_\infty}{|x|})u = f, \quad (4.157)$$

in  $\mathbb{R}^3 \setminus \Omega$ , where  $\Omega$  is a bounded region if  $u$  satisfies one of the conditions listed in Prop 18, in particular, the Uniform Sommerfeld radiation condition (4.150)

$$\partial_r u(x) - ik_0 u(x) = o(r^{-1}) \quad , \quad \text{as } r = |x| \rightarrow \infty \text{ uniformly in } \frac{x}{|x|} \in \mathbb{S}(0, 1),$$

or the  $L^2$ -radiation condition (4.151),

$$\lim_{R \rightarrow \infty} \int_{\mathbb{S}(0, R)} |(\partial_r u)(x) - ik_0 u(x)|^2 d\sigma(x) = 0. \quad \triangle$$

**Proposition 19.** With definition of outgoing given by Definition 3, we have the following statements.

- For  $k_0 > 0$ , if  $u \in H^2_{loc}(\mathbb{R}^3)$  is an outgoing solution to  $(-\Delta - k_0^2 + \frac{\alpha_\infty}{|x|})u = 0$  and satisfies the outgoing radiation condition, then  $u \equiv 0$ .
- For  $k_0 > 0$ , if  $u \in H^2_{loc}(\mathbb{R}^3)$  is an outgoing solution to  $(-\Delta - k_0^2 + \frac{\alpha_\infty}{|x|})u = f$ ,  $f \in L^2_c(\mathbb{R}^3)$ , then  $u$  is unique.

*Proof.* If  $u$  is an outgoing solution in  $\mathbb{R}^3$ , then by the exterior representation formula (4.153)

$$u(x) = \int_{\mathbb{S}(0, \epsilon)} \left( (\partial_n u)(y) \Phi_{k_0}^+(x, y) - u(y) (\partial_n(y) \Phi_{k_0}^+(x, y)) \right) d\sigma(y), \quad (4.158)$$

in  $\mathbb{R}^3 \setminus \mathbb{B}_{(0, \epsilon)}$  for all  $\epsilon < |x|$ . Let  $\epsilon \rightarrow 0$ , we obtain that  $u(x) \rightarrow 0$ .

For the second statement, suppose  $u_1$  and  $u_2$  are two outgoing solutions of the inhomogeneous equation, then  $u = u_1 - u_2$  solves the homogeneous equation and is still outgoing. By the first part,  $u \equiv 0$ . □

## 4.7 Rellich's lemma

The following theorem is also proved in [26, Thm 1.2]. This is usually needed to show uniqueness of exterior boundary value problem.

**Lemma 20** (Rellich estimate). Consider a solution  $u \in \mathcal{C}^2(\mathbb{R}^3 \setminus \mathbb{B}_{(0, r)})$

$$(-\Delta - k_0^2 + \frac{\alpha_\infty}{|x|})u = 0 \quad \text{on } \mathbb{R}^3 \quad , \quad \text{with } k_0 > 0,$$

which does not vanish identically, then  $\exists C > 0$ , and  $\tilde{\mathfrak{r}} > \mathfrak{r}$  such that

$$\forall r > \tilde{\mathfrak{r}} \quad , \quad \int_{\mathfrak{r} \leq |x| \leq r} |u(x)|^2 dx \geq Cr. \quad (4.159)$$

*Proof. Step 1* In the region  $\mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})}$ , with RHS being 0, the equation has the radial symmetry and a general solution can be decomposed as expansions of spherical harmonics, i.e.

$$u(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell}^m(r) Y_{\ell}^m(\theta, \phi),$$

where the coefficients  $u_{\ell}^m(r)$  are

$$u_{\ell}^m(r) = \int_{\mathbb{S}^1} u(r\varpi) \overline{Y_{\ell}^m(\varpi)} d\varpi = \int_0^{\pi} \int_0^{2\pi} u(r, \phi, \theta) \overline{Y_{\ell}^m(\theta, \phi)} \sin \theta d\phi d\theta.$$

By the orthogonality of  $\{Y_{\ell}^m\}$ , we also have

$$\int_{\mathbb{S}^2} |u(s, \varpi)|^2 d\varpi = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |u_{\ell}^m(s)|^2.$$

As a result,

$$\int_{\mathfrak{r} \leq |x| \leq r} |u(x)|^2 dx = \int_{\mathfrak{r}}^r \int_{\mathbb{S}^1} |u(s, \varpi)|^2 s^2 d\varpi ds = \int_{\mathfrak{r}}^r \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |u_{\ell}^m(s)|^2 s^2 ds.$$

By hypothesis that  $u \not\equiv 0$  on  $\mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})}$ , there exists radius  $s_0$  and mode  $(m, \ell)$  so that

$$|u_{\ell}^m(s_0)| > 0. \quad (4.160)$$

This quantity will be as a lower bound for the  $L^2$  norm of  $u$  on the annulus  $\mathfrak{r} \leq s \leq r$ ,

$$\int_{\mathfrak{r} \leq |x| \leq r} |u(x)|^2 dx \geq \int_{\mathfrak{r}}^r |u_{\ell}^m(s)|^2 s^2 ds > 0. \quad (4.161)$$

**Step 2a** We will look for  $\tilde{\mathfrak{r}}$  and  $C > 0$  so that if  $r > \tilde{\mathfrak{r}}$  then

$$\int_{\mathfrak{r}}^r |u_{\ell}^m(s)|^2 s^2 ds > Cr.$$

By (4.174) (which gives expansion in spherical harmonic and Whittaker functions) and (4.160), for some  $\tilde{a}$  and  $\tilde{b}$  with  $|\tilde{a}|^2 + |\tilde{b}|^2 > 0$ ,

$$u_{\ell}^m(s) = \frac{1}{s} \left( \tilde{a} W_{-\chi, \ell + \frac{1}{2}}(-2ik s) + \tilde{b} W_{\chi, \ell + \frac{1}{2}}(2ik s) \right).$$

Using the asymptotic properties (4.49) of the Whittaker function in Appendix C.2, we have, for some  $a$  and  $b$  with  $|a|^2 + |b|^2 > 0$ ,

$$u_{\ell}^m(s) = \frac{1}{s} \left( a e^{-\frac{\pi}{2}\eta_0} \sin(k_0 r - \eta_0 \log(2k_0 s)) + b e^{-\frac{\pi}{2}\eta_0} \cos(k_0 r - \eta_0 \log(2k_0 s)) + O(s^{-2}) \right). \quad (4.162)$$

In fact,  $b = \tilde{a} + \tilde{b}$  and  $a = i(\tilde{a} - \tilde{b})$ .

We next rewrite the two dominant terms in (4.162) as,

$$a \sin(k_0 r - \eta_0 \log(2k_0 s)) + b \cos(k_0 r - \eta_0 \log(2k_0 s)) = \sin(k_0 r - \eta_0 \log(2k_0 s) + \theta_0),$$

where the angle  $\theta_0$  is given by

$$\cos \theta_0 = \frac{a}{\sqrt{a^2 + b^2}} \quad , \quad \sin \theta_0 = \frac{b}{\sqrt{a^2 + b^2}} .$$

We can write

$$\begin{aligned} u_\ell^m(s) &= e^{-\frac{\pi}{2}\eta_0} \sqrt{a^2 + b^2} \left( \sin(k_0 r - \eta_0 \log(2k_0 s) + \theta_0) + O(s^{-1}) \right); \\ \Rightarrow |u_\ell^m(s)|^2 s^2 &= e^{-\pi\eta_0} (a^2 + b^2) \left( \sin(k_0 r - \eta_0 \log(2k_0 s) + \theta_0) + O(s^{-1}) \right)^2; \\ &= e^{-\pi\eta_0} (a^2 + b^2) \left( \sin^2(k_0 r - \eta_0 \log(2k_0 s) + \theta_0) + O(s^{-1}) \right); \\ &= e^{-\pi\eta_0} \frac{a^2 + b^2}{2} \left( 1 - \cos 2(k_0 r - \eta_0 \log(2k_0 s) + \theta_0) + O(s^{-1}) \right). \end{aligned}$$

For the last equality, we use the identity  $\sin^2 \phi = \frac{1 - \cos 2\phi}{2}$ .

After this step we have obtained

$$\begin{aligned} &\int_{\mathfrak{r}}^r |u_\ell^m(s)|^2 s^2 ds \\ &= e^{-\pi\eta_0} \frac{a^2 + b^2}{2} \left( r - \mathfrak{r} + \int_{\mathfrak{r}}^r \cos 2(k_0 s - \eta_0 \log(2k_0 s) + \theta_0) ds \right) + O(\log r). \end{aligned} \tag{4.163}$$

**Step 2b** We next show that the second integral in (4.163)

$$\mathbb{I} = \int_{\mathfrak{r}}^r \cos 2(k_0 s - \eta_0 \log(2k_0 s) + \theta_0) ds .$$

is  $O(1)$  as  $r \rightarrow \infty$ . We first define

$$g(s) := k_0 s - \eta_0 \log(2k_0 s) + \theta_0 \quad \Rightarrow \quad g'(s) = 2k_0 - 2\eta_0 \frac{1}{s} = \frac{2k_0 s - 2\eta_0}{s} .$$

In terms of  $g$ , we write

$$\mathbb{I} = \int_{\mathfrak{r}}^r \frac{1}{g'(s)} \cos g(s) \times g'(s) ds = - \int_{\mathfrak{r}}^r \frac{1}{g'(s)} (\sin g(s))' ds .$$

Using integration by parts,

$$\mathbb{I} = - \frac{\sin g(s)}{g'(s)} \Big|_{\mathfrak{r}}^r + \int_{\mathfrak{r}}^r \sin g(s) \left( \frac{1}{g'(s)} \right)' ds. \tag{4.164}$$

Since  $|\sin(\cdot)| \leq 1$  and

$$\lim_{r \rightarrow \infty} \frac{1}{g'(r)} = 2k_0 ,$$

the first term on the RHS of (4.164) reads

$$- \frac{\sin g(r)}{g'(r)} + \frac{\sin g(\mathfrak{r})}{g'(\mathfrak{r})} = O(1) \quad , \quad \text{as } r \rightarrow \infty. \tag{4.165}$$

We next consider the second term on the RHS of (4.164). First recall that  $\eta_0 = \frac{\alpha_\infty}{2k_0} > 0$  since  $\alpha_\infty > 0$  and  $k_0 > 0$ . Hence,

$$g'' = 2\eta_0 \frac{1}{s^2} > 0 \quad \text{and} \quad \left( \frac{1}{g'(s)} \right)' = \frac{g''(s)}{(g'(s))^2} > 0. \tag{4.166}$$

Now using  $|\sin(\cdot)| \leq 1$  to bound

$$\left| \int_{\mathfrak{r}}^r \sin g(s) \left( \frac{1}{g'(s)} \right)' ds \right| \leq \int_{\mathfrak{r}}^r \left| \left( \frac{1}{g'(s)} \right)' \right| ds \stackrel{(4.166)}{=} \int_{\mathfrak{r}}^r \left( \frac{1}{g'(s)} \right)' ds = \frac{1}{g'(r)} - \frac{1}{g'(\mathfrak{r})}.$$

Since

$$\lim_{r \rightarrow \infty} \frac{1}{g'(r)} = \frac{1}{2k_0},$$

we thus have

$$\frac{1}{g'(r)} - \frac{1}{g'(\mathfrak{r})} = O(1).$$

As a result of this,

$$\int_{\mathfrak{r}}^r \sin g(s) \left( \frac{1}{g'(s)} \right)' ds = O(1). \quad (4.167)$$

Putting together (4.165) and (4.167), we obtain

$$\mathbb{I} = O(1) \quad , \quad \text{as } r \rightarrow \infty. \quad (4.168)$$

**Step 2c** From (4.168) and (4.163), we then conclude the existence of  $C > 0$  and  $\tilde{\mathfrak{r}} > 0$

$$\int_{\mathfrak{r}}^r |u_{\ell}^{\text{m}}(s)|^2 s^2 ds = e^{-\pi\eta_0} \frac{a^2 + b^2}{2} r + O(1) + O(\log r).$$

Here we have gathered into  $O(1)$  the terms  $e^{-\pi\eta_0} \frac{a^2 + b^2}{2} (-\mathfrak{r} + \mathbb{I})$ . The final Rellich estimate (4.159) now follows after using (4.161). □

## 4.8 General solutions for the homogeneous equation

In this subsection, we will describe a generic solution of the homogeneous problem of operator (4.2)

$$\left( -\Delta_x - k^2 + \frac{\alpha_{\infty}}{|x|} \right) u = 0. \quad (4.169)$$

Recall that by separation of variable, this is reduced to an ODE on each mode  $(\ell, m)$

$$\left( -\frac{d^2}{dr^2} - k^2 - \frac{\alpha_{\infty}}{r} + \frac{\ell(\ell+1)}{r^2} \right) u_{\ell}^m = 0 \quad , \quad \ell = 0, 1, 2, \dots$$

By Remark 21, the range of angle for  $z = 2e^{i\frac{\pi}{2}} k r$  is in the definition range  $(-\frac{\pi}{2}, \frac{3\pi}{2})$  of

$$W_{\chi, \ell + \frac{1}{2}}(z) \quad \text{and} \quad W_{-\chi, \ell + \frac{1}{2}}(e^{-\pi i} z), \quad (4.170)$$

a pair of fundamental solutions for (4.5) at  $\infty$ , and in the definition range  $(-\pi, \pi)$  of the fundamental pair near the origin,

$$\mathcal{M}_{\chi, \ell + \frac{1}{2}}(e^{-i\pi} z) \quad \text{and} \quad W_{\chi, \ell + \frac{1}{2}}(e^{-i\pi} z). \quad (4.171)$$

These fundamental pairs are listed in Subsubsection 4.2.4 with their definition given in (4.26)–(4.29) for the Buchholtz function  $\mathcal{M}_{\chi, \ell + \frac{1}{2}}$  and in (4.32)–(4.33) for the Whittaker function  $W_{\chi, \ell + \frac{1}{2}}$ . We obtain readily the following results.

**Proposition 21.** *If  $u \in L_{loc}^2$  is a solution to*

$$\left( -\Delta_x - k^2 + \frac{\alpha_{\infty}}{|x|} \right) u = 0, \quad (4.172)$$

- in a sphere  $|x| \leq R$ , then  $u$  is given by

$$u = \sum_{\ell=0}^{\infty} \sum_{m=-1}^{\ell} c_{\ell}^m \frac{\mathcal{M}_{\chi, \ell + \frac{1}{2}}(2ik|x|)}{|x|} Y_{\ell}^m(\theta, \phi), \quad (4.173)$$

- and in an annulus  $0 < R_1 \leq |x| \leq R_2$  is given by

$$u = \sum_{\ell=0}^{\infty} \sum_{m=-1}^{\ell} \frac{1}{|x|} \left( a_{\ell}^m W_{-\chi, \ell + \frac{1}{2}}(e^{-i\pi} 2ik|x|) + b_{\ell}^m W_{\chi, \ell + \frac{1}{2}}(2ik|x|) \right) Y_{\ell}^m(\theta, \phi). \quad (4.174)$$

- If  $u$  is, in addition, outgoing by Definition 3, then on  $0 < R_1 \leq |x| \leq R_2$ ,

$$u = \sum_{\ell=0}^{\infty} \sum_{m=-1}^{\ell} a_{\ell}^m \frac{W_{-\chi, \ell + \frac{1}{2}}(e^{-i\pi} 2ik|x|)}{|x|} Y_{\ell}^m(\theta, \phi). \quad (4.175)$$

**Remark 24.** The series (4.174) and (4.173) converge on compact subsets of  $\mathbb{R}^3 \setminus \{0\}$ .  $\triangle$

**Remark 25.** In the general spherically symmetric case, we still have  $\rho(x) = \rho(|x|)$ , but  $\frac{\rho'}{\rho}$  is not reduced to a constant. However, on each mode  $(\ell, m)$ , we still obtain an ODE of the form

$$\left( -\frac{d^2}{dr^2} - k_0^2 + v(r) \right) u_{\ell}^m = 0.$$

This is a specific case of the general problem considered in [7, Chapter 2],

$$\left( -\frac{d^2}{dr^2} - f^2(r) \right) u = 0 \quad , \quad f(r) = \sqrt{k_0^2 - v(r)} > 0. \quad (4.176)$$

For  $k_0^2 \neq 0$ , in case of a decaying potential  $v(r)$  that is

$$v(r) \rightarrow 0 \quad \text{as } r \rightarrow \infty. \quad (4.177)$$

with further condition, cf. [7, Eqn 4.45], for a  $x_0$  chosen arbitrarily large,

$$\int_{x_0}^{\infty} |v'(r)|^2 dr < \infty \quad , \quad \int_{x_0}^{\infty} |v''(r)| dr < \infty. \quad (4.178)$$

Applying Theorem 4.5 and 4.6 of [7] gives that the equation (4.176), has a pair of solutions with the following asymptotics, as  $r \rightarrow \infty$ ,

$$\exp \left( \pm i k_0 \int_{r_0}^r \sqrt{1 - \frac{v(s)}{k_0^2}} ds \right) (1 + o(1)).$$

In our case, by (2.19) and (2.11) and supposing constant speed,

$$v(r) = \frac{\alpha^2(r) - \alpha_{\infty}^2}{4} + \frac{\partial_r \alpha(r) - \alpha'_{\infty}}{2} + \frac{\alpha_{\infty}(r)}{r} + \frac{\ell(\ell+1)}{r^2}.$$

In order to apply this result, we assume that  $\alpha_{\infty}(r)$  is such that  $v(r)$  satisfies (4.177) and (4.178) and that  $k^2 \geq v(r)$ .  $\triangle$



#### 4.9 Exact Dirichlet-to-Neumann map

**Definition 4.** Consider a bounded domain  $\Omega \subset \mathbb{R}^3$  with smooth boundary  $\Gamma$ . Denote respectively by  $|_{\Gamma}^{\pm}$  the outer and inner trace along  $\Gamma$ . Consider the Schrödinger equation with Coulomb potential,

$$\left( -\Delta - k^2 + \frac{\alpha_{\infty}}{|x|} \right) u = 0. \quad (4.179)$$

For  $g \in L^2(\Gamma)$ ,

- the outer D-t-N operator  $\mathbf{T}^+$  associated with (4.179) and  $\Gamma$  is defined as

$$\mathbf{T}^+ g = \partial_n u|_{\Gamma}^+ \quad \text{where} \quad \begin{array}{l} u \text{ is the outgoing solution to (4.179) in } \mathbb{R}^n \setminus \Omega; \\ \text{with boundary condition } u|_{\Gamma}^+ = g \end{array};$$

- while the inner D-t-N operator  $\mathbf{T}^-$  is

$$\mathbf{T}^- g = \partial_n u|_{\Gamma}^- \quad \text{where} \quad \begin{array}{l} u \text{ is the unique solution to (4.179) in } \Omega \\ \text{with boundary condition } u|_{\Gamma}^- = g. \end{array}$$

△

**Proposition 22.** Consider equation (4.179) in exterior of the sphere  $\mathbb{B}_{(0,R)}$  with boundary denoted by  $\Gamma$ . The outer D-t-N along  $\Gamma$  associated with this equation is given by

$$\mathbf{T}^+(u|_{\Gamma}) = \sum_{\ell=0}^{\infty} \gamma_{\ell} \sum_{m=-\ell}^{\ell} u_{\ell}^m Y_{\ell}^m(\theta, \phi), \quad (4.180)$$

where  $u_{\ell}^m$  are the coefficients of the expansion of  $u|_{\Gamma}$  in the spherical harmonic basis  $Y_{\ell}^m$ , i.e.

$$\begin{aligned} u|_{\Gamma}(\theta, \phi) &= \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell}^m Y_{\ell}^m(\theta, \phi), \\ \text{with } u_{\ell}^m &:= \int_0^{\pi} \int_0^{2\pi} u(R, \theta, \phi) \overline{Y_{\ell}^m(\theta, \phi)} \sin \theta d\phi d\theta, \end{aligned} \quad (4.181)$$

and  $\gamma_{\ell}$  are the modal coefficients of  $\mathbf{T}^+$  at level  $\ell$  (called modal D-t-N coefficients),

$$\gamma_{\ell} := -2ik \frac{W'_{-\chi, \ell + \frac{1}{2}}(-2ikR)}{W_{-\chi, \ell + \frac{1}{2}}(-2ikR)} - \frac{1}{R}, \quad \chi = \frac{i\alpha_{\infty}}{2k}. \quad (4.182)$$

*Proof.* From (4.173), an outgoing solution  $u_{\text{out}}$  in  $R \leq |x| \leq R'$  is given by

$$u_{\text{out}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell}^m \frac{W_{-\chi, \ell + \frac{1}{2}}(-2ik|x|)}{|x|} Y_{\ell}^m(\theta, \phi), \quad \chi = \frac{i\alpha_{\infty}}{2k}.$$

The sequence  $a_{\ell}^m$  is next determined from the outer Dirichlet trace of  $u_{\text{outgoing}}$  along  $\Gamma$  given by  $u|_{\Gamma}$ . Upon imposing the boundary condition on each mode  $(m, \ell)$ , with  $u_{\ell}^m$  given in (4.181), we obtain

$$a_{\ell}^m \frac{W_{-\chi, \ell + \frac{1}{2}}(-2ikR)}{R} = u_{\ell}^m. \quad (4.183)$$

Since the series converges absolutely and uniformly in  $R \leq |x| \leq R'$ , we can differentiate term-by-term in the radial direction to obtain the outer normal trace  $u_{\text{out}}$  along  $\Gamma$  is then

$$\partial_n u_{\text{out}}|_{\Gamma^+} = - \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell}^m \left( 2ik \frac{W'_{-\chi, \ell + \frac{1}{2}}(-2ikR)}{R} + \frac{W_{-\chi, \ell + \frac{1}{2}}(-2ikR)}{R^2} \right) Y_{\ell}^m(\theta, \phi).$$

Replace  $a_\ell^m$  by expression (4.183), with simplification we obtain

$$\partial_n u_{\text{out}}|_{\Gamma^+} = - \sum_{\ell=0}^{\infty} \left( 2ik \frac{W'_{-\chi, \ell + \frac{1}{2}}(-2ikR)}{W_{-\chi, \ell + \frac{1}{2}}(-2ikR)} + \frac{1}{R} \right) \sum_{m=\ell}^{\ell} u_\ell^m Y_\ell^m(\theta, \phi).$$

□

## 5 Results for the original problem

We rephrase the results obtained for the conjugated operator (2.5)

$$\mathcal{L} = \rho^{-1/2} \mathcal{L}_{\text{orig}} \rho^{1/2} = -\Delta - \frac{\omega^2}{c^2} + \rho^{1/2} \Delta \rho^{-1/2},$$

in terms of those for the original one (2.1)

$$\mathcal{L}_{\text{orig}} u := -\nabla \cdot (\rho^{-1} \nabla u) - \frac{\omega^2}{\rho c^2} u.$$

### 5.1 Global outgoing solutions

We first recall the constructed resolvent for the conjugated operator  $\mathcal{L}$  in Subsection 3.3, denoted by  $\mathfrak{R}_{\omega^2}(\mathbf{k}^2) := \left( -\Delta + \mathbf{q}(x) - \frac{\omega^2}{c^2} \right)^{-1}$ , cf. (3.69) in the presence of attenuation, and (3.71) (Approach 1) or (3.84) (Approach 2) without attenuation. The ‘outgoing’ resolvent for the original operator in (1.1) is given as

$$\rho^{1/2} \mathfrak{R}_{\omega^2}(\mathbf{k}^2) \rho^{1/2}. \quad (5.1)$$

Here, ‘outgoing’ or physical means that  $w$  is  $L^2$  in the presence of attenuation and  $\mathbf{k}_0$ -outgoing in the case without attenuation. As a result, ‘outgoing’ or physical for the original equation means that  $\rho^{-1/2}u$  is  $L^2$  in the presence of attenuation and  $\mathbf{k}_0$ -outgoing in the case without attenuation.

**Definition 5** (Outgoing solution for the original problem). *For  $f$  with  $\rho^{1/2}f \in \mathfrak{B}$  (Remark 9) for the case without attenuation, or  $\rho^{1/2}f \in L^2$  with attenuation, a solution  $u$  to  $\mathcal{L}_{\text{orig}}u = f$  is called outgoing if  $u = \rho^{1/2}w$  where  $w$  is the (unique) outgoing/physical solution to  $\mathcal{L}w = \rho^{1/2}f$ . Specifically, with  $w = \mathcal{R}_{\omega^2}(\mathbf{k}^2) \rho^{1/2}f$ , the outgoing solution is then*

$$u = \rho^{1/2} \mathfrak{R}_{\omega^2}(\mathbf{k}^2) \rho^{1/2} f. \quad \triangle$$

**Remark 26** (Global outgoing solution to the inhomogeneous equation in the *Atmo* model). *For completeness of discussion, we consider the case in which *Atmo* model is applied for the whole  $\mathbb{R}^3$ , i.e.*

$$\rho(x) = d e^{-\alpha_\infty |x|}, \quad c = c_\infty, \quad x \in \mathbb{R}^3.$$

*In this case, with  $\gamma \geq 0$ , the normalized wavenumber is given by (4.15), and we have specific expression for the resolvent of the conjugated operator  $\mathcal{L}$ . For<sup>23</sup>  $g \in \mathfrak{B}$ , cf. (4.140)–(4.141),*

$$\begin{aligned} \mathfrak{R}_{\omega^2}(\mathbf{k}^2) g &= \tilde{\mathcal{R}}(\mathbf{k}^2) g = \int_{y \in \mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) g(y) dy, \quad \text{Im } \mathbf{k}^2 \neq 0, \\ \mathfrak{R}_{\omega_0^2}(\mathbf{k}_0^2) g &= \tilde{\mathcal{R}}^+(\mathbf{k}_0^2) g = \int_{y \in \mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) g(y) dy, \quad \mathbf{k}_0 > 0. \end{aligned}$$

*Under the current assumption, density  $\rho$  decays exponentially, thus for  $f \in L^2(\mathbb{R}^3)$ ,  $\rho^{1/2}f$  satisfies condition  $\rho^{1/2}f \in \mathfrak{B}$  without attenuation and  $\rho^{1/2}f \in L^2$  for the case with attenuation. In another word, one*

<sup>23</sup>stronger assumptions are either  $L_\sigma^2$  with  $\sigma > 1/2$  or simply  $L_{\text{comp}}^2$ .

can readily apply the constructed resolvent  $\tilde{\mathcal{R}}(\mathbf{k}^2)$  to  $\rho^{1/2}f$ . The outgoing solution  $u$  to  $\mathcal{L}_{\text{orig}}u = f$  with  $f \in L^2(\mathbb{R}^3)$  is then given by

$$\begin{aligned} u &= d e^{-\frac{\alpha_\infty}{2}|x|} \int_{y \in \mathbb{R}^3} \Phi_{\mathbf{k}}(x, y) e^{-\frac{\alpha_\infty}{2}|y|} f(y) dy \quad , \quad \text{Im } \mathbf{k}^2 \neq 0, \\ u &= d e^{-\frac{\alpha_\infty}{2}|x|} \int_{y \in \mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) e^{-\frac{\alpha_\infty}{2}|y|} f(y) dy \quad , \quad \mathbf{k}_0 > 0. \end{aligned} \quad (5.2)$$

For convenience, we recall here the explicit kernel given in (4.70),

$$\Phi_{\mathbf{k}}(x, y) := -\frac{\Gamma(1+\chi)}{4\pi|x-y|} \begin{vmatrix} W_{-\chi, 1/2}(-i\mathbf{k}s) & M_{-\chi, 1/2}(-i\mathbf{k}t) \\ W'_{-\chi, 1/2}(-i\mathbf{k}s) & M'_{-\chi, 1/2}(-i\mathbf{k}t) \end{vmatrix},$$

with the auxiliary variable defined in (4.71),

$$s = |x| + |y| + |x - y| \quad , \quad t = |x| + |y| - |x - y|.$$

The normalized wavenumber (4.15) is

$$\begin{aligned} \mathbf{k} &:= \mathfrak{g}_2 \left( \frac{\omega^2}{c^2} - \frac{\alpha^2}{4} \right) = \mathfrak{g}_2 \left( \frac{\omega_0^2}{c^2} - \frac{\alpha^2}{4} + i \frac{\gamma}{c^2} \omega_0^2 \right); \\ \eta &:= \frac{\alpha}{2\mathbf{k}} \quad ; \quad \chi := i\eta. \end{aligned}$$

The outgoing resolvent without absorption (i.e.  $\gamma = 0$ ) is given in (4.75) as a limit as  $\gamma \rightarrow 0^+$  of the above kernel,

$$\Phi_{\mathbf{k}_0}^+(x, y) = -\frac{\Gamma(1+\chi_0)}{4\pi|x-y|} \begin{vmatrix} W_{-\chi, 1/2}(-i\mathbf{k}_0 s) & M_{-\chi, 1/2}(-i\mathbf{k}_0 t) \\ W'_{-\chi, 1/2}(-i\mathbf{k}_0 s) & M'_{-\chi, 1/2}(-i\mathbf{k}_0 t) \end{vmatrix}. \quad \triangle$$

## 5.2 Expansion of outgoing solutions to the homogeneous equation in the Atmo model

In this case, we consider equation  $\mathcal{L}_{\text{orig}}u_{\text{orig}} = 0$  in the exterior of a sphere  $\mathbb{B}_{(0,R)}$  with  $R \geq R_a$ . Recall in this case that the sound speed  $c$  is constant as well as density height scale  $H(r)$  and  $\alpha(r) = \frac{1}{H(r)}$ . To be consistent with the notation from the general case, we will work with notation

$$c(r) = c_\infty \quad , \quad \alpha(r) = \alpha_\infty.$$

The wavenumber  $\mathbf{k}$  in this case is given in (4.15)

$$\mathbf{k} = \sqrt{\frac{\omega_0^2}{c^2} - \frac{\alpha^2}{4} + i \frac{\gamma}{c^2} \omega_0^2} \quad ; \quad \chi = \frac{i\alpha}{2\mathbf{k}} \quad , \quad \gamma \geq 0.$$

The relation between  $u_{\text{orig}}$  solution to

$$-\nabla \cdot (\rho^{-1} \nabla u) - \frac{\omega^2}{\rho c_\infty^2} u = 0$$

and  $u$  solution to the conjugated problem  $\mathcal{L}u = 0$  is  $u_{\text{orig}} = \rho^{1/2}w$ . With

$$\rho = \rho_{\mathbf{S}}(R_a) \exp(-\alpha_\infty|x|),$$

in the **Atmo** model, this relation has the form,

$$u_{\text{orig}} = e^{-\frac{1}{2}\alpha_\infty|x|} \sqrt{\rho_{\mathbf{S}}(R_a)} u,$$

where  $|x|u$  is described in terms of the Whittaker functions, cf. Prop 21. In short, in  $R_a < r < R'_a$ ,  $u_{\text{orig}}$  is given by

$$u_{\text{orig}}(x) = \frac{e^{-\frac{\alpha_\infty}{2}|x|}}{|x|} \sum_{\ell=0}^{\infty} \sum_{m=-1}^{\ell} a_\ell^m W_{-\chi, \ell+\frac{1}{2}}(-2ik|x|) Y_\ell^m(\theta, \phi).$$

Without attenuation, the wavenumber reduces to

$$k_0 = \sqrt{\frac{\omega_0^2}{c^2} - \frac{\alpha_\infty^2}{4}}, \quad \chi = \frac{i\alpha_\infty}{2k_0}.$$

A general outgoing solution to (1.1) in  $r > R_a$  is given by

$$u_{\text{orig}}^{\text{out}}(x) = \frac{e^{-\frac{\alpha_\infty}{2}|x|}}{|x|} \sum_{\ell=0}^{\infty} \sum_{m=-1}^{\ell} a_\ell^m W_{-\chi_0, \ell+\frac{1}{2}}(-2ik_0|x|) Y_\ell^m(\theta, \phi),$$

while an incoming one by

$$u_{\text{orig}}^{\text{in}}(x) = \frac{e^{-\frac{\alpha_\infty}{2}|x|}}{|x|} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_\ell^m W_{\chi_0, \ell+\frac{1}{2}}(2ik_0|x|) Y_\ell^m(\theta, \phi).$$

### 5.3 Exact D-t-N in the Atmo model

Under the same notation as in previous subsection, i.e. we work with constants  $R_a > 0$ ,  $c_\infty > 0$ ,  $\alpha_\infty > 0$  and  $d > 0$ ,

$$\rho(r) = d \exp(-\alpha_\infty|x|) \quad , \quad R > R_a,$$

and consider equation

$$-\nabla \cdot (\rho^{-1} \nabla u) - \frac{\omega^2}{\rho c_\infty^2} u = 0, \quad \text{in } \mathbb{R}^3 \setminus \mathbb{B}_{(0,R)}.$$

Recall that the constant  $R_a$  represents the height of the atmosphere, and  $d = \rho_S(R_a)$  with  $\rho_S$  from model S. Also denote the boundary of  $\mathbb{B}_{(0,R_a)}$  by  $\Gamma$ .

**Proposition 23.** *The outer D-t-N along  $\Gamma$  associated with the above equation is given as*

$$\mathbf{T}_{\text{orig}}^+(u|_\Gamma) = \sum_{\ell=0}^{\infty} \gamma_\ell \sum_{m=-\ell}^{\ell} u_\ell^m Y_\ell^m(\theta, \phi), \quad (5.3)$$

where  $u_\ell^m$  are the coefficients of the expansion of  $u|_\Gamma$  in the spherical harmonic basis  $Y_\ell^m$ , i.e.

$$u|_\Gamma(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_\ell^m Y_\ell^m(\theta, \phi), \quad (5.4)$$

$$\text{with } u_\ell^m := \int_0^\pi \int_0^{2\pi} u(R, \theta, \phi) \overline{Y_\ell^m(\theta, \phi)} \sin \theta d\phi d\theta,$$

and  $\gamma_\ell^{\text{orig}}$  are called the radiation impedance coefficients of  $\mathbf{T}_{\text{orig}}^+$  at level  $\ell$ ,

$$\gamma_\ell^{\text{orig}} := -\frac{1}{R} - \frac{\alpha_\infty}{2} - 2ik \frac{W'_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}{W_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}, \quad \eta = \frac{\alpha_\infty}{2k}. \quad (5.5)$$

with  $k$  defined in (4.15).

*Proof.* From Prop 21, an outgoing solution  $u_{\text{out}}$  to  $\mathcal{L}_{\text{orig}}u = 0$  in  $R \leq |x| \leq R'$  is given by

$$u_{\text{out}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell}^m \frac{e^{-\frac{\alpha_{\infty}}{2}|x|}}{|x|} W_{-\chi, \ell+\frac{1}{2}}(-2ik|x|) Y_{\ell}^m(\theta, \phi) \quad , \quad \chi = \frac{i\alpha_{\infty}}{2k}.$$

The sequence  $a_{\ell}^m$  is next determined from the (outer Dirichlet trace of  $u_{\text{outgoing}}$  along  $\Gamma$  given by  $u|_{\Gamma}$ . Upon imposing the boundary condition on each mode  $(m, \ell)$ , with  $u_{\ell}^m$  given in (5.4), we obtain

$$a_{\ell}^m \frac{e^{-\frac{\alpha_{\infty}}{2}R}}{R} W_{-\chi, \ell+\frac{1}{2}}(-2ikR) = u_{\ell}^m. \quad (5.6)$$

Since the series converges absolutely and uniformly in  $R \leq |x| \leq R'$ , we differentiate term-by-term in the radial direction to obtain the outer normal trace  $u_{\text{out}}$  along  $\Gamma$ ,

$$\begin{aligned} \partial_n u_{\text{out}}|_{\Gamma}^+ &= - \sum_{\ell=0}^{\infty} \sum_{m=\ell}^{\ell} a_{\ell}^m e^{-\frac{\alpha_{\infty}}{2}R} \left( \frac{W_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}{R^2} \right. \\ &\quad \left. + \frac{\alpha_{\infty}}{2} \frac{W_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}{R} + 2ik \frac{W'_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}{R} \right) Y_{\ell}^m(\theta, \phi). \end{aligned}$$

Replace  $a_{\ell}^m$  by expression (5.6), with simplification we obtain

$$\partial_n u_{\text{out}}|_{\Gamma}^+ = - \sum_{\ell=0}^{\infty} \sum_{m=\ell}^{\ell} u_{\ell}^m \left( \frac{1}{R} + \frac{\alpha_{\infty}}{2} + 2ik \frac{W'_{-i\eta, \ell+\frac{1}{2}}(-2ikR)}{W_{-i\eta, \ell+\frac{1}{2}}(-2ikR)} \right) Y_{\ell}^m(\theta, \phi).$$

□

## 6 Radiation Boundary Conditions (RBC) in the Atmo model

The framework of potential scattering gives rise to the normalized wavenumber  $k$  (2.18), which is (4.15) in the **Atmo** model. The defined ‘outgoing’ conjugated solution is shown to satisfy a Sommerfeld-type radiation condition with in terms of  $k$  (and not the original complex frequency  $\omega$  (4.13)). In this section, we compare how two approaches affect the form of the radiation boundary condition and the choice of gauge function (or ‘parameters of interest’) in approximating the transparent nonlocal condition, with some preliminary numerical experiments in Subsection 6.6. Another novelty of the current discussion is the **Whittaker** function family, which allows for the evaluation of the *exact* D-t-N impedance coefficient, cf. Prop 23. We thus have a true reference coefficient, in addition to the nonlocal transparent one (see below discussion). Another important point is that this is defined for the case with or without absorption. Lack of the true D-t-N, a numerical approximation was employed in [5] to create a reference solution, however is only applicable in the case of absorption  $\gamma > 0$ .

More in-depth discussion and numerical analysis are reserved to a following up report. For the current discussion, we restrict ourselves to the atmosphere described by the **Atmo** model. We expect that in the general case (under applicable assumption), the minimal condition  $\partial_r u - iku = 0$  should work as well as the zeroth-order Sommerfeld radiation condition for the Helmholtz equation. On the other hand, from the theoretical analysis, it does not come as a surprise that condition  $\partial_r u - i\omega u = 0$  does not capture the oscillatory behavior of the solution and hence fails to distinguish between the incoming and outgoing one.

**Notation** We denote  $(\cdot)^{1/2}$  the choice of square root  $\mathbf{g}_1$  (4.11a), (i.e. the Principal branch) with  $\text{Arg}_1(z) \in (-\pi, \pi]$ .

## 6.1 Relations among RBCs

We first recall that under separation of variables, the original problem (2.1),

$$\left( -\nabla \cdot (\rho^{-1} \nabla u) - \frac{\omega^2}{\rho c_\infty^2} \right) u_{\text{orig}} = 0, \quad (6.1)$$

gives, on each mode  $(\ell, m)$ ,

$$\left( -\frac{d^2}{dr^2} - \left( \frac{2}{r} + \alpha_\infty \right) \frac{d}{dr} - \frac{\omega^2}{c_\infty^2} + \frac{\ell(\ell+1)}{r^2} \right) [u_{\text{orig}}]_\ell^m = 0. \quad (6.2)$$

On the other hand, under the change of unknown (2.3) (relisted below in (6.8)) the original problem becomes the conjugated problem (4.2),

$$\left( -\Delta - \frac{\omega^2}{c^2} + \frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{r} \right) u = 0. \quad (6.3)$$

This gives, on each mode  $\ell$ , the ODE (4.3)

$$\left( -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) u_\ell^m = 0. \quad (6.4)$$

We further remove the first-order term and work with

$$\left( -\frac{d^2}{dr^2} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) w_\ell^m = 0. \quad (6.5)$$

This is called the reduced 1D problem. Note that this problem is only defined on each mode.

In summary, we have the following quantities and equations.

1.  $u_{\text{orig}}$  solves the original problem (6.1) in  $\mathbb{R}^3$ , which after separation of variables is equivalent to solving  $[u_{\text{orig}}]_\ell^m$  solution to the 1D (6.2)
2.  $u$  solves the conjugated problem (6.3) in  $\mathbb{R}^3$ , which after separation of variables is equivalent to  $u_\ell^m$  solution to the 1D (6.4).
3.  $w_\ell^m$  solves the reduced 1D problem (6.5).

The coefficients  $[u_{\text{orig}}]_\ell^m$ ,  $u_\ell^m$  and  $w_\ell^m$  are related by

$$[u_{\text{orig}}]_\ell^m = d e^{-\frac{\alpha_\infty}{2} r} u_\ell^m = d \frac{e^{-\frac{\alpha_\infty}{2} r}}{r} w_\ell^m, \quad (6.6)$$

$$u_\ell^m = r^{-1} w_\ell^m. \quad (6.7)$$

The 3D solutions of the original and conjugate problems are related by

$$u_{\text{orig}} = d e^{-\frac{\alpha_\infty}{2} r} u. \quad (6.8)$$

**Relations among the modal RBCs** The above relations (6.6) and (6.7) lead to the following relations among the RBCs of discussed ODEs. We denote by  $\mathbf{Z}_\bullet^\ell$  a *radiation impedance coefficient* in the Robin-type boundary condition

$$\boxed{\partial_r w = \mathbf{Z}_\bullet^\ell w, \quad w = w_\ell^m.} \quad (6.9)$$

used to truncate the reduced ODE (6.5) to a finite interval so that the resulting solution approximates the outgoing solution. The RBC for the ODE (6.4) is given by

$$\boxed{\partial_r u = -\frac{1}{R} u + \mathbf{Z}_\bullet^\ell u, \quad u = [u]_\ell^m.} \quad (6.10)$$

The RBC for the ODE (6.2) is given by

$$\boxed{\partial_r u = -\left( \frac{1}{R} + \frac{\alpha_\infty}{2} \right) u + \mathbf{Z}_\bullet^\ell u, \quad u = [u_{\text{orig}}]_\ell^m.} \quad (6.11)$$

**Relations between the 3D RBCs** To obtain the RBC in 3D for the conjugated problem (6.3), the terms involving  $\ell$  in  $\mathbf{Z}_\bullet^\ell$  will have to be reinterpreted as differential operators (or in fact pseudo-differential operators) in the tangential variables. Denote the resulting operators by  $\mathbf{Z}_\bullet$ , the RBC for (6.3) is

$$\partial_r \mathbf{u} = -\frac{1}{R} \mathbf{u} + \mathbf{Z}_\bullet \mathbf{u} \quad , \quad \mathbf{u} = u. \quad (6.12)$$

From relation (6.8), those for (6.1) are of the form

$$\partial_r \mathbf{u} = -\left(\frac{1}{R} + \frac{\alpha_\infty}{2}\right) \mathbf{u} + \mathbf{Z}_\bullet \mathbf{u} \quad , \quad \mathbf{u} = u_{\text{orig}}. \quad (6.13)$$

Exact radiation condition and its approximation were constructed in [5] by working directly with (6.1), and thus of the form (6.13) or the modal version (6.11) in radial symmetry. Same approach was used in [13], see Remark 27. On the other hand, we work with conjugated problem and thus 3D RBC of the form (6.10) or its completely reduced modal version (6.9) in radial symmetry.

**Remark 27.** *As in Remark 2, in the spherical symmetry, the completely reduced ODE (6.5) can be obtained from the original problem (6.1), by a separation of variable then a removal of the first order term  $(\frac{2}{r} + \alpha_\infty) \frac{d}{dr}$ , see Appendix A.2. This amounts to doing all-at-once the change of unknown  $w = r \rho^{-1/2} u_{\text{orig}}$ . This is mentioned in [13, Eqn 8]. However, for spherical symmetry, [13] employs the radiation conditions constructed in [5] using the original equation i.e. the ODE (6.2). They also employ the same idea to construct boundary conditions for cylindrical symmetry, cf. [13, section 3.2]. As a result, all of their radiation conditions (listed in Subsection 6.5), like those in [5] contain the term  $\frac{1}{R} + \frac{1}{2H}$  (which is  $\frac{1}{R} + \frac{\alpha_\infty}{2}$  in our current notation). This was also noted in [13], see the discussion right after Eqn (13) there.  $\triangle$*

## 6.2 Nonlocal modal radiation impedance coefficients

For convenience of discussion, we define

$$Q_\ell := \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} - \frac{\alpha_\infty}{r} - \frac{\ell(\ell+1)}{r^2} = k^2 - \frac{\alpha_\infty}{r} - \frac{\ell(\ell+1)}{r^2}. \quad (6.14)$$

Recall that  $\omega$  and  $k$  are given by (4.13) and (4.15) respectively using the second branch  $\mathbf{g}_2$ . See also Remark 17 for the case  $\gamma \geq 0$ .

In the current discussion, we work with nonnegative absorption  $\gamma \geq 0$ . We rewrite (6.5) using the quantity  $Q_\ell$  as

$$\frac{d^2}{dr^2} w_\ell^m = -Q_\ell w_\ell^m.$$

Define the nonlocal radiation impedance coefficient,

$$\mathbf{Z}_{\text{nonlocal}}^\ell := i \mathbf{g}_1(Q_\ell).$$

In [5], the outgoing wave at  $\partial \mathbb{B}_{(0,R)}$  is defined by condition,

$$\partial_r [u_{\text{orig}}]_\ell^m = \left( -\frac{1}{R} - \frac{\alpha_\infty}{2} + \mathbf{Z}_{\text{exact,S}} \right) [u_{\text{orig}}]_\ell^m, \quad (6.15)$$

while that for the conjugated problem is

$$\partial_r w_\ell^m = \mathbf{Z}_{\text{nonlocal}}^\ell w_\ell^m. \quad (6.16)$$

With  $(\cdot)^{1/2} = \mathbf{g}_1(\cdot)$  and  $\gamma \geq 0$ , we will verify below that  $\mathbf{Z}_{\text{exact}}$  can be written as

$$\begin{aligned} \mathbf{Z}_{\text{nonlocal}}^\ell &= i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) \right)^{1/2} \\ &= i k \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right)^{1/2}. \end{aligned} \quad (6.17)$$

Verification of (6.17) We can write

$$Q_\ell = \frac{\omega^2}{c_\infty^2} \left( 1 - \frac{\alpha_\infty^2}{4} \frac{c_\infty^2}{\omega^2} - \frac{\alpha_\infty}{r} \frac{c_\infty^2}{\omega^2} - \frac{\ell(\ell+1)}{r^2} \frac{c_\infty^2}{\omega^2} \right).$$

Since  $\omega^2 = \omega_0^2 + i\gamma$ , and  $\gamma \geq 0$ , we have  $\text{Arg}_1(Q_\ell) \in [0, \pi]$  and  $\text{Arg}_1\left(\frac{\omega^2}{c_\infty^2}\right) \in [0, \frac{\pi}{2}]$ , thus

$$\text{Arg}_1(Q_\ell) - \text{Arg}_1\left(\frac{\omega^2}{c_\infty^2}\right) \in \left[-\frac{\pi}{2}, \pi\right] \subset (-\pi, \pi].$$

With property (J.4) satisfied, and the second statement of Prop 33 gives

$$\mathfrak{g}_1(Q_\ell) = \mathfrak{g}_1\left(\frac{\omega^2}{c_\infty^2}\right) \mathfrak{g}_1\left(1 - \frac{c_\infty^2}{\omega^2} \left(\frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2}\right)\right).$$

With this, we obtain the first equality in (6.17) by now using Remark 17 which gives the equality of the two branches  $\mathfrak{g}_1$  and  $\mathfrak{g}_2$  under the current assumption  $\gamma \geq 0$ .

We can also factor  $Q_\ell$  in terms of  $k^2$ ,

$$Q_\ell = k^2 \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right).$$

However, by its definition,  $\text{Re } k^2$  can be positive or negative, thus

$$\text{Arg}_1(k^2) \in [0, \pi] \quad \text{and} \quad \text{Arg}_1(Q_\ell) - \text{Arg}_1(k^2) \in [-\pi, \pi].$$

The above quantity can only take on value  $-\pi$  when  $Q_\ell > 0$  and  $k^2 < 0$ . This cannot happen, since

$$\alpha_\infty > 0, \ell \geq 0 \Rightarrow k^2 > Q_\ell.$$

As a result, assumption (J.4) is satisfied, and the second statement of Prop 33 gives

$$\mathfrak{g}_1(Q_\ell) = \mathfrak{g}_1(k^2) \mathfrak{g}_1\left(\frac{Q_\ell}{k^2}\right).$$

As before, we obtain the second equality in (6.17) by using Remark 17. □

### 6.3 New approximations of the nonlocal modal radiation impedance coefficients

Approximate radiation boundary conditions were constructed in [5], by asymptotic expansion of

$$\left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty^2}{4} - \frac{\alpha_\infty}{r} - \frac{\ell(\ell+1)}{r^2} \right) \right)^{1/2},$$

using as small quantities (also called as *gauge function*)  $\omega$  or  $\frac{\ell(\ell+1)}{R_a^2 \omega^2}$ . Approximation obtained with the second quantity is called small-angle-incidence (SAI) approximation. Here we will approximate

$$\left( 1 - \frac{1}{k^2} \left( \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) \right)^{1/2}$$

using  $k$  or SAI like quantities defined in terms of  $k$  as gauge functions. We will use expansion (J.9) in Appendix J.3,

$$\begin{aligned} \mathfrak{g}_1(-z+1) &= \sum_{k=0}^{\infty} \binom{1/2}{k} (-z)^k = 1 + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k 2^{2k-1}} \binom{2k-2}{k-1} (-z)^k \\ &= 1 - \frac{1}{2}z - \frac{1}{8}z^2 - \frac{1}{16}z^3 - \frac{5}{128}z^4 + \dots, \quad |z| < 1. \end{aligned}$$



Approach 1 With the small quantity (gauge function) as

$$\varepsilon = \frac{1}{k^2} \left( \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right),$$

we obtain as first-order approximation,

$$\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right)^{1/2} = 1 + \mathcal{O}(\varepsilon), \quad (6.18)$$

and second-order approximation,

$$\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right)^{1/2} = 1 - \frac{1}{2} \frac{1}{k^2} \left( \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) + \mathcal{O}(\varepsilon^2). \quad (6.19)$$

If we assume further that

$$\frac{\ell(\ell+1)}{r} \ll \alpha_\infty,$$

then we have the following approximation,

$$\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right)^{1/2} \sim 1 - \frac{1}{2} \frac{1}{k^2} \frac{\alpha_\infty}{r}. \quad (6.20)$$

Approach 2 Another approach is to write

$$\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(rk)^2} \right)^{1/2} = \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} \right)^{1/2} \left( 1 - \frac{\frac{\ell(\ell+1)}{(rk)^2}}{1 - \frac{\alpha_\infty}{r} \frac{1}{k^2}} \right)^{1/2}.$$

The small quantity is considered as

$$\varepsilon = \frac{\frac{\ell(\ell+1)}{(rk)^2}}{1 - \frac{\alpha_\infty}{r} \frac{1}{k^2}}.$$

The first order approximation gives

$$\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{2k^2} \right)^{1/2} (1 + \mathcal{O}(\varepsilon)), \quad (6.21)$$

while the second one gives

$$\begin{aligned} & \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} \right)^{1/2} \left( 1 - \frac{1}{2} \frac{\frac{\ell(\ell+1)}{(rk)^2}}{1 - \frac{\alpha_\infty}{r} \frac{1}{k^2}} + \mathcal{O}(\varepsilon^2) \right) \\ &= \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} \right)^{1/2} - \frac{1}{2} \frac{\frac{\ell(\ell+1)}{(rk)^2}}{\left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} \right)^{1/2}} + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (6.22)$$

In summary, we gather the results of (6.18) – (6.22), which were obtained by using the new gauge

function  $k$  and multiply with  $ik$ . Here  $R_a$  is the radius of artificial boundary  $\Gamma_a = \partial\mathbb{B}_{(0,R_a)}$ .

$$\begin{aligned}
\mathbf{Z}_{\text{S-HF-0}} &\stackrel{(6.18)}{=} ik \quad ; \\
\mathbf{Z}_{\text{S-HF-1a}} &\stackrel{(6.19)}{=} ik - \frac{i}{2k} \frac{1}{R_a} \alpha_\infty \quad ; \\
\mathbf{Z}_{\text{S-HF-1b}}^\ell &\stackrel{(6.20)}{=} ik - \frac{i}{2k} \frac{1}{R_a} \left( \alpha_\infty + \frac{\ell(\ell+1)}{R_a} \right) \quad ; \\
\mathbf{Z}_{\text{S-SAI-0}}^\ell &\stackrel{(6.21)}{=} ik \left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2} \quad ; \\
\mathbf{Z}_{\text{S-SAI-1}}^\ell &\stackrel{(6.22)}{=} ik \left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2} - \frac{i}{2} \frac{\frac{\ell(\ell+1)}{R_a^2 k}}{\left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2}} .
\end{aligned} \tag{6.23}$$

#### 6.4 Coefficients from literature

We recall the coefficients obtained in [5] and [13] (by using  $\omega$  as the gauge function).

$$\begin{aligned}
\mathbf{Z}_{\text{A-HF-0}} &= i \frac{\omega}{c_\infty} \quad , \\
\mathbf{Z}_{\text{A-HF-1}}^\ell &= i \frac{\omega}{c_\infty} + \frac{c_\infty}{2i\omega} \left( \frac{\ell(\ell+1)}{R_a^2} + \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \quad ,
\end{aligned}$$

and

$$\begin{aligned}
\mathbf{Z}_{\text{A-SAI-0}}^\ell &= i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2} \quad , \\
\mathbf{Z}_{\text{A-SAI-1}}^\ell &= i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2} + \frac{\frac{c_\infty}{2i\omega} \frac{\ell(\ell+1)}{R_a^2}}{\left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2}} .
\end{aligned}$$

The two SAI families, A-SAI and S-SAI, turn out to coincide. This is verified below,

$$\begin{aligned}
\mathbf{Z}_{\text{A-SAI-0}}^\ell &= i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2} = i \left( \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty}{R_a} - \frac{\alpha_\infty^2}{4} \right)^{1/2} \\
&= i \left( k^2 - \frac{\alpha_\infty}{R_a} \right)^{1/2} = ik \left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2} = \mathbf{Z}_{\text{S-SAI-0}}^\ell .
\end{aligned}$$

It remains to verify the second term in the A-SAI-1.

$$\begin{aligned}
\frac{\frac{c_\infty}{2i\omega} \frac{\ell(\ell+1)}{R_a^2}}{\left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2}} &= \frac{\frac{1}{2i} \frac{\ell(\ell+1)}{R_a^2}}{\frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right) \right)^{1/2}} \\
&= \frac{\frac{1}{2i} \frac{\ell(\ell+1)}{R_a^2}}{\left( k^2 - \frac{\alpha_\infty}{R_a} \right)^{1/2}} = -\frac{i}{2} \frac{\frac{1}{2i} \frac{\ell(\ell+1)}{R_a^2} k}{\left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2}} .
\end{aligned}$$

We will thus only use one notation for them

$$\begin{aligned}
\mathbf{Z}_{\text{SAI-0}}^\ell &= \mathbf{Z}_{\text{A-SAI-0}}^\ell = \mathbf{Z}_{\text{S-SAI-0}}^\ell ; \\
\mathbf{Z}_{\text{SAI-1}}^\ell &= \mathbf{Z}_{\text{A-SAI-1}}^\ell = \mathbf{Z}_{\text{S-SAI-1}}^\ell .
\end{aligned} \tag{6.24}$$

Another condition suggested in [5] is obtained by removing all terms involving  $\frac{1}{R_a}$  in coefficient  $\mathbf{Z}_{\mathbf{A-SAI-1}}^\ell$  and working with original modal (6.2). In particular, from the condition, at an artificial boundary  $r = R_a$ ,

$$\partial_r \mathbf{u} = - \left( \frac{1}{R_a} + \frac{\alpha_\infty}{2} \right) \mathbf{u} + \mathbf{Z}_{\mathbf{A-SAI-1}}^\ell \mathbf{u} \quad , \quad \mathbf{u} = u_\ell^m, \quad (6.25)$$

the new condition called **Atmo RBC 1** is created by dropping all terms with  $\frac{1}{R_a}$  (still using with ODE (6.2))

$$\partial_r \mathbf{u} = \left( -\frac{\alpha_\infty}{2} + i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{4 \omega^2} \right)^{1/2} \right) \mathbf{u} \quad , \quad \text{for } \mathbf{u} = [u_{\text{orig}}]_\ell^m. \quad (6.26)$$

In our notation<sup>24</sup>

$$\mathbf{Z}_{\mathbf{A-RBC-1}} := \frac{1}{R_a} + i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{4 \omega^2} \right)^{1/2} = \frac{1}{R_a} + \mathbf{Z}_{\mathbf{S-HF-0}}. \quad (6.29)$$

See also Remark 28.

**Remark 28.** In our analysis, we know that in condition (6.25) the first factor  $\frac{1}{R_a}$  does not play the same role as in the other  $\frac{1}{R_a}$  appearing in the definition of  $\mathbf{Z}_{\mathbf{A-SAI-1}}^\ell$ . The first one is crucial and appears in both outgoing and incoming solution, i.e. part of every solution, while those in  $\mathbf{Z}_{\mathbf{A-SAI-1}}^\ell$  actually contribute to distinguishing the incoming from the outgoing one. We thus suggest using the same idea but however dropping only the  $\frac{1}{R_a}$  term in  $\mathbf{Z}_{\mathbf{A-SAI-1}}^\ell$ , and work with

$$i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{\omega^2 4} \right)^{1/2}.$$

But this turns out to be

$$i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{\omega^2 4} \right)^{1/2} = i \left( \frac{\omega^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} \right)^{1/2} = i k = \mathbf{Z}_{\mathbf{S-HF-0}}. \quad \triangle$$

We also put in our notation a modal radiation boundary condition called **Naive Sommerfeld** discussed in [5] and [13]. In particular, at an artificial boundary  $r = R_a$ , the following RBC

$$\partial_r \mathbf{u} = i \frac{\omega}{c_\infty} \mathbf{u} \quad , \quad \text{for } \mathbf{u} = [u_{\text{orig}}]_\ell^m, \quad (6.30)$$

is applied to ODE (6.2). In our notation, this is equivalent<sup>25</sup> to working impedance coefficient defined as

$$\mathbf{Z}_{\text{Naive}} := \frac{1}{R_a} + \frac{\alpha_\infty}{2} + i \frac{\omega}{c_\infty}. \quad (6.33)$$

<sup>24</sup>Using **A-RBC-1** with the original modal ODE (6.2) is equivalent to working with the conjugated modal ODE (6.4) and RBC,

$$\partial_r \mathbf{u} = \left( \frac{1}{R_a} + i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{4 \omega^2} \right)^{1/2} \right) \mathbf{u} \quad , \quad \text{for } \mathbf{u} = u_\ell^m. \quad (6.27)$$

or the reduced ODE (6.5) and RBC,

$$\partial_r \mathbf{u} = i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2 \alpha_\infty^2}{4 \omega^2} \right)^{1/2} \mathbf{u} \quad , \quad \text{for } \mathbf{u} = w_\ell^m. \quad (6.28)$$

<sup>25</sup>Due to the relation (6.10)–(6.11) among the RBC among the three ODEs, working with the original modal ODE (6.2) and RBC (6.31) is equivalent to working with the conjugated modal ODE (6.4) and RBC,

$$\partial_r \mathbf{u} = \left( \frac{\alpha_\infty}{2} + i \frac{\omega}{c_\infty} \right) \mathbf{u} \quad , \quad \text{for } \mathbf{u} = u_\ell^m, \quad (6.31)$$

or the reduced ODE (6.5) and RBC,

$$\partial_r \mathbf{u} = \left( \frac{1}{R_a} + \frac{\alpha_\infty}{2} + i \frac{\omega}{c_\infty} \right) \mathbf{u} \quad , \quad \text{for } \mathbf{u} = w_\ell^m. \quad (6.32)$$

## 6.5 List of modal radiation impedance coefficients

For convenience of numerical comparison, we gather in a list all of the modal radiation impedance coefficients mentioned above. They are to be used in Robin-type boundary conditions (6.10), (6.10) or (6.11) according to the chosen problem (reduced (6.5), conjugated modal (6.4), or original modal (6.2) respectively). The 3D versions are (6.12) for the conjugated problem (6.3), or (6.13) for original problem (6.1). Recall that  $(\cdot)^{1/2}$  to mean the choice of square root  $\mathfrak{g}_1$  (4.11a), (i.e. the Principal branch) i.e. with  $\text{Arg}_1(z) \in (-\pi, \pi]$ .

1. The reference coefficient  $\mathbf{Z}_{\text{DtN}}^\ell$  comes from the modal D-t-N coefficients (6.17)  $\gamma_\ell$  cf. (4.182), see also Prop 23 or 22,

$$\mathbf{Z}_{\text{DtN}}^\ell := -2ik \frac{W'_{-\chi, \ell + \frac{1}{2}}(-2ikR_a)}{W_{-\chi, \ell + \frac{1}{2}}(-2ikR_a)} \quad , \quad \chi = \frac{i\alpha_\infty}{2k}. \quad (6.34)$$

Note that this is the DtN impedance coefficient for the reduced ODE 6.5.

2. The nonlocal modal radiation coefficient  $\mathbf{Z}_{\text{nonlocal}}^\ell$  is the same in both approaches (either using  $\omega$  or  $k$ ) and is given (6.17),

$$\begin{aligned} \mathbf{Z}_{\text{nonlocal}}^\ell &= i \frac{\omega}{c_\infty} \left( 1 - \frac{c_\infty^2}{\omega^2} \left( \frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{R_a} + \frac{\ell(\ell+1)}{R_a^2} \right) \right)^{1/2} \\ &= ik \left( 1 - \frac{\alpha_\infty}{r} \frac{1}{k^2} - \frac{\ell(\ell+1)}{(R_a k)^2} \right)^{1/2}. \end{aligned}$$

3. The HF family

$$\begin{aligned} \mathbf{Z}_{\text{S-HF-0}} &\stackrel{(6.18)}{=} ik \quad ; \\ \mathbf{Z}_{\text{S-HF-1a}} &\stackrel{(6.19)}{=} ik - \frac{i}{2k} \frac{1}{R_a} \alpha_\infty \quad ; \\ \mathbf{Z}_{\text{S-HF-1b}}^\ell &\stackrel{(6.20)}{=} ik - \frac{i}{2k} \frac{1}{R_a} \left( \alpha_\infty + \frac{\ell(\ell+1)}{R_a} \right) \quad ; \\ \mathbf{Z}_{\text{A-HF-0}} &= i \frac{\omega}{c_\infty} \quad ; \\ \mathbf{Z}_{\text{A-HF-1}}^\ell &= i \frac{\omega}{c_\infty} + \frac{c_\infty}{2i\omega} \left( \frac{\ell(\ell+1)}{R_a^2} + \frac{\alpha_\infty}{R_a} + \frac{\alpha_\infty^2}{4} \right). \end{aligned} \quad (6.35)$$

4. The SAI family

$$\begin{aligned} \mathbf{Z}_{\text{SAI-0}} &\stackrel{(6.21)}{=} ik \left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2} \quad ; \\ \mathbf{Z}_{\text{SAI-1}}^\ell &\stackrel{(6.22)}{=} ik \left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2} - \frac{i}{2} \frac{\frac{\ell(\ell+1)}{R_a^2 k}}{\left( 1 - \frac{\alpha_\infty}{R_a} \frac{1}{k^2} \right)^{1/2}}, \end{aligned} \quad (6.36)$$

and

$$\mathbf{Z}_{\text{A-RBC-1}} := \frac{1}{R_a} + \mathbf{Z}_{\text{S-HF-0}}. \quad (6.37)$$

5. We will also include the Naive Sommerfeld (in our notation)

$$\mathbf{Z}_{\text{Naive}} := \frac{1}{R_a} + \frac{\alpha_\infty}{2} + i \frac{\omega}{c_\infty}. \quad (6.38)$$

## 6.6 Numerical experiments

We test how well the radial ABC can approximate the outgoing solution given by the Whittaker function  $W$ . For simplicity, we work with the reduced ODE (6.5). In particular, we consider the truncated outer Dirichlet problem on  $R_{\min} \leq r \leq R_a$ ,

$$\begin{cases} \left( -\frac{d^2}{dr^2} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) w = 0 & , \quad R_{\min} \leq r \leq R_a; \\ w(R_{\min}) = 1; \\ w'(R_a) = \mathbf{Z}_\bullet w(R_a). \end{cases} \quad (6.39)$$

Here  $\mathbf{Z}_\bullet$  are given in the list of ABCs in (6.23). The numerical solutions corresponding to a coefficient  $\mathbf{Z}_\bullet$  is labeled as

$$w_{\mathbf{Z}_\bullet, \ell, \omega_0} \quad \text{or simply} \quad w_{\mathbf{Z}_\bullet},$$

if we ignore the dependence on  $\ell$  and  $\omega_0$ .

The above solutions will be compared with the exact solution,

$$w_{\text{ref}, \ell, \omega_0} = w_{\text{D-t-N}, \ell, \omega_0},$$

or simply written as

$$w_{\text{ref}} = w_{\text{D-t-N}}.$$

This is defined as the unique solution to problem,

$$\begin{cases} \left( -\frac{d^2}{dr^2} - k^2 + \frac{\alpha_\infty}{r} + \frac{\ell(\ell+1)}{r^2} \right) w_{\text{ref}} = 0 & , \quad R_{\min} \leq r \leq R_a; \\ w_{\text{ref}}(R_{\min}) = 1; \\ w_{\text{ref}} \text{ k - outgoing.} \end{cases} \quad (6.40)$$

The explicit expression for the analytic solution is,

$$w_{\text{ref}} = w_{\text{D-t-N}} = \frac{W_{-\chi, \ell + \frac{1}{2}}(-2ikr)}{W_{-\chi, \ell + \frac{1}{2}}(-2ikR_{\min})}. \quad (6.41)$$

We recall that with  $\mathfrak{g}_2(\cdot)$  the branch of square root using argument  $[0, \pi)$ ,

$$\chi = \frac{i\alpha_\infty}{2k} \quad , \quad k = \mathfrak{g}_2\left(\frac{\omega_0^2}{c_\infty^2} - \frac{\alpha_\infty^2}{4} + i\frac{\gamma}{c_\infty^2}\omega_0^2\right) \quad , \quad \omega = \omega_0 \mathfrak{g}_2(1 + i\gamma). \quad (6.42)$$

In our experiments, we fix the following parameters,

$$c_\infty = 3, \quad R_{\min} = 1, \quad R_a = 1.2, \quad \alpha_\infty = 50. \quad (6.43)$$

We will compare the solution in varying  $l$ ,  $\gamma$  and  $\omega_0$  (hence  $\omega$ ).

**Remark 29.** For the resolution of Problem (6.39), we employ a finite difference discretization of order six and the Whittaker function is computed using *Matlab* intrinsic function `whittakerW(.,.,.)`. However, despite our relatively common range of values, we already observe some numerical instability in the computation of Whittaker function in *Matlab*, these can be seen in Figures 19, 20, 21 and 22, with the artifact shapes near the cut-off frequency near  $\ell = 100$ . For more precise computations, we instead implemented the hypergeometric functions from the *arb* library, [22], within a *Fortran* interface in order to conduct similar experiments in [6].

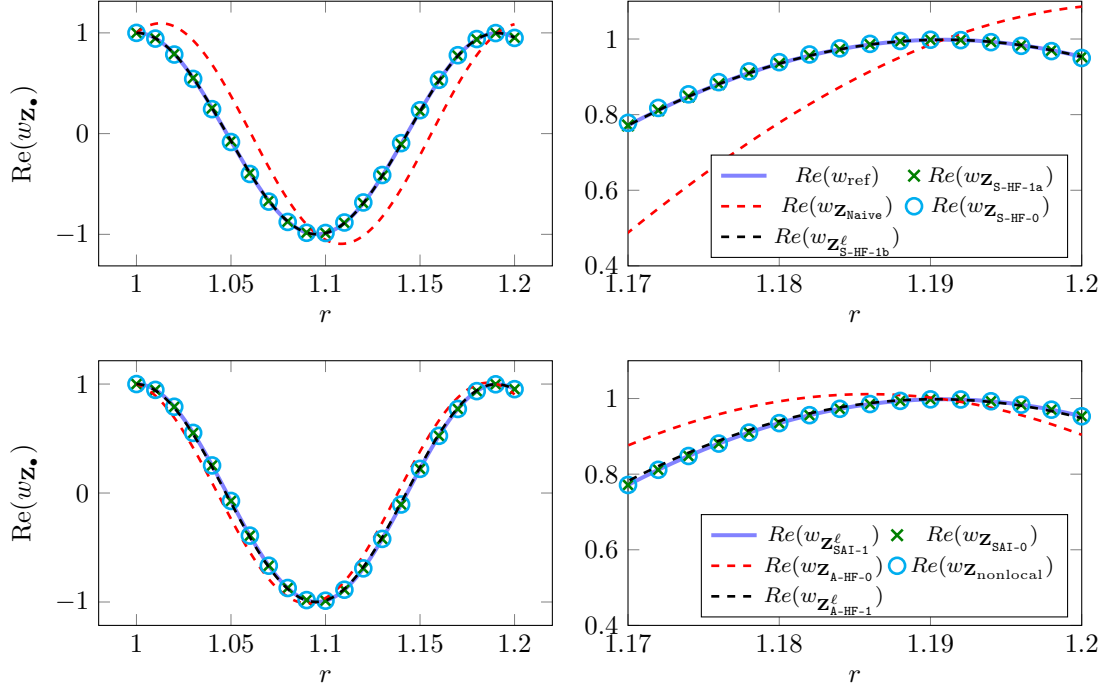


Figure 13: Comparison of  $w_{\mathbf{z}}$  solution to (6.39) on  $[1, 1.2]$  with the analytical solution  $w_{\text{ref}}$  in (6.41). Here the comparison is in terms of the real part of the solution. The parameters used are  $\omega_0 = 2\pi 20$ ,  $\alpha_\infty = 50$ ,  $l = 3$  and  $\gamma = 0$ . Evolution of the global profile (left) and zoom towards the end (right).

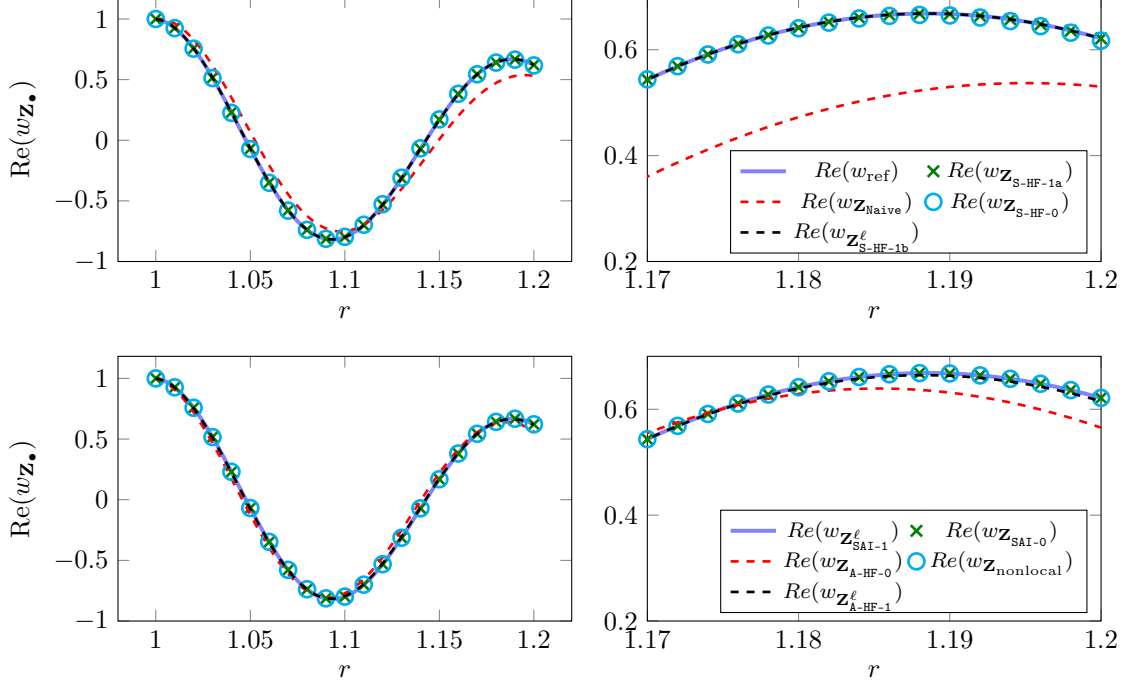


Figure 14: Comparison of  $w_{\mathbf{z}}$  solution to (6.39) on  $[1, 1.2]$  with the analytical solution  $w_{\text{ref}}$  in (6.41). Here the comparison is in terms of the real part of the solution. The parameters used are  $\omega_0 = 2\pi 20$ ,  $\alpha_\infty = 50$ ,  $l = 3$  and  $\gamma = 5$ . Evolution of the global profile (left) and zoom towards the end (right).

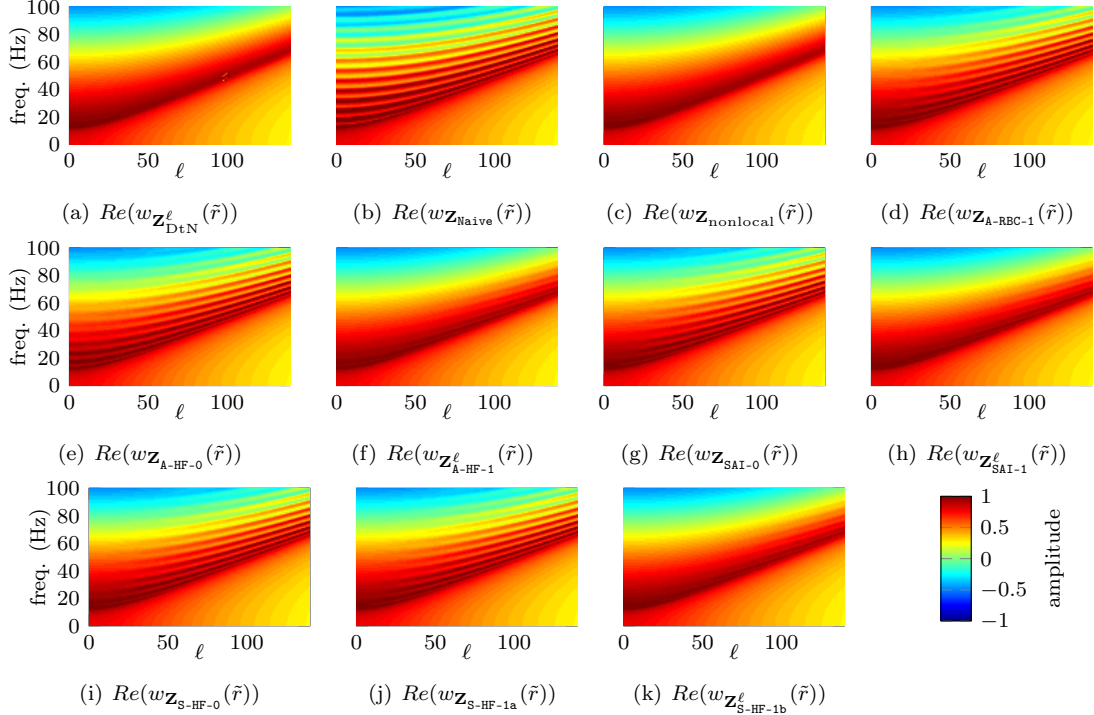


Figure 15: Comparison of the solutions  $Re(w_{\bullet, \ell, \omega_0}(\tilde{r}))$  as a function of the frequency  $\omega_0$  and  $\ell$  in  $\tilde{r} = 1.01$  without attenuation ( $\gamma = 0$ ).

**Experiment group 1** Here, for a chosen  $\ell = 3$  and  $\omega_0 = 2\pi 20$ , we plot  $w_{\bullet}$  on  $[R_{\min}, R_a]$  against the reference solution  $w_{\text{ref}}$  given in (6.41). This is carried out for  $\gamma = 5$  in Figure 14 and without attenuation, i.e.  $\gamma = 0$ , in 13. This comparison shows that the solutions can be grouped into two distinct groups. Lower accuracy coefficients are  $Z_{A-HF-0}$  and  $Z_{Naive}$ . The remaining coefficients belong to the higher accuracy group. However, within this group, the plots coincide with that of  $w_{\text{ref}}$ , and it is not possible to *visually* distinguish one from another.

**Experiment group 2** In order to have a better comparison, we compute the solutions for a wide range of  $\ell$  and frequencies  $\omega_0$  with  $\ell$  taking integer values between 0 to 140 and  $\omega_0$  varying from  $2\pi 1$  to  $2\pi 100$ . It results in 14 100 test-cases, which are then doubled due to the presence or absence of attenuation. There are three subgroups of figures.

1. We first plot the solution  $w_{\bullet, \ell, \omega_0}(r)$  in a fixed position  $r = 1.01$ , for every choice of  $\ell$  and  $\omega_0$ . In Figures 15 and 16, the results are shown for  $\gamma = 0$  and  $\gamma = 5$  respectively.
2. We proceed similarly for fixed point  $r = 1.10$  in Figures 17 and 18. This is closer to  $R_a$  and further away from  $R_{\min}$ .
3. We quantify the comparison in terms of errors. We consider global  $L^2$  error and error at a fixed point  $r$ ,

$$E_{\bullet}(\ell, \omega_0) := \frac{\|w_{\bullet, \ell, \omega_0} - w_{\text{ref}, \ell, \omega_0}\|_{L^2(R_{\min}, R_a)}}{\|w_{\text{ref}, \ell, \omega_0}\|_{L^2(R_{\min}, R_a)}}, \quad e_{\bullet}(\ell, \omega_0, r) := |w_{\bullet, \ell, \omega_0}(r) - w_{\text{ref}, \ell, \omega_0}(r)|. \quad (6.44)$$

The comparisons using error norm  $e_{\bullet}$  are shown in Figure 19 for  $\gamma = 0$  and 20 for  $\gamma = 5$ , while those using error norm  $E_{\bullet}$  are in Figures 21 for  $\gamma = 0$  and 22 for  $\gamma = 5$ .

From the pictures of the solutions in one position, i.e. in Figure 15 – 18 we can already observe some differences between the coefficients:

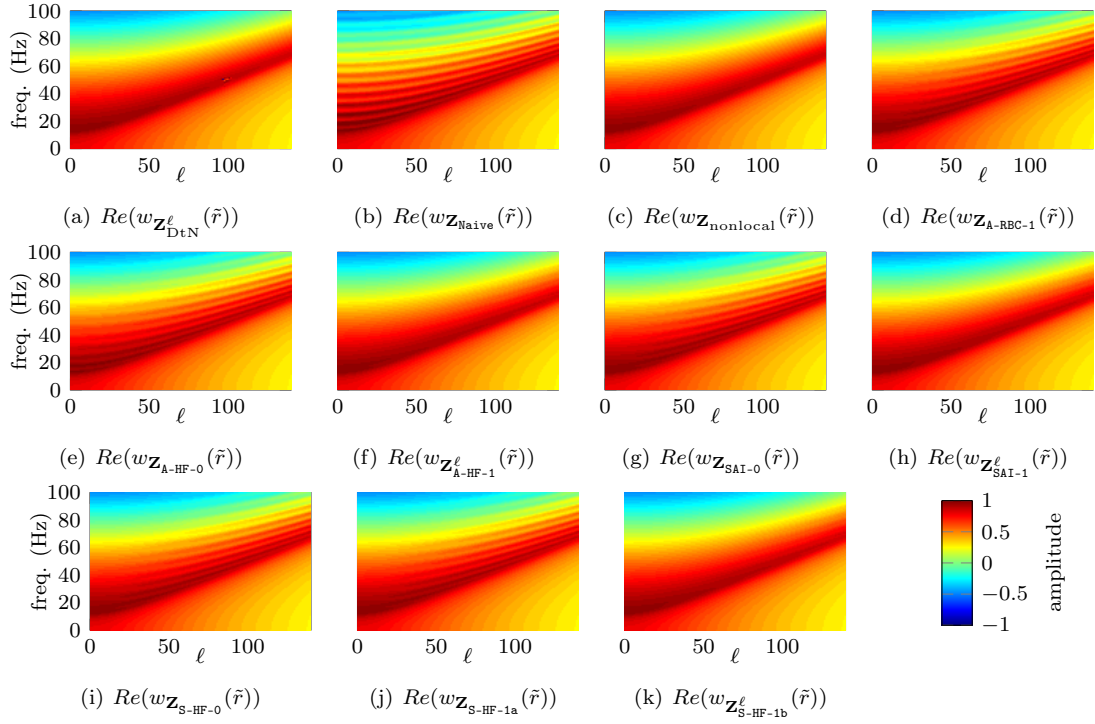


Figure 16: Comparison of the solutions  $Re(w_{\bullet, \ell, \omega_0}(\tilde{r}))$  as a function of the frequency  $\omega_0$  and  $\ell$  in  $\tilde{r} = 1.01$  with attenuation  $\gamma = 5$ .

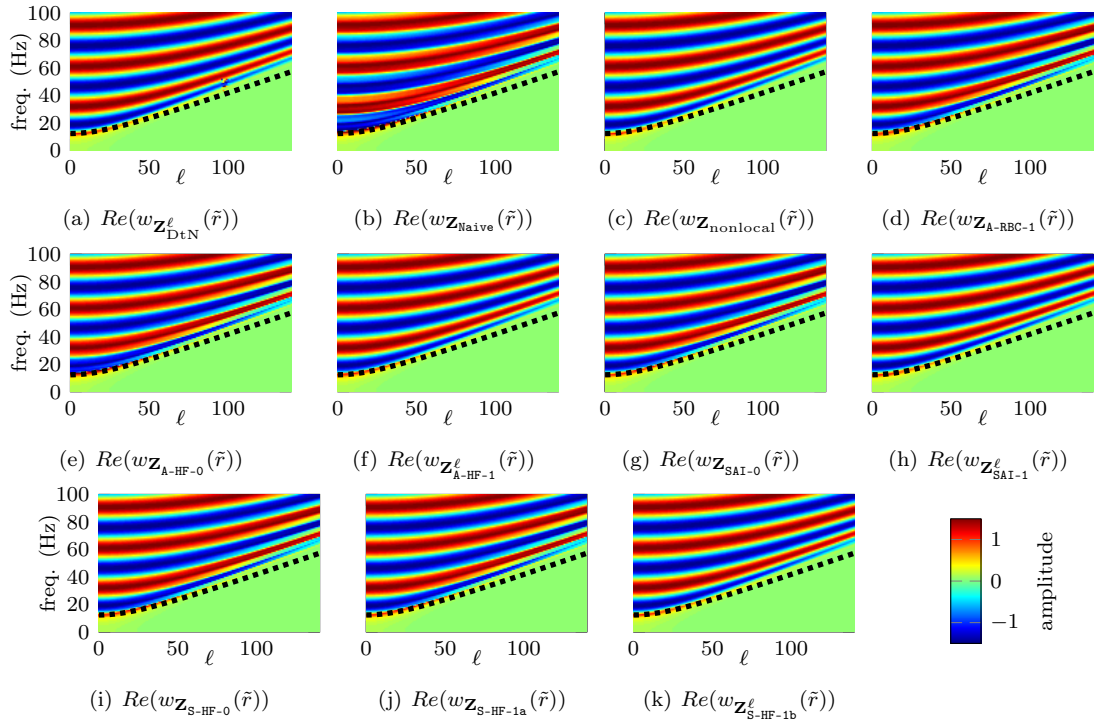


Figure 17: Comparison of the solutions  $Re(w_{\bullet, \ell, \omega_0}(\tilde{r}))$  as a function of the frequency  $\omega_0$  and  $\ell$  in  $\tilde{r} = 1.1$  without attenuation ( $\gamma = 0$ ). The black dashed line indicates the cutoff frequency given in (6.45).



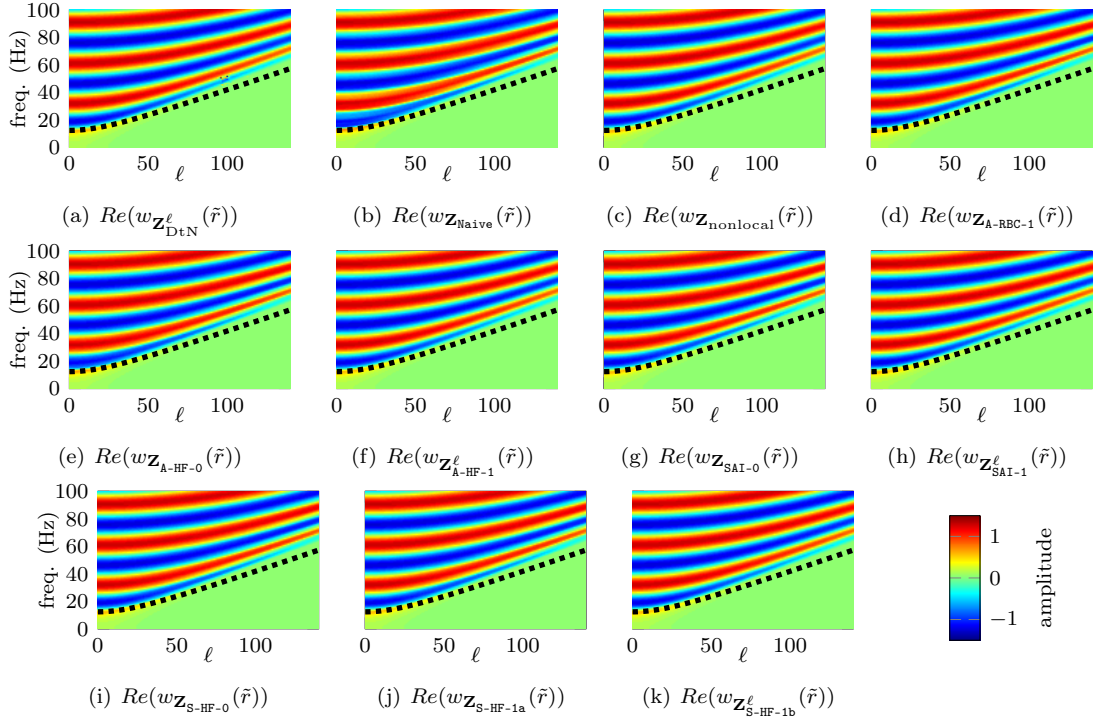


Figure 18: Comparison of the solutions  $Re(w_{\bullet, \ell, \omega_0}(\tilde{r}))$  as a function of the frequency  $\omega_0$  and  $\ell$  in  $\tilde{r} = 1.1$  with attenuation  $\gamma = 5$ . The black dashed line indicates the cutoff frequency given in (6.45).

1. There are more pronounced differences when the fixed point in consideration is closer to  $R_{\min}$ . In this case  $r = 1.01$  in Figures 15 and 16, compared to  $r = 1.1$  for Figures 17 and 18. In particular, there are no ridges in the figure for the reference solution, which however appear in those for the coefficients independent of  $\ell$ . The difference is most pronounced with  $\mathbf{Z}_{\text{Naive}}$ . Visually, it seems that  $\mathbf{Z}_{\text{nonlocal}}$ ,  $\mathbf{Z}_{\text{SAI-1}}^\ell$ ,  $\mathbf{Z}_{\text{S-HF-1b}}^\ell$  and  $\mathbf{Z}_{\text{A-HF-1}}^\ell$  give better performance.
2. The observations are confirmed in the presence of attenuation, which does not impact the performance of the coefficients.
3. When we move away from the initial point, see Figures 17 and 18 for  $r = 1.10$ , it is now very hard to distinguish any difference between the approaches.
4. We observe in all cases, the plots resemble one another below the cut-off frequency, i.e. for

$$\omega_0 < c_\infty \sqrt{\frac{\alpha_\infty^2}{4} + \frac{\alpha_\infty}{R_a} + \frac{\ell(\ell+1)}{R_a^2}}. \quad (6.45)$$

This corresponds with the green area (under the black dashed line) on the bottom right of the subfigures of Figures 17 and 18.

We give in Table 1 the mean of the error  $E$  over the investigated range of frequency and  $\ell$ , where we conclude that

$$\begin{aligned} \text{mean}(E_{\mathbf{Z}_{\text{nonlocal}}}) &< \text{mean}(E_{\mathbf{Z}_{\text{SAI-1}}^\ell}) < \text{mean}(E_{\mathbf{Z}_{\text{S-HF-1b}}^\ell}) < \text{mean}(E_{\mathbf{Z}_{\text{A-HF-1}}^\ell}) < \text{mean}(E_{\mathbf{Z}_{\text{SAI-0}}}) \\ &< \text{mean}(E_{\mathbf{Z}_{\text{S-HF-1a}}}) < \text{mean}(E_{\mathbf{Z}_{\text{S-HF-0}}}) < \text{mean}(E_{\mathbf{Z}_{\text{A-RBC-1}}}) < \text{mean}(E_{\mathbf{Z}_{\text{A-HF-0}}}) < \text{mean}(E_{\mathbf{Z}_{\text{Naive}}}). \end{aligned} \quad (6.46)$$

We have the following observations concerning the results using error norm  $e_\bullet$  shown in Figure 19 and 20, and error norm  $E_\bullet$  in Figures 21 and 22

1. Each  $\mathbf{Z}_\bullet$  yields lower error in the presence of attenuation than without.

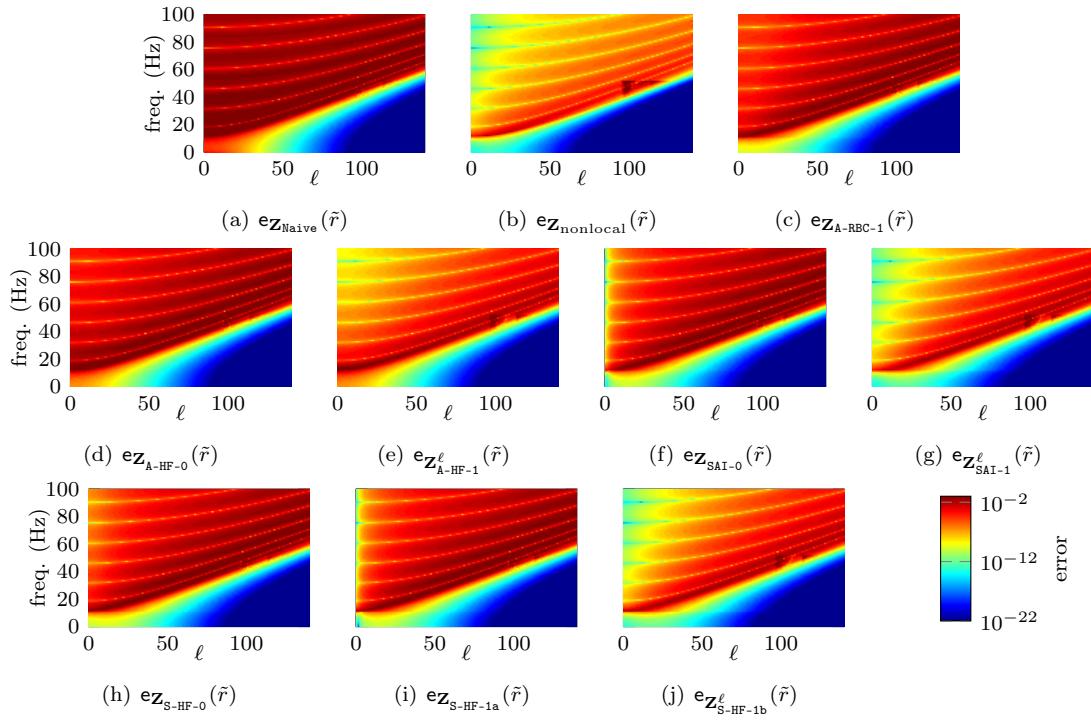


Figure 19: Comparison of the error  $\mathbf{e}_\bullet(\ell, \omega_0, \tilde{r})$  as a function of the frequency  $\omega_0$  and  $\ell$  in  $\tilde{r} = 1.1$  without attenuation ( $\gamma = 0$ ).

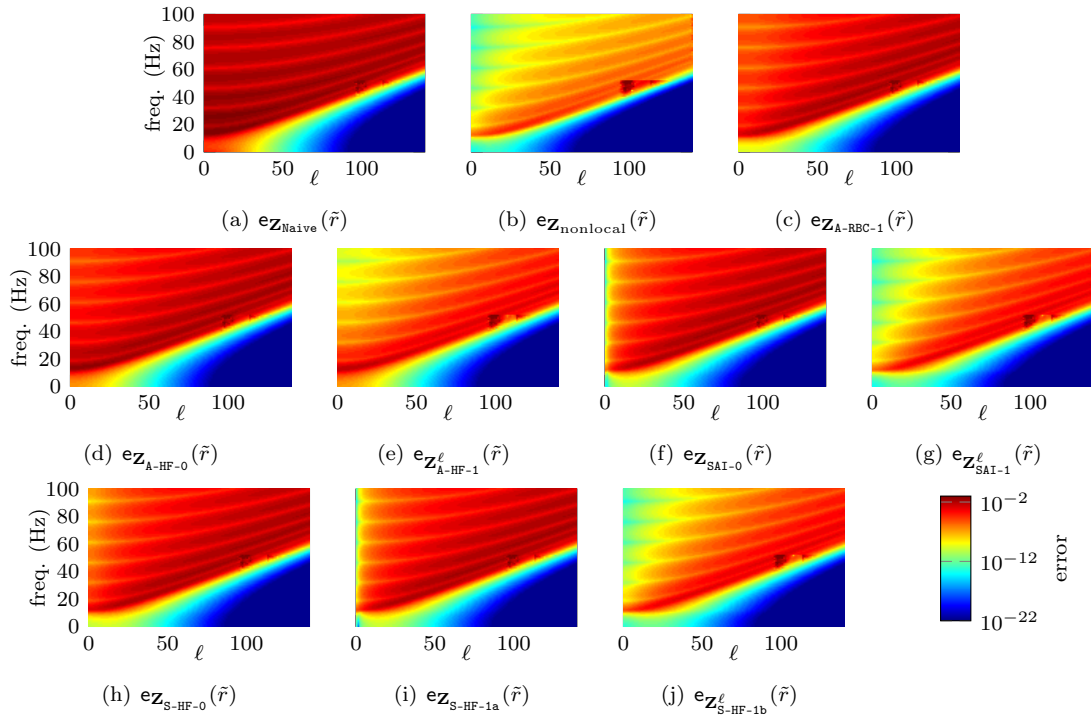


Figure 20: Comparison of the error  $\mathbf{e}_\bullet(\ell, \omega_0, \tilde{r})$  as a function of the frequency and  $\ell$  in  $\tilde{r} = 1.1$  with attenuation  $\gamma = 5$ .

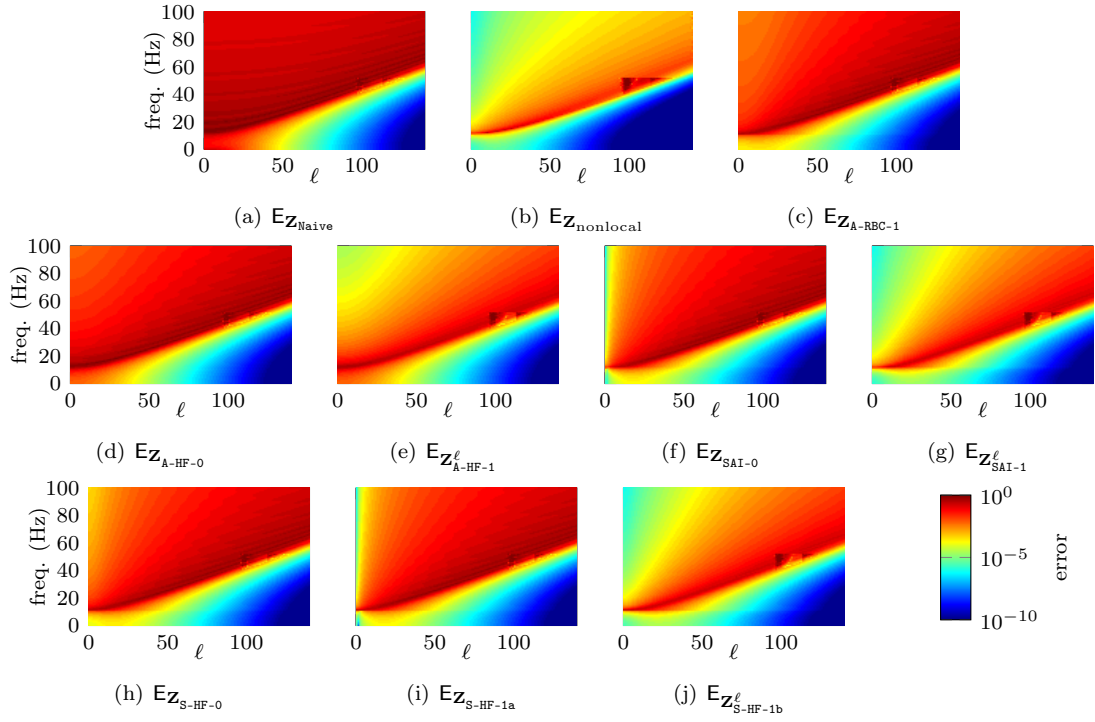


Figure 21: Comparison of the error  $E_{\bullet}(\ell, \omega_0)$  as a function of the frequency  $\omega_0$  and  $\ell$  without attenuation ( $\gamma = 0$ ).

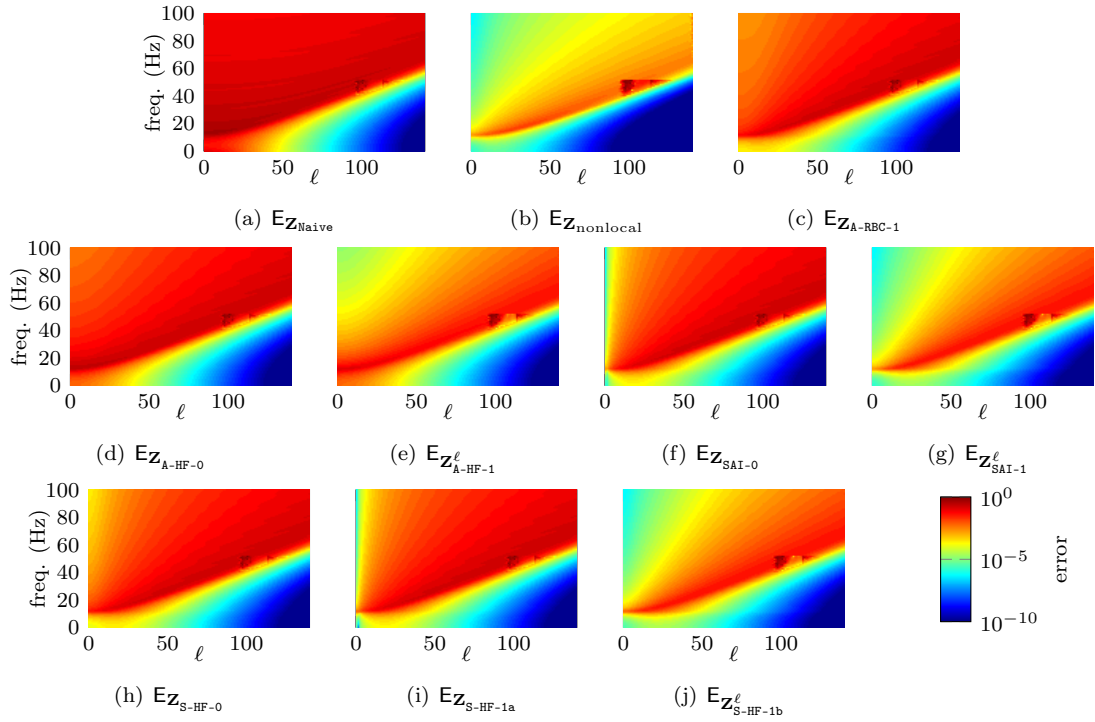


Figure 22: Comparison of the error  $E_{\bullet}(\ell, \omega_0)$  as a function of the frequency  $\omega_0$  and  $\ell$  with attenuation  $\gamma = 5$ .

2. It does not come as a surprise that the coefficients dependent on  $\ell$  behave better than the independent ones, since they are higher order approximates of the nonlocal.
3. Small angle approximation **SAI** represents in each group a better approximation than the **HF** ones. In particular, among higher order approximations with dependence on  $\ell$ ,  $\mathbf{Z}_{\text{SAI-1}}^\ell$  performs better than  $\mathbf{Z}_{\text{S-HF-1b}}^\ell$  and  $\mathbf{Z}_{\text{A-HF-1}}^\ell$ , while among lower order ones independent of  $\ell$ ,  $\mathbf{Z}_{\text{SAI-0}}$  performs better than  $\mathbf{Z}_{\text{S-HF-1a}}$  and  $\mathbf{Z}_{\text{S-HF-0}}$ .
4. The fact the  $\mathbf{Z}_{\text{S-HF-0}}$  performs better than  $\mathbf{Z}_{\text{A-RBC-1}}$  shows that the term  $\frac{1}{R_a}$  should be factored out, and not considered as part of a impedance coefficient, see Remark 28.
5. Within the coefficients that are independent of  $\ell$ ,  $\mathbf{Z}_{\text{SAI-0}}$ ,  $\mathbf{Z}_{\text{S-HF-1a}}$  and  $\mathbf{Z}_{\text{S-HF-0}}$  give the higher performance than the **A-RBC-1** and **A-HF-0**. They have the advantage of being simpler to implement in a 3D discretization (since dependence on  $\ell$  translates to a tangential differential operator),
6. The new **S-HF** family performs better than the **A-HF** with

$$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{S-HF-1b}}^\ell}) < \text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{A-HF-1}}^\ell}) \quad \text{and} \quad \text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{S-HF-0}}}) < \text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{A-HF-0}}}).$$

The comparison between  $\mathbf{Z}_{\text{S-HF-1b}}^\ell$  and  $\mathbf{Z}_{\text{A-HF-1}}^\ell$ , and between  $\mathbf{Z}_{\text{A-RBC-1}}$  and  $\mathbf{Z}_{\text{A-HF-1}}^\ell$  confirm that  $k$  is the correct wavenumber to work with, and not  $\omega/c$ . This also means that with  $\mathbf{Z}_{\text{A-RBC-1}}$  gives the Sommerfeld-like condition, comparable to the Sommerfeld radiation condition cf. [4, Sec 4.3] for Helmholtz equation, while with  $\mathbf{Z}_{\text{S-HF-0}}$ , we retrieve a condition with similar performance with the first-order radiation condition [4, Eqn. 21] for Helmholtz equation.

As a conclusion, for a discretization in 3D and in time domain,  $\mathbf{Z}_{\text{SAI-0}}$  and  $\mathbf{Z}_{\text{S-HF-1a}}$  are the best options in terms of ‘simplicity *vs.* accuracy ratio’. The second one is  $\mathbf{Z}_{\text{S-HF-0}}$ . This last one has the further advantage of lending itself readily to simulation in time domain.

	$\gamma = 0$	$\gamma = 5$
$\text{mean}(\mathbf{E}_{\text{nonlocal}})$	0.0045	0.0021
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{SAI-1}}^\ell})$	0.0132	0.0057
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{S-HF-1b}}^\ell})$	0.0136	0.0058
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{A-HF-1}}^\ell})$	0.0175	0.0076
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{SAI-0}}})$	0.0670	0.0312
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{S-HF-1a}}})$	0.0672	0.0312
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{S-HF-0}}})$	0.0684	0.0318
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{A-RBC-1}}})$	0.0691	0.0323
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{A-HF-0}}})$	0.0838	0.0398
$\text{mean}(\mathbf{E}_{\mathbf{Z}_{\text{Naive}}})$	0.1505	0.0779

Table 1: Mean of  $\mathbf{E}$  for  $0 \leq \ell \leq 140$  and  $2\pi 1 \leq \omega_0 \leq 2\pi 100$ , i.e., mean of the error pictured in Figures 21 and 22. Within each group, one observes that small-angle-incidence (**SAI**) approximation gives better accuracy than the high frequency (**HF**) one, and that the new **S-HF** family performs better than the **A-HF**. Radiation boundary conditions with  $\mathbf{Z}_{\text{SAI-0}}$ ,  $\mathbf{Z}_{\text{S-HF-1a}}$  and  $\mathbf{Z}_{\text{S-HF-0}}$  (highlighted in blue) represent the best options in terms of ‘simplicity *vs.* accuracy ratio’.

## 7 Conclusion

The main theme of the current report is the characterization and construction of ‘outgoing’ solutions (also called physical) to the scalar wave equation that is based on the model **S+Atmo**. In the absence

of attenuation, outgoing solutions are characterized by their  $L^2$ -boundedness, while in the presence of attenuation, they are defined by Limiting Absorption Principle (LAP), which are obtained by taking limits from above the continuous spectrum  $[0, \infty)$  (in  $\mathbb{C}_{k^2}$  with  $k^2$  the energy level in operator  $-\Delta - k^2 + \text{potential}$ ) of corresponding attenuated ( $L^2$ ) solutions.

Two techniques have been used to construct and define the uniqueness of the outgoing solutions. In both cases, the equation is first rewritten, using the Liouville transform, as a potential scattering problem for Schrödinger equation. The conjugated form of the operator makes appear the constant wavenumber  $k^2$  which gathers zero-th energy level and limiting values at infinity of the potential (so that the normalized potential now decays to zero at infinity). In the general case, results are obtained by means of the long-range potential scattering theory by Saito and Ikebe, with slight modifications to accommodate the weak singularity at the origin and the dependence on  $\omega$  of the potential. When the Atmo model is extended to the whole domain, results for existence and uniqueness of the outgoing solution is redone by working directly with the explicit expression of the Green kernel of the resolvent given by Whittaker functions.

The results concerning the fundamental outgoing kernel also have implications in numerical implementation. They provide the expression for the D-t-N map, which is used as a reference to evaluate the accuracy of radiation boundary conditions. We have also carried out some preliminary comparisons which confirm that  $k$  is the correct wavenumber to work with. This is predicted theoretically by the fact that the outgoing solution satisfies a Sommerfeld-like radiation condition in the newly defined wavenumber  $k$ . The numerical experiments also show that, in terms of ‘simplicity *vs.* accuracy ratio’ for a discretization in 3D and in time domain,  $\mathbf{Z}_{\text{SAI-0}}$  and  $\mathbf{Z}_{\text{S-HF-1a}}$  are best options, while a second-to-best one is given by  $\mathbf{Z}_{\text{S-HF-0}}$ . The latter two coefficients are newly introduced in this report by working with the wavenumber  $k$  and in the conjugated form of the operator.

As future work, further numerical experiments will be included in a second report more dedicated towards radiation boundary conditions. We will test the performance of the new and old radiation boundary conditions on more realistic cases e.g. S+Atmo and other models of atmosphere. We also plan to implement the boundary conditions with  $\mathbf{Z}_{\text{SAI-0}}$ ,  $\mathbf{Z}_{\text{S-HF-1a}}$  and  $\mathbf{Z}_{\text{S-HF-0}}$  in 3D discretization using Hybridizable Discontinuous Galerkin and in domains with non-spherical geometry.

## A More details on Liouville transform

Here we show details of the calculation of the potential resulted from Liouville transformation discussed in Section 2.

### A.1 General symmetry

**Proposition 24.** For  $\rho > 0$ , if  $u$  is a solution of

$$-\nabla \cdot \left( \frac{1}{\rho} \nabla u \right) - \frac{\omega^2}{\rho c^2} u = f,$$

then  $w = \rho^{-1/2} u$  solves

$$-\Delta w + \mathbf{q} w - \frac{\omega^2}{c^2} w = \rho^{1/2} f,$$

where

$$\mathbf{q} := \rho^{1/2} \Delta \rho^{-1/2}. \quad (\text{A.1})$$

*Proof.* We first consider the following identities,

$$\begin{aligned} \nabla(\rho^{1/2} w) &= (\nabla \rho^{1/2}) w + \rho^{1/2} \nabla w \\ \Rightarrow \nabla \cdot [\rho^{-1} \nabla(\rho^{1/2} w)] &= \nabla \cdot [\rho^{-1} (\nabla \rho^{1/2}) w + \rho^{-1/2} \nabla w] \\ &= w \underbrace{\nabla \cdot (\rho^{-1} \nabla \rho^{1/2})}_{-\Delta \rho^{-1/2}} + \underbrace{(\rho^{-1} \nabla \rho^{1/2}) \cdot \nabla w + (\nabla \rho^{-1/2}) \cdot \nabla w}_0 + \rho^{-1/2} \Delta w. \end{aligned}$$

The above cancellation is due to the identity,

$$\rho^{-1} \nabla \rho^{1/2} = -\nabla \rho^{-1/2}, \quad (\text{A.2})$$

since

$$\rho^{-1} \nabla \rho^{1/2} = \rho^{-1} \frac{1}{2} \rho^{-1/2} \nabla \rho = \frac{1}{2} \rho^{-3/2} \nabla \rho, \quad \nabla \rho^{-1/2} = -\frac{1}{2} \rho^{-3/2} \nabla \rho.$$

Using the above identities, we obtain the PDE satisfied by  $w$

$$\begin{aligned} -\nabla \cdot [\rho^{-1} \nabla (\rho^{1/2} w)] - \frac{\omega^2}{\rho c^2} \rho^{1/2} w &= f \\ \Leftrightarrow w \Delta \rho^{-1/2} - \rho^{-1/2} \Delta w - \frac{\omega^2}{\rho c^2} \rho^{1/2} w &= f. \end{aligned}$$

Since  $\rho \neq 0$ , thus we can divide both sides by  $\rho^{-1/2}$ , and obtain

$$-\Delta w + w \rho^{1/2} \Delta \rho^{-1/2} - \frac{\omega^2}{c^2} w = \rho^{1/2} f.$$

□

We next describe in more details the potential  $\mathbf{q}$ . We recall the definition of  $\alpha(x)$  in (2.8),

$$\alpha(x) := -\frac{\frac{x}{|x|} \cdot \nabla \rho}{\rho(x)} = -\frac{\partial_r \rho}{\rho}.$$

**Proposition 25.** *Potential  $\mathbf{q} := \rho^{1/2} \Delta \rho^{-1/2}$  defined in (A.1) can be written as,*

$$\begin{aligned} \mathbf{q} &= \frac{3}{4} \left\| \frac{\nabla \rho}{\rho} \right\|^2 - \frac{1}{2} \frac{\Delta \rho}{\rho} \\ &= \frac{\alpha(x)^2}{2} + \frac{\partial_r \alpha(x)}{2} + \frac{\alpha(x)}{|x|} + \frac{1}{4|x|^2} \left( \frac{3 \|\nabla_{\mathbb{S}^2} \rho\|^2}{\rho^2} - \frac{2 \Delta_{\mathbb{S}^2} \rho}{\rho} \right). \end{aligned} \quad (\text{A.3})$$

*Proof. Part 1* We calculate the gradient and Laplacian of  $\rho^{-1/2}$ .

$$\begin{aligned} \nabla \rho^{-1/2} &= -\frac{1}{2} \rho^{-1/2} \frac{\nabla \rho}{\rho} \\ \Rightarrow \Delta \rho^{-1/2} &= \nabla \cdot \nabla \rho^{-1/2} = -\frac{1}{2} \nabla(\rho^{-1/2}) \cdot \frac{\nabla \rho}{\rho} - \frac{1}{2} \rho^{-1/2} \nabla \cdot \frac{\nabla \rho}{\rho}. \end{aligned}$$

We further rewrite the last term in the above right-hand-side,

$$\begin{aligned} \nabla \cdot \left( \frac{\nabla \rho}{\rho} \right) &= \nabla \rho^{-1} \cdot \nabla \rho + \rho^{-1} \nabla \cdot \nabla \rho = -\rho^{-2} \nabla \rho \cdot \nabla \rho + \rho^{-1} \Delta \rho \\ &= -\frac{\nabla \rho}{\rho} \cdot \frac{\nabla \rho}{\rho} + \rho^{-1} \Delta \rho. \end{aligned}$$

We thus obtain

$$\Delta \rho^{-1/2} = \frac{1}{4} \rho^{-1/2} \left\| \frac{\nabla \rho}{\rho} \right\|^2 + \frac{1}{2} \rho^{-1/2} \left\| \frac{\nabla \rho}{\rho} \right\|^2 - \frac{1}{2} \rho^{-1/2} \rho^{-1} \Delta \rho,$$

and

$$\mathbf{q} := \rho^{1/2} \Delta \rho^{-1/2} = \frac{3}{4} \left\| \frac{\nabla \rho}{\rho} \right\|^2 - \frac{1}{2} \frac{\Delta \rho}{\rho}.$$

**Part 2** Consider the gradient in terms of  $\alpha$ ,

$$\begin{aligned}\nabla \rho &= (\partial_r \rho) \mathbf{e}_r + \frac{\nabla_{\mathbb{S}^2} \rho}{r} \quad \text{where} \quad \mathbf{e}_r = \frac{x}{|x|} \\ \Rightarrow \frac{\nabla \rho}{\rho} &= -\alpha(x) \mathbf{e}_r + \frac{1}{r} \frac{\nabla_{\mathbb{S}^2} \rho}{\rho} \quad \Rightarrow \quad \left\| \frac{\nabla \rho}{\rho} \right\|^2 = \alpha^2(x) + \frac{1}{r^2} \frac{\|\nabla_{\mathbb{S}^2} \rho\|^2}{\rho^2}.\end{aligned}$$

Similarly, we rewrite the Laplacian in terms of  $\alpha$ ,

$$\Delta \rho = \partial_r^2 \rho + \frac{2}{r} \partial_r \rho + \frac{\Delta_{\mathbb{S}^2} \rho}{r^2}.$$

By the definition of  $\alpha$ , we have

$$-\rho(x) \alpha(x) = \partial_r \rho \quad \Rightarrow \quad -(\partial_r \rho) \alpha - \rho(\partial_r \alpha) = \partial_r^2 \rho \quad \Rightarrow \quad \frac{\partial_r^2 \rho}{\rho} = \alpha^2 - \partial_r \alpha.$$

Thus

$$\frac{\Delta \rho}{\rho} = \alpha^2(x) - \partial_r \alpha - \frac{2}{r} \alpha(x) + \frac{1}{r^2} \frac{\Delta_{\mathbb{S}^2} \rho}{\rho}.$$

And we obtain

$$\begin{aligned}\mathfrak{q}(x) &= \frac{3}{4} \left( \alpha^2(x) + \frac{1}{r^2} \frac{\|\nabla_{\mathbb{S}^2} \rho\|^2}{\rho^2} \right) - \frac{1}{2} \left( \alpha^2 - \partial_r \alpha - \frac{2}{r} \alpha + \frac{1}{r^2} \frac{\Delta_{\mathbb{S}^2} \rho}{\rho} \right) \\ &= \frac{1}{2} \alpha(x)^2 + \frac{1}{2} \partial_r \alpha(x) + \frac{\alpha(x)}{|x|} + \frac{1}{4|x|^2} \left( \frac{3\|\nabla_{\mathbb{S}^2} \rho\|^2}{\rho^2} - \frac{2\Delta_{\mathbb{S}^2} \rho}{\rho} \right).\end{aligned}$$

□

## A.2 Radial symmetry calculation

In radial symmetry, the original ODE on each mode (6.2) can be rewritten as the reduced conjugated problem (6.5) by the basic technique in ODE to remove first order derivative term. In the current discussion, we assume  $\alpha$  is constant and  $k^2 = \frac{\omega^2}{c^2}$ .

We consider

$$\left( -\frac{d^2}{dr^2} - \left( \frac{2}{r} + \alpha_\infty \right) \frac{d}{dr} - \frac{\omega^2}{c_\infty^2} + \frac{\ell(\ell+1)}{r^2} \right) u = f. \quad (\text{A.4})$$

We carry out the change of unknown,

$$u = h(r) w(r),$$

where  $h$  is chosen as

$$h(r) = e^{-\frac{1}{2} \int (2r^{-1} + \alpha)} = r^{-1} e^{-\frac{\alpha}{2} r}.$$

In another word,  $h$  satisfies the ODE

$$h'(r) = -\frac{1}{2} \left( \frac{2}{r} + \alpha \right) h.$$

Hence we have,

$$\begin{aligned}h'' &= -\frac{1}{2} \left( \frac{2}{r} + \alpha \right) h' + \frac{1}{r^2} h \\ \Rightarrow h'' + \left( \frac{2}{r} + \alpha \right) h' &= \frac{1}{2} \left( \frac{2}{r} + \alpha \right) h' + \frac{1}{r^2} h = -\frac{1}{4} \left( \frac{2}{r} + \alpha \right)^2 h + \frac{1}{r^2} h \\ \Rightarrow \frac{h'' + \left( \frac{2}{r} + \alpha \right) h'}{h} &= -\frac{1}{r^2} - \frac{\alpha}{r} - \frac{1}{4} \alpha^2 + \frac{1}{r^2} = -\frac{\alpha}{r} - \frac{\alpha^2}{4}.\end{aligned}$$

Substitute the above calculation into (A.4) satisfied by  $u$ ,

$$u'' + \left(\frac{2}{r} + \alpha\right) u' - \frac{\ell(\ell+1)}{r^2} u + k^2 u = -f,$$

we obtain that for  $w$ ,

$$\begin{aligned} & (h''w + 2h'w' + hw'') + \left(\frac{2}{r} + \alpha\right)(h'w + hw') - \frac{\ell(\ell+1)}{r^2}hw + k^2hw = -f; \\ \Rightarrow & hw'' + w' \underbrace{\left[2h' + \left(\frac{2}{r} + \alpha\right)h\right]}_0 + w \left[h'' + \left(\frac{2}{r} + \alpha\right)h'\right] - \frac{\ell(\ell+1)}{r^2}hw + k^2hw = -f. \end{aligned}$$

Divide both sides by  $h$ , we are left with the reduced conjugated ODE,

$$w'' + \left[\frac{\omega^2}{c^2} - V(r)\right]w = h^{-1}f, \quad V(r) = \frac{\alpha_\infty}{r} + \frac{\alpha_\infty^2}{4} + \frac{\ell(\ell+1)}{r^2}.$$

## B Some elements of spectral and perturbation theory

**Basics notations from spectral theory** We first recall the notions of spectrum and resolvent for a general operator for an operator  $A$  densely defined on a complex Hilbert space  $\mathcal{H}$  and with domain  $D(A)$ .

- The **resolvent set**  $\rho(A)$  is defined as

$$\rho(A) := \{\lambda \in \mathbb{C} \mid A - \lambda \text{ is invertible with bounded inverse defined on } \mathcal{H}\}.$$

- The **spectrum**  $\sigma(A)$  is the complement

$$\sigma(A) := \mathbb{C} \setminus \rho(A).$$

$\lambda$  is an eigenvalue of  $A$  if there exists  $f \neq 0$  such that  $(A - \lambda)f = 0$ , i.e.  $A - \lambda$  is not injective (thus not invertible).  $\dim \text{Ker}(A - \lambda)$  is called the geometric multiplicity and  $\ker(A - \lambda)$  is the geometric eigenspace of  $A - \lambda$ .

- We have the disjoint decomposition of  $\sigma(A)$  into the **discrete spectrum**

$$\sigma_{\text{dis}}(A) := \{\lambda \in \sigma(A) \mid \lambda \text{ is an isolated eigenvalue of } A \text{ with finite algebraic multiplicity}\},$$

and the remaining part called the **essential spectrum**<sup>26</sup>,

$$\sigma_{\text{ess}}(A) := \sigma(A) \setminus \sigma_{\text{dis}}(A).$$

**Spectral properties for self-adjoint operators** For self-adjoint  $A$ ,

$$\sigma(A) \subset \mathbb{R}.$$

In addition, the essential spectrum is characterized as

$$\sigma_{\text{ess}}(A) = \{\lambda \in \sigma(A) \mid \exists \{u_n\} \subset D(A), \|u\| = 1, u_n \xrightarrow{w} 0, (A - \lambda)u_n \xrightarrow{s} 0\}.$$

In this case, the geometric multiplicity is equal to algebraic multiplicity. Thus the spectrum of self-adjoint  $A$  consists of only discrete eigenvalues (with finite multiplicity) and  $\lambda$  for which there exists a Weyl sequence,

$$\sigma(A) = \sigma_{\text{dis}}(A) \sqcup \{\lambda \in \sigma(A) \mid \exists \{u_n\} \subset D(A), \|u\| = 1, u_n \xrightarrow{w} 0, (A - \lambda)u_n \xrightarrow{s} 0\}.$$

$\sqcup$  denotes the disjoint union. We have further have the characterization,

$$\lambda \in \sigma(A) \Leftrightarrow \exists u_n, u_n \in D(A), \|u_n\| = 1, \|(A - \lambda)u_n\| \rightarrow 0, n \rightarrow \infty.$$

Note that if  $\lambda \in \sigma_{\text{ess}}(A)$  and  $\lambda$  is not an eigenvalue, then the element of a Weyl sequence can be considered as approximate eigenfunctions.

<sup>26</sup>The essential spectrum can also be characterized by one of the following three conditions. For  $\lambda \in \sigma(A)$ ,  $\sigma \in \sigma_{\text{ess}}(A)$  iff  $\lambda$  is not an eigenvalue, or  $\lambda$  is an accumulation point of the set of eigenvalues or  $\dim \text{Ker}(A - \lambda) = \infty$ . Essential spectrum is a closed set.



**Perturbation theory regarding self-adjointness** We following the exposition of [17, 13.1 p.132]. Suppose that  $A$  is self-adjoint and  $B$  closed.

- $B$  is **relative  $A$ -bounded** if  $D(A) \subset D(B)$ . If  $\rho(A) \neq \emptyset$ , then there exist constants  $a, b > 0$  such that

$$\|Bu\| \leq a \|Au\| + b \|u\|, \quad \forall u \in D(A). \quad (\text{B.1})$$

Smallest such constant  $a$  is called the relative  **$A$ -bound** of  $B$ .

An example is the **Kato-Rellich class** which by definition consists of  $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ . Such potentials have relative  $A$ -bound zero, i.e.  $\|Vu\| \leq b \|u\|$ . For proof see [17, Exp 13.4 p.133].

- The Kato-Rellich gives condition so that  $A + B$  is self-adjoint.

**Theorem 26** (Kato-Rellich [17, Thm 13.5]). *Let  $A$  be self-adjoint and  $B$  a closed, symmetric and  $A$ -bounded operator with relative  $A$ -bounded less than one. Then  $A + B$  is self-adjoint on  $D(A)$ .*

**Perturbation theory regarding essential spectrum** We follow the exposition of [17, Chapter 14 p.139]

- For  $A$  a closed operator with  $\rho(A) \neq \emptyset$ , an operator  $B$  is **relatively  $A$ -compact** if  $D(A) \subset D(B)$  and  $B(A - z)^{-1}$  is compact for some (and thus all)  $z \in \rho(A)$ .

For  $A$  self-adjoint, all  $A$ -relatively compact operators are  $A$ -bounded with relative bound zero,

- Weyl Theorem gives the condition under which essential spectrum of an operator is invariant under relatively compact perturbation.

**Theorem 27** ([17, Theorem 14.6]). *Let  $A$  and  $B$  be self-adjoint operators let  $A - B$  by  $A$ -compact, then*

$$\sigma_{ess}(A) = \sigma_{ess}(B).$$

- Not all Kato-Rellich potentials are relatively compact (e.g  $V = 1$ ) but a subclass is. By definition, cf. [17, Def 14.7],  $V$  is **Kato-type** if  $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)_\epsilon$ , which means that for any  $\epsilon > 0$ , we can decompose  $V$  as

$$V = V_1 + V_2, \quad V_1 \in L^2, \quad \|V_2\|_{L^\infty} < \epsilon. \quad (\text{B.2})$$

Examples of Kato potential includes

- $V$  real-valued, continuous and vanishes at infinity, i.e.  $V(x) \rightarrow 0$  as  $|x| \rightarrow \infty$ , and
- allows the potential to have singularity e.g. Coulomb potential  $V(x) = \frac{\alpha}{|x|}$ .

- A real Kato potential is relatively  $\Delta$ -compact, cf. Thm 14.9 of [17].

## C Collected facts on Whittaker functions

We have introduced the Whittaker equation

$$\partial_z^2 W + \left[ -\frac{1}{4} + \frac{\chi}{z} + \frac{\frac{1}{4} - \mu^2}{z^2} \right] W = G. \quad (\text{C.1})$$

### C.1 Properties of derivatives

In this subsection, we list the formula to calculate the derivative of the Whittaker functions and their properties near zero and infinity. These information are employed in the derivation of the properties of the Green kernel  $\Phi_k(x, y)$  (4.70).

**Connection formulae for derivatives** We cite the differentiation identities which are Eqn 13.15.15, 13.15.25 and 13.15.26 in [32] respectively,

$$\frac{d^n}{dz^n} \left( e^{\frac{1}{2}z} z^{\mu-\frac{1}{2}} M_{\kappa,\mu}(z) \right) = (-1)^n (-2\mu)_n e^{\frac{1}{2}z} z^{\mu-\frac{1}{2}(n+1)} M_{\kappa-\frac{1}{2}n, \mu-\frac{1}{2}n}(z), \quad (\text{C.2a})$$

$$\frac{d^n}{dz^n} \left( e^{-\frac{1}{2}z} z^{\mu-\frac{1}{2}} W_{\kappa,\mu}(z) \right) = (-1)^n e^{-\frac{1}{2}z} z^{\mu-\frac{1}{2}(n+1)} W_{\kappa+\frac{1}{2}n, \mu-\frac{1}{2}n}(z), \quad (\text{C.2b})$$

$$\left( z \frac{d}{dz} \right)^n \left( e^{-\frac{1}{2}z} z^{\kappa-1} W_{\kappa,\mu}(z) \right) = (-1)^n e^{-\frac{1}{2}z} z^{\kappa+n-1} W_{\kappa+n, \mu}(z). \quad (\text{C.2c})$$

We simplify these identities for one-time differentiation.

**Lemma 28.** *The first order derivative of  $M_{\kappa,\mu}$  and  $W_{\kappa,\mu}$  can be obtained by the following connection formulae.*

$$M'_{\kappa,\mu}(z) = \left( -\frac{1}{2} + \frac{\frac{1}{2}-\mu}{z} \right) M_{\kappa,\mu}(z) + \frac{2\mu}{\sqrt{z}} M_{\kappa-\frac{1}{2}, \mu-\frac{1}{2}}(z); \quad (\text{C.3a})$$

$$W'_{\kappa,\mu}(z) = \left( \frac{1}{2} - \frac{\mu-\frac{1}{2}}{z} \right) W_{\kappa,\mu}(z) - \frac{1}{\sqrt{z}} W_{\kappa+\frac{1}{2}, \mu-\frac{1}{2}}(z); \quad (\text{C.3b})$$

$$W'_{\kappa,\mu}(z) = \left( \frac{1}{2} - \frac{\kappa}{z} \right) W_{\kappa,\mu}(z) - \frac{1}{z} W_{\kappa+1, \mu}(z). \quad (\text{C.3c})$$

When  $\mu = \frac{1}{2}$ , they simplify further to,

$$M'_{\kappa, \frac{1}{2}}(z) = -\frac{M_{\kappa, \frac{1}{2}}(z)}{2} + \frac{M_{\kappa-\frac{1}{2}, 0}(z)}{\sqrt{z}}; \quad (\text{C.4a})$$

$$W'_{\kappa, \frac{1}{2}}(z) = \frac{W_{\kappa, \frac{1}{2}}(z)}{2} - \frac{W_{\kappa+\frac{1}{2}, 0}(z)}{\sqrt{z}}; \quad (\text{C.4b})$$

$$W'_{\kappa, \frac{1}{2}}(z) = \left( \frac{1}{2} - \frac{\kappa}{z} \right) W_{\kappa, \frac{1}{2}}(z) - \frac{W_{\kappa+1, \frac{1}{2}}(z)}{z}. \quad (\text{C.4c})$$

*Proof.* For one time differentiation, we set  $n = 1$  and the left-hand-sides of (C.2) simplify to

$$\begin{aligned} \frac{d}{dz} \left( e^{\frac{1}{2}z} z^{\mu-\frac{1}{2}} M_{\kappa,\mu}(z) \right) &= \left( \frac{1}{2} M_{\kappa,\mu}(z) + \frac{\mu-\frac{1}{2}}{z} M_{\kappa,\mu}(z) + M'_{\kappa,\mu}(z) \right) e^{\frac{1}{2}z} z^{\mu-\frac{1}{2}}; \\ \frac{d}{dz} \left( e^{-\frac{1}{2}z} z^{\mu-\frac{1}{2}} W_{\kappa,\mu}(z) \right) &= \left( -\frac{1}{2} W_{\kappa,\mu}(z) + \frac{\mu-\frac{1}{2}}{z} W_{\kappa,\mu}(z) + W'_{\kappa,\mu}(z) \right) e^{-\frac{1}{2}z} z^{\mu-\frac{1}{2}}; \\ z \frac{d}{dz} z \left( e^{-\frac{1}{2}z} z^{\kappa-1} W_{\kappa,\mu}(z) \right) &= z \frac{d}{dz} \left( e^{-\frac{1}{2}z} z^{\kappa} W_{\kappa,\mu}(z) \right) \\ &= \left( -\frac{1}{2} W_{\kappa,\mu}(z) + \frac{\kappa}{z} W_{\kappa,\mu}(z) + W'_{\kappa,\mu}(z) \right) e^{-\frac{1}{2}z} z^{\kappa+1}. \end{aligned}$$

By definition of the Pochhammer's symbol (4.23),  $(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$ , and identity  $(-a)_n = (-1)^n (a-n+1)_n$  and  $\Gamma(a+1) = a\Gamma(a)$ , we have

$$(-2\mu)_n = (-1)^n (2\mu-n+1)_n = (-1)^n \frac{\Gamma(2\mu+1)}{\Gamma(2\mu-n+1)}.$$

For  $n = 1$ , this takes on value

$$(-2\mu)_1 = -\frac{\Gamma(2\mu+1)}{\Gamma(2\mu)} = -2\mu.$$

The first identity (C.2a), after canceling out  $e^{\frac{1}{2}z} z^{\mu-\frac{1}{2}}$ , gives

$$\frac{1}{2}M_{\kappa,\mu}(z) + \frac{\mu-\frac{1}{2}}{z}M_{\kappa,\mu}(z) + M'_{\kappa,\mu}(z) = (2\mu)z^{-\frac{1}{2}}M_{\kappa-\frac{1}{2},\mu-\frac{1}{2}}(z).$$

After rearrangement, we obtain (C.3a).

The second identity (C.2b), after canceling out  $e^{-\frac{1}{2}z} z^{\mu-\frac{1}{2}}$ , can be written as

$$\left(-\frac{1}{2} + \frac{\mu-\frac{1}{2}}{z}\right)W_{\kappa,\mu}(z) + W'_{\kappa,\mu}(z) = -z^{-\frac{1}{2}}W_{\kappa+\frac{1}{2},\mu-\frac{1}{2}}(z).$$

After rearrangement, we obtain (C.3b). Similarly, after canceling out  $e^{-\frac{1}{2}z} z^{\kappa+1}$ , the third identity (C.2b) is written as,

$$-\frac{1}{2}W_{\kappa,\mu}(z) + \frac{\kappa}{z}W_{\kappa,\mu}(z) + W'_{\kappa,\mu}(z) = -\frac{1}{z}W_{\kappa+1,\mu}(z).$$

After rearrangement, we obtain (C.3c).

□

**Remark 30** (Concerning typos in [27]). We note that identity (C.3c) agrees with the last identity concerning derivative of  $W$  on p. 302 of [27]. We however note the following typo in [27]. On page 302 of [27], the fifth-to-last identity of [27] is

$$\begin{aligned} 2W_{\kappa+\frac{1}{2},\mu-\frac{1}{2}}(z) &= \frac{1-2\mu+z}{\sqrt{z}}W_{\kappa,\mu}(z) - \sqrt{z}W'_{\kappa,\mu}(z) \\ \Leftrightarrow \frac{1}{\sqrt{z}}W_{\kappa+\frac{1}{2},\mu-\frac{1}{2}}(z) &= \left(\frac{1}{2} - \frac{\mu-\frac{1}{2}}{z}\right)W_{\kappa,\mu}(z) - \frac{1}{2}W'_{\kappa,\mu}(z) \\ \Leftrightarrow \frac{1}{2}W'_{\kappa,\mu}(z) &= \left(\frac{1}{2} - \frac{\mu-\frac{1}{2}}{z}\right)W_{\kappa,\mu}(z) - \frac{1}{\sqrt{z}}W_{\kappa+\frac{1}{2},\mu-\frac{1}{2}}(z). \end{aligned}$$

According the fifth-to-last identity in [27], the right-hand-side of the above expression gives  $\frac{1}{2}W'_{\kappa,\mu}(z)$ . However, according to the verified identity (C.3b), this should give  $W'_{\kappa,\mu}(z)$ . To resolve this incoherence, we numerically verify the identities by using high-order finite difference to calculate the derivatives of  $W_{\kappa,\mu}$ , and this process shows that identity (C.3b) is the correct one. Hence, there is a typo in the fifth-last equation in [27, p. 302].

In this new version of our report, we note that (C.3a) now agrees with the first identity with  $M_{\kappa,\mu}$  on p. 302 of [27] which is

$$\begin{aligned} 2\mu M_{\kappa-\frac{1}{2},\mu-\frac{1}{2}}(z) &= \sqrt{z}M'_{\kappa,\mu}(z) + \frac{2\mu-1+z}{2\sqrt{z}}M_{\kappa,\mu}(z) \\ \Leftrightarrow M'_{\kappa,\mu}(z) &= \left(-\frac{1}{2} + \frac{\frac{1}{2}-\mu}{z}\right)M_{\kappa,\mu}(z) + \frac{2\mu}{\sqrt{z}}M_{\kappa-\frac{1}{2},\mu-\frac{1}{2}}(z). \end{aligned}$$

△

**Proposition 29.** Behavior as  $z \rightarrow 0$

$$M_{\kappa,1/2}(0) = 0 \quad ; \quad \lim_{z \rightarrow 0} M'_{\kappa,1/2}(z) = 1.$$

Asymptotic as  $z \rightarrow \infty$ , and  $\text{Arg } z \in (-\frac{1}{2}\pi, \frac{3}{2}\pi)$ ,

$$M_{\kappa,1/2}(z) \sim e^{\frac{1}{2}z} z^{-\kappa} \left( \frac{1}{\Gamma(1-\kappa)} + O(z^{-1}) \right) + e^{-\frac{1}{2}z} z^{\kappa} \left( \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} + O((-z)^{-1}) \right),$$

and

$$M'_{\kappa, \frac{1}{2}}(z) \sim e^{\frac{1}{2}z} z^{-\kappa} \left( \frac{1}{2\Gamma(1-\kappa)} + O(z^{-1}) \right) + e^{-\frac{1}{2}z} z^{\kappa} \left( -\frac{1}{2\Gamma(1+\kappa)} e^{(1-\kappa)\pi i} + O((-z)^{-1}) \right).$$

*Proof.* By [32, Eqn (13.14.6) p 334]

$$M_{\kappa, n}(z) = e^{-\frac{1}{2}z} z^{\frac{1}{2}+n} \left( 1 + \sum_{k=1}^{\infty} \frac{(\frac{1}{2}+n+\kappa)_k}{(1+2n)_k k!} z^k \right), \quad 2n \neq -1, -2, -3, \dots \quad (C.5)$$

converges for all  $z \in \mathbb{C}$ . In particular,

$$M_{\kappa, n}(z) = e^{-1/2z} z \left( 1 + \sum_{k=1}^{\infty} \frac{(1+\kappa)_k}{(2)_k k!} z^k \right) \quad (C.6)$$

converges for all  $z \in \mathbb{C}$ , and

$$M_{\kappa, 1/2}(0) = 0. \quad (C.7)$$

To obtain the limit of the derivative, we first use the connection formula (C.4a),

$$M'_{\kappa, \frac{1}{2}} = \frac{1}{\sqrt{z}} M_{\kappa-\frac{1}{2}, 0}(z) - \frac{1}{2} M_{\kappa, \frac{1}{2}}(z). \quad (C.8)$$

The limit of the first term is obtained by using (C.5) (with  $n = 0$ )

$$M_{\kappa-\frac{1}{2}, 0}(z) = e^{-\frac{1}{2}z} z^{\frac{1}{2}} \left( 1 + \sum_{k=1}^{\infty} \frac{(\frac{1}{2}+\kappa)_k}{(1)_k k!} z^k \right) \Rightarrow \lim_{z \rightarrow 0} \frac{1}{\sqrt{z}} M_{\kappa-\frac{1}{2}, 0}(z) = 1.$$

Together with (C.7), we obtain that  $\lim_{z \rightarrow 0} M' = 1$ .

We next consider the behavior as  $z \rightarrow \infty$ . By [32, 13.19.2] and using also [32, 13.7.2], we have

$$\begin{aligned} M_{\kappa, \mu} &\sim \frac{1}{\Gamma(\frac{1}{2}+\mu-\kappa)} e^{\frac{1}{2}z} z^{-\kappa} \sum_{k=0}^{\infty} \frac{(\frac{1}{2}-\mu+\kappa)_k (\frac{1}{2}+\mu+\kappa)_k}{k!} z^{-k} \\ &+ \frac{e^{(\frac{1}{2}+\mu-\kappa)\pi i}}{\Gamma(\frac{1}{2}+\mu+\kappa)} e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=0}^{\infty} \frac{(\frac{1}{2}+\mu-\kappa)_k (\frac{1}{2}-\mu-\kappa)_k}{k!} (-z)^{-k}, \end{aligned} \quad (C.9)$$

$$\text{Arg } z \in (-\frac{1}{2}\pi, \frac{3}{2}\pi) \quad \text{and} \quad (2\mu \neq -1, -2, -3 \quad \text{or} \quad \mu - \kappa \neq -\frac{1}{2}, -\frac{3}{2}, \dots).$$

Here, we use the condition<sup>27</sup> of [32, 13.7.2]. In particular for  $\mathcal{M}_{\kappa, 1/2}$  and  $\mathcal{M}_{\kappa-1/2, 0}$ , we have, for  $\text{Arg } z \in (-\frac{1}{2}\pi, \frac{3}{2}\pi)$ ,

$$\begin{aligned} M_{\kappa, 1/2} &\sim \frac{1}{\Gamma(1-\kappa)} e^{\frac{1}{2}z} z^{-\kappa} \sum_{k=0}^{\infty} \frac{(\kappa)_k (1+\kappa)_k}{k!} z^{-k} \\ &+ \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=0}^{\infty} \frac{(1-\kappa)_k (-\kappa)_k}{k!} (-z)^{-k}, \end{aligned} \quad (C.10)$$

<sup>27</sup>The verbatim statement is that, unless  $a = 0, -1, \dots$  and  $b - a = 0, -1, \dots$  then asymptotic (13.7.2) holds. This is equivalent to, if

$$a \neq 0, -1, \dots \quad \text{or} \quad b - a \neq 0, -1, \dots,$$

then we have the asymptotics (13.7.2) in [32]. Since  $a = \frac{1}{2} + \mu - \kappa$ , and  $b = 1 + 2\mu$  this translates to if

$$\frac{1}{2} + \mu - \kappa \neq 0, -1, \dots \quad \text{or} \quad 1 + 2\mu \neq 0, -1$$

When  $\mu = 1/2$ , this gives

$$1 - \kappa \neq 0, -1, \dots \quad \text{or} \quad 2 \neq 0, -1, \dots$$

This condition is always satisfied for  $\mu = \frac{1}{2}$ .

and

$$\begin{aligned} M_{\kappa-\frac{1}{2},0} &\sim \frac{1}{\Gamma(1-\kappa)} e^{\frac{1}{2}z} z^{-\kappa+\frac{1}{2}} \sum_{k=0}^{\infty} \frac{(\kappa)_k (\kappa)_k}{k!} z^{-k} \\ &\quad + \frac{e^{(1-\kappa)\pi i}}{\Gamma(\kappa)} e^{-\frac{1}{2}z} z^{\kappa-\frac{1}{2}} \sum_{k=0}^{\infty} \frac{(1-\kappa)_k (1-\kappa)_k}{k!} (-z)^{-k}. \end{aligned}$$

Thus

$$\begin{aligned} \frac{M_{\kappa-\frac{1}{2},0}}{z^{1/2}} &\sim \frac{1}{\Gamma(1-\kappa)} e^{\frac{1}{2}z} z^{-\kappa} \sum_{k=0}^{\infty} \frac{(\kappa)_k (\kappa)_k}{k!} z^{-k} \\ &\quad - \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=1}^{\infty} \frac{\kappa (1-\kappa)_{k-1} (1-\kappa)_{k-1}}{(k-1)!} (-z)^{-k}. \end{aligned}$$

We combine these asymptotics to obtain that for  $M'$

$$\begin{aligned} M'_{\kappa,\frac{1}{2}} &= \frac{1}{\sqrt{z}} M_{\kappa-\frac{1}{2},0}(z) - \frac{1}{2} M_{\kappa,\frac{1}{2}}(z) \\ &\sim e^{\frac{1}{2}z} z^{-\kappa} \frac{1}{\Gamma(1-\kappa)} \sum_{k=0}^{\infty} \frac{(\kappa)_k}{k!} \left( -\frac{1}{2} (1+\kappa)_k + (\kappa)_k \right) z^{-k} \\ &\quad + \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} e^{-\frac{1}{2}z} z^{\kappa} \left( -\frac{1}{2} + \sum_{k=1}^{\infty} \left( -\frac{1}{2} \frac{(1-\kappa)_k (-\kappa)_k}{k!} - \frac{\kappa (1-\kappa)_{k-1} (1-\kappa)_{k-1}}{(k-1)!} \right) (-z)^{-k} \right). \end{aligned}$$

The coefficients of the series can be further simplified, using the identity  $\Gamma(a+1) = a\Gamma(a)$ ,

$$\begin{aligned} &-\frac{1}{2} \frac{(1-\kappa)_k (-\kappa)_k}{k!} - \frac{\kappa (1-\kappa)_{k-1} (1-\kappa)_{k-1}}{(k-1)!} \\ &= -\frac{1}{2k!} \frac{\Gamma(1-\kappa+k)}{\Gamma(1-\kappa)} \frac{\Gamma(k-\kappa)}{\Gamma(-\kappa)} - \frac{\kappa}{(k-1)!} \left( \frac{\Gamma(k-\kappa)}{\Gamma(1-\kappa)} \right)^2 \\ &= -\frac{1}{2k!} \frac{(k-\kappa)}{(-\kappa)} \left( \frac{\Gamma(k-\kappa)}{\Gamma(-\kappa)} \right)^2 - \frac{\kappa}{(k-1)!(-\kappa)^2} \left( \frac{\Gamma(k-\kappa)}{\Gamma(-\kappa)} \right)^2 \\ &= \left( \frac{k-\kappa}{2\kappa} - \frac{k}{\kappa} \right) \frac{1}{k!} \left( \frac{\Gamma(k-\kappa)}{\Gamma(-\kappa)} \right)^2 = -\frac{k+\kappa}{2\kappa} \frac{1}{k!} ((-\kappa)_k)^2 \end{aligned}$$

and

$$\begin{aligned} -\frac{1}{2} (1+\kappa)_k + (\kappa)_k &= -\frac{1}{2} \frac{\Gamma(1+\kappa+k)}{\Gamma(1+\kappa)} + (\kappa)_k = -\frac{1}{2} \frac{\Gamma(\kappa+k)}{\Gamma(\kappa)} \frac{(\kappa+k)}{\kappa} + (\kappa)_k \\ &= \left( -\frac{1}{2} \frac{(\kappa+k)}{\kappa} + 1 \right) (\kappa)_k = \frac{\kappa-k}{2\kappa} (\kappa)_k. \end{aligned}$$

Thus

$$\begin{aligned} M'_{\kappa,\frac{1}{2}}(z) &\sim e^{\frac{1}{2}z} z^{-\kappa} \frac{1}{\Gamma(1-\kappa)} \sum_{k=0}^{\infty} \frac{(\kappa)_k (\kappa)_k (\kappa-k)}{k! 2\kappa} z^{-k} \\ &\quad - \frac{1}{2} \frac{e^{(1-\kappa)\pi i}}{\Gamma(1+\kappa)} e^{-\frac{1}{2}z} z^{\kappa} \left( 1 + \sum_{k=1}^{\infty} \frac{(k+\kappa)}{\kappa} \frac{(-\kappa)_k (-\kappa)_k}{k!} (-z)^{-k} \right). \end{aligned}$$

□

**Proposition 30.** *Behavior for  $z \rightarrow 0$*

$$\begin{aligned} W_{\kappa, \frac{1}{2}}(z) &= \frac{1}{\Gamma(1-\kappa)} + O(z \ln z) \quad , \quad z \rightarrow 0; \\ W'_{\kappa, \frac{1}{2}}(z) &= \frac{\ln z}{\Gamma(-\kappa)} + \frac{\psi(-\kappa) + 2\gamma}{\Gamma(-\kappa)} + \frac{1}{\Gamma(1-\kappa)} + O(z \ln z) \quad , \quad z \rightarrow 0. \end{aligned} \quad (\text{C.11})$$

*Behavior for  $z \rightarrow \infty$*

$$\begin{aligned} W_{\kappa, \frac{1}{2}}(z) &= e^{-\frac{1}{2}z} z^{\kappa} \left( 1 + O(|z|^{-1}) \right), \quad |\text{Arg } z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty; \\ W'_{\kappa, \frac{1}{2}}(z) &= e^{-\frac{1}{2}z} z^{\kappa} \left( -\frac{1}{2} + O(|z|^{-1}) \right), \quad |\text{Arg } z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty, \end{aligned}$$

*and the radiating property*

$$e^{\frac{1}{2}z} z^{-\kappa} \left( W'_{\kappa, \frac{1}{2}}(z) + \frac{1}{2} W_{\kappa, \frac{1}{2}}(z) \right) = O(|z|^{-1}). \quad (\text{C.12})$$

*Proof.* For the behavior at 0, we use the second identity in (C.4b),

$$W'_{\kappa, \frac{1}{2}}(z) = \frac{W_{\kappa, \frac{1}{2}}(z)}{2} - \frac{W_{\kappa+\frac{1}{2}, 0}(z)}{\sqrt{z}}.$$

Result (C.11) now follows by using the properties of  $W_{\kappa+\frac{1}{2}, 0}(z)$  as  $z \rightarrow 0$ , cf. (4.39)

$$W_{\kappa+\frac{1}{2}, 0}(z) = -\frac{\sqrt{z}}{\Gamma(-\kappa)} \left( \ln z + \psi(-\kappa) + 2\gamma \right) + O(z^{3/2} \ln z),$$

and that of  $W_{\kappa, \frac{1}{2}}(z)$ ,

$$W_{\kappa, \frac{1}{2}}(z) = \frac{1}{\Gamma(1-\kappa)} + O(z \ln z).$$

Thus

$$W'_{\kappa, \frac{1}{2}}(z) = \frac{1}{2} \left( \frac{1}{\Gamma(1-\kappa)} + O(z \ln z) \right) + \left( \frac{\ln z + \psi(-\kappa) + 2\gamma}{\Gamma(-\kappa)} + O(z \ln z) \right).$$

In a similar manner, to obtain the behavior of the derivative at  $\infty$ , we use the relation (C.4),

$$-\frac{W_{\kappa+1, \mu}(z)}{z} + \left( \frac{1}{2} - \frac{\kappa}{z} \right) W_{\kappa, \mu}(z) = W'_{\kappa, \mu}(z).$$

From the relation, we have

$$W'_{\kappa, \mu}(z) + \frac{1}{2} W_{\kappa, \mu}(z) = -\frac{W_{\kappa+1, \mu}(z)}{z} + W_{\kappa, \mu}(z) - \frac{\kappa}{z} W_{\kappa, \mu}(z),$$

we observe that the two terms

$$\frac{\kappa}{z} W_{\kappa, \mu}(z) \quad \text{and} \quad -\frac{W_{\kappa+1, \mu}(z)}{z} + W_{\kappa, \mu}(z),$$

consist of only of lower order terms. This is due to

$$\begin{aligned} W_{\kappa, \frac{1}{2}}(z) &\sim e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=0}^{\infty} \frac{(1-\kappa)_k (-\kappa)_k}{k!} (-z)^{-k} \quad , \quad |\text{Arg } z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty, \\ z^{-1} W_{\kappa+1, \frac{1}{2}}(z) &\sim e^{-\frac{1}{2}z} z^{\kappa} \sum_{k=0}^{\infty} \frac{(2-\kappa-1)_k (-\kappa-1)_k}{k!} (-z)^{-k} \quad , \quad |\text{Arg } z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty. \end{aligned}$$

□

## C.2 Asymptotics and Limiting behavior (with regards to incoming or outgoing convention)

Here we show the calculation for the statement in subsection 4.2.3, which shows the highest order term in the asymptotic expansion of the Whittaker function when  $z \rightarrow \infty$ , as well as their relation when  $\gamma \rightarrow 0+$  or  $\gamma \rightarrow 0-$ . With (4.63), we are in the applicable range  $(-\frac{3\pi}{2}, \frac{3\pi}{2})$  of (4.61) to obtain the behavior at  $\infty$ , for  $W_{\kappa,\mu}(z)$  and  $W_{-\kappa,\mu}(e^{-i\pi}z)$  with  $z$  defined in (4.6). We expand the leading term explicitly in terms of  $r$  and  $k_\gamma$ ,  $\eta_\gamma$ , defined in (4.15).

First we need the following identities involving the principal branch  $\log$ , i.e.  $-\pi < \text{Im}(\log z) \leq \pi$ . This means

$$\log(-|s|) = \ln|s| + i\pi \quad , \quad s \in \mathbb{R} \setminus \{0\}. \quad (\text{C.13})$$

Recall

$$0 \leq \text{Arg}(k_\gamma) \leq \frac{\pi}{2} \quad \gamma \geq 0 \quad ; \quad \frac{\pi}{2} < \text{Arg}(k_\gamma) < \pi \quad , \quad \gamma < 0,$$

We have

$$\begin{aligned} \gamma > 0 \quad : \quad & \log(2e^{i\frac{\pi}{2}} k_\gamma r) = \log(2k_\gamma r) + i\frac{\pi}{2} \quad ; \\ & \log(2e^{-i\frac{\pi}{2}} k_\gamma r) = \log(2k_\gamma r) - i\frac{\pi}{2}; \end{aligned} \quad (\text{C.14})$$

$$\begin{aligned} \gamma < 0 \quad : \quad & \log(2e^{i\frac{\pi}{2}} k_\gamma r) = \log(2k_\gamma r) + i\frac{\pi}{2} - i2\pi \quad ; \\ & \log(2e^{-i\frac{\pi}{2}} k_\gamma r) = \log(2k_\gamma r) - i\frac{\pi}{2} . \end{aligned} \quad (\text{C.15})$$

- For  $\gamma > 0$ , we have

$$\begin{aligned} \gamma > 0 \quad : \quad W_{i\eta_\gamma,\mu}(z) &\sim e^{-\frac{z}{2}} z^{i\eta_\gamma} = e^{-\frac{z}{2} + i\eta_\gamma \log(z)} \\ &\stackrel{(4.61),(4.63)}{=} \exp\left(-ik_\gamma r + i\eta_\gamma \log(2e^{i\frac{\pi}{2}} k_\gamma r)\right) \\ &\stackrel{(\text{C.14})}{=} \exp\left(-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right) \quad ; \end{aligned} \quad (\text{C.16})$$

Similarly

$$\begin{aligned} \gamma > 0 \quad : \quad W_{-i\eta_\gamma,\mu}(e^{-i\pi}z) &\sim e^{-\frac{1}{2}(e^{-i\pi}z)}(e^{-i\pi}z)^{-i\eta_\gamma} \sim e^{\frac{z}{2} - i\eta_\gamma \log(e^{-i\pi}z)} \\ &= \exp\left(ik_\gamma r - i\eta_\gamma \log(2e^{-i\frac{\pi}{2}} k_\gamma r)\right) \\ &\stackrel{(\text{C.14})}{=} \exp\left(ik_\gamma r - i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right). \end{aligned} \quad (\text{C.17})$$

Using  $k_\gamma \rightarrow k_0$ ,  $\eta_\gamma \rightarrow \eta_0$ ,  $\kappa_\gamma \rightarrow \kappa_0$ , as  $\gamma \rightarrow 0^+$ , cf. (4.19), taking limits as  $\gamma \rightarrow 0^+$ , we obtain

$$\exp\left(-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right) \longrightarrow \exp\left(-ik_0 r + i\eta_0 \log(2k_0 r) - \frac{\pi}{2}\eta_0\right) \quad , \quad \gamma \rightarrow 0^+$$

$$\exp\left(ik_\gamma r - i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right) \longrightarrow \exp\left(ik_0 r - i\eta_0 \log(2k_0 r) - \frac{\pi}{2}\eta_0\right) \quad , \quad \gamma \rightarrow 0^+.$$

- For  $\gamma < 0$ , we use (C.15),

$$\begin{aligned} \gamma < 0 \quad : \quad W_{i\eta_\gamma,\mu}(z) &\stackrel{(\text{C.15})}{\sim} \exp\left(-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r) - \frac{3\pi}{2}\eta_\gamma\right); \\ W_{-i\eta_\gamma,\mu}(e^{-i\pi}z) &\stackrel{(\text{C.15})}{\sim} \exp\left(ik_\gamma r - i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right). \end{aligned}$$

Using  $k_\gamma \rightarrow -k_0$ ,  $\eta_\gamma \rightarrow -\eta_0$ ,  $\kappa_\gamma \rightarrow -\kappa_0$  as  $\gamma \rightarrow 0^-$ , cf. (4.19), taking limits as  $\gamma \rightarrow 0^-$ ,

$$\begin{aligned}
 \exp\left(-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r) - \frac{3\pi}{2}\eta_\gamma\right) &\longrightarrow \exp\left(ik_0 r - i\eta_0 \log(-2k_0 r) + \frac{3\pi}{2}\eta_0\right) \\
 &\stackrel{(C.13)}{=} \exp\left(ik_0 r - i\eta_0 (\log(2k_0 r) + i\pi) + \frac{3\pi}{2}\eta_0\right) \\
 &= \exp\left(ik_0 r - i\eta_0 \log(2k_0 r) + \eta_0\pi + \frac{3\pi}{2}\eta_0\right) \\
 &= \exp\left(ik_0 r - i\eta_0 \log(2k_0 r) + \frac{5\pi}{2}\eta_0\right); \\
 \exp\left(ik_\gamma r - i\eta_\gamma \log(2k_\gamma r) - \frac{\pi}{2}\eta_\gamma\right) &\longrightarrow \exp\left(-ik_0 r + i\eta_0 \log(-2k_0 r) + \frac{\pi}{2}\eta_0\right) \\
 &\stackrel{(C.13)}{=} \exp\left(-ik_0 r + i\eta_0 (\log(2k_0 r) + i\pi) + \frac{\pi}{2}\eta_0\right) \\
 &= \exp\left(-ik_0 r + i\eta_0 \log(2k_0 r) - \pi\eta_0 + \frac{\pi}{2}\eta_0\right) \\
 &= \exp\left(-ik_0 r + i\eta_0 \log(2k_0 r) - \frac{\pi}{2}\eta_0\right).
 \end{aligned}$$

The properties of  $L^2$  comes from Remark 20.

## D Definition of the Kummer functions

Equation (4.21) has a regular singularity at  $z = 0$  with indices 0 and  $1 - b$ , and an irregular singularity at infinity of rank one. When  $b$  is not an integer, method of Fröbenius can be used to construct two linearly independent solution. The first Kummer function, also called **confluent hypergeometric function**,  $M(a, b; z)$  or  ${}_1F_1(a, b; z)$  cf. [32, Eqn 13.2.2],

$$M(a, b; z) = {}_1F_1(a, b; z) := \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k k!} z^k, \quad b \neq -1, -2, -3, \dots \quad (D.1)$$

Here  $(\bullet)_k$  is the Pochhammer's symbol, cf. [32, Eqn 5.2(iii)],

$$(a)_k := \frac{\Gamma(a+k)}{\Gamma(a)}. \quad (D.2)$$

When  $b$  is not an integer, then in the neighborhood of  $z = 0$ , a pair of linearly independent solution to the Kummer equation are given by,

$$M(a, b; z) \quad \text{and} \quad z^{1-b} M(a-b+1, 2-b; z), \quad b \neq 0, -1, -2, \dots \quad (D.3)$$

$M(a, b; z)$  is entire in  $z$  and  $a$  while meromorphic in  $b$ , with single order poles at  $b = -1, -2, -3, \dots$ . This results in  $M_{\kappa, \ell + \frac{1}{2}}(z)$  not defined for  $2\ell + 2 = -1, -2, -3, \dots$  (i.e.  $2 + 2\ell \in \mathbb{Z}^-$ ). However, these are

also the same poles of the Gamma function, the limiting value  $\lim_{b \rightarrow -n} \frac{M(a, b; z)}{\Gamma(b)}$  exists. In fact, the function

$$\mathbf{M}(a, b; z) := \frac{M(a, b; z)}{\Gamma(b)} \quad (D.4)$$

is entire in  $a, b$  and  $z$ , and cf. [8, Eqn 8a p.4]

$$\lim_{b \rightarrow -n} \frac{M(a, b; z)}{\Gamma(b)} = \mathbf{M}(a, -n; z) = \frac{(a)_{n+1}}{(n+1)!} z^{n+1} M(a+n+1, n+2; z), \quad n = 0, 1, 2, \dots \quad (D.5)$$



Using the simplification<sup>28</sup>, this can be written as, cf. [8, Eqn 8a p.4]

$$\lim_{b \rightarrow -n} \frac{M(a, b; z)}{\Gamma(b)} = z^{n+1} \sum_{k=0}^{\infty} \frac{(a)_{n+1+k}}{(n+1+k)!} \frac{z^k}{k!} = \sum_{k=n+1}^{\infty} \frac{(a)_k}{(k-n-1)!} \frac{z^k}{k!}. \quad (\text{D.6})$$

Note that  $\Gamma(k-n) = (k-n-1)!$ .

Despite the fact that the limiting value exists at  $b = -1, -2, -3, \dots$ , the pair (D.3) are linearly dependent when  $b \in \mathbb{Z}$ . In this case, we have to generate another independent solution by differentiating with respect to the parameter  $b$ . This gives rise to the second Kummer function, also called **Tricomi confluent hypergeometric** function,  $U(a, b, z)$ , which is uniquely determined by the property

$$U(a, b; z) \sim z^{-a} \quad , \quad z \rightarrow \infty \quad , \quad |\text{Arg } z| \leq \frac{3}{2}\pi - \delta. \quad (\text{D.7})$$

In general, this is a multi-valued function (due to the factor  $z^{-a}$  (with the origin being a branch point and the point at infinity an essential singularity). The principal branch is that of  $\ln z$ , by convention in [32, 13.14.22]. We list its specific definitions under the assumption<sup>29</sup>  $a \neq 0, -1, -2, \dots$

- When  $b$  is not an integer, cf. [27, p.263-264]

$$\begin{aligned} U(a, b; z) &:= \frac{\pi}{\sin(\pi b)} \left( \frac{M(a, b; z)}{\Gamma(b) \Gamma(1+a-b)} - z^{1-b} \frac{M(a+1-b, 2-b; z)}{\Gamma(a) \Gamma(2-b)} \right) \\ &\quad , \quad -\pi < \text{Arg } z \leq \pi, \quad b \notin \mathbb{Z} \\ &= \frac{\Gamma(1-b)}{\Gamma(1+a-b)} M(a, b; z) + \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b} M(1+a-b, 2-b; z). \end{aligned} \quad (\text{D.8})$$

The second equality is obtained by using

$$\frac{\pi}{\sin(\pi b)} = \Gamma(b) \Gamma(1-b) = -\Gamma(b-1) \Gamma(2-b).$$

- When  $b$  is an integer, then for  $b = n+1$ ,  $n = 0, 1, 2$ , and  $a \neq 0, -1, -2$ , cf. [32, 13.2.9],

$$\begin{aligned} U(a, n+1, z) &:= \frac{1}{\Gamma(a)} \sum_{k=1}^n \frac{(k-1)! (1-a+k)_{n-k}}{(n-k)!} z^{-k} + \frac{(-1)^{n+1}}{n! \Gamma(a-n)} M(a, n+1; z) \ln z \\ &\quad \frac{(-1)^{n+1}}{n! \Gamma(a-n)} (\psi(a+k) - \psi(1+k) - \psi(n+k+1)) \quad , \quad n = 0, 1, 2, \dots \end{aligned} \quad (\text{D.9})$$

Here  $\psi$  is the Digamma function listed in Notations.

- When  $b = -n$ ,  $n = 0, 1, 2, \dots$ , then

$$U(a, -n, z) = z^{n+1} U(a+n+1, n+2, z) \quad , \quad n = 0, 1, 2, \dots \quad (\text{D.10})$$

where the expression on the right-hand-side is given defined by (D.9).

---

<sup>28</sup>Note that  $\Gamma(k) = (k-1)!$  for  $k \in \mathbb{Z}^+$ ,

$$\begin{aligned} (a)_{n+1} (a+n+1)_k &= \frac{\Gamma(a+n+1)}{\Gamma(a)} \frac{\Gamma(a+n+1+k)}{\Gamma(a+n+1)} = \frac{\Gamma(a+n+1+k)}{\Gamma(a)} = (a)_{n+1+k} \\ (n+1)! (n+2)_k &= (n+1)! \frac{\Gamma(n+2+k)}{\Gamma(n+2)} = (n+1)! \frac{(n+1+k)!}{(n+1)!} = (n+1+k)!. \end{aligned}$$

<sup>29</sup>This is sufficient since in our application  $\kappa = i \frac{\alpha}{2k}$  is not integer, while  $\mu = \ell + \frac{1}{2}$  with  $\ell = 0, 1, 2, \dots$

**Basis of independent solutions** We list a basis of independent solution, cf. [27, 6.3 and 6.3.1 p 269].

- $b = n + 1$  for  $n = 1, 2, 3, \dots$ , two linearly independent solutions are, are

$$M(a, n + 1; z) \quad \text{and} \quad \frac{n! \Gamma(a - n)}{(-1)^{n+1}} U(a, n + 1, z). \quad (\text{D.11})$$

In cf. [32, 13.2.47], the second basis function is written <sup>30</sup>in the form (D.12).

- $b = -n$ , for  $n = 0, 1, 2, \dots$ , using (D.10), two linearly independent solutions are

$$z^{n+1} M(a + n + 1, n + 2; z) \quad \text{and} \quad \frac{(n + 1)! \Gamma(a - 1)}{(-1)^n} U(a, -n, z) = z^{n+1} \frac{(n + 1)! \Gamma(a - 1)}{(-1)^n} U(a + n + 1, n + 2; z). \quad (\text{D.13})$$

In [32, 13.2.30], the second basis function is written<sup>31</sup> as (D.14).

A basis of solutions for Kummer's equation in the neighborhood of infinity is given by

$$\begin{aligned} U(a, b, z) \quad , \quad e^z U(b - a, b, e^{-\pi i} z) \quad , \quad -\frac{1}{2}\pi \leq \text{Arg } z \leq \frac{3}{2}\pi; \\ U(a, b, z) \quad , \quad e^z U(b - a, b, e^{\pi i} z) \quad , \quad -\frac{3}{2}\pi \leq \text{Arg } z \leq \frac{1}{2}\pi. \end{aligned} \quad (\text{D.15})$$

## E Justification of integration under the integral sign

### E.1 Volume integral

<sup>30</sup>By algebraic derivation, we can rewrite  $\frac{n! \Gamma(a - n)}{(-1)^{n+1}} U(a, n + 1, z)$ ,  $n = 1, 2, 3, \dots$ , as

$$\sum_{k=1}^n \frac{n! (k - 1)!}{(n - k)! (1 - a)_k} z^{-k} - \underbrace{M(a, n + 1; z) \ln z - \sum_{k=0}^{\infty} \frac{(a)_k}{(n + 1)_k} \frac{z^k}{k!} (\psi(a + k) - \psi(1 + k) - \psi(n + k + 1))}_{:=\mathbb{J}}. \quad (\text{D.12})$$

Using the definition of  $U$  given in (D.9) in this case, we have

$$\frac{n! \Gamma(a - n)}{(-1)^{n+1}} U(a, n + 1, z) = -\mathbb{J} + \frac{n! \Gamma(a - n)}{(-1)^{n+1}} \frac{1}{\Gamma(a)} \sum_{k=1}^{\infty} \frac{(k - 1)! (1 - a + k)_{n-k}}{(n - k)!} z^{-k}$$

Consider the coefficients of the second series,

$$\begin{aligned} \frac{n! \Gamma(a - n)}{(-1)^{n+1}} \frac{1}{\Gamma(a)} \frac{(k - 1)! (1 - a + k)_{n-k}}{(n - k)!} &= \frac{n! (k - 1)!}{(n - k)!} \frac{\Gamma(1 - a)}{\Gamma(1 - a + k)} \frac{\Gamma(a - n)}{\Gamma(a)} \frac{\Gamma(1 - a + k + n - k)}{\Gamma(1 - a)} \\ &= \frac{n! (k - 1)!}{(n - k)! (1 - a)_k} \times \underbrace{\frac{1}{(-1)^{n+1}} \frac{\Gamma(a - n) \Gamma(1 - (a - n))}{\Gamma(a) \Gamma(1 - a)}}_{-1}. \end{aligned}$$

That the second factor is  $-1$ , is due to the identity, for  $a \neq \mathbb{Z}$ ,

$$\Gamma(a) \Gamma(1 - a) = \frac{\pi}{\sin(\pi a)},$$

and

$$\Gamma(a - n) \Gamma(1 - (a - n)) = \frac{\pi}{\sin(\pi(a - n))} = \frac{\pi}{\sin(\pi a) \cos(\pi n)} = \frac{\pi}{(-1)^n \sin(\pi a)}.$$

<sup>31</sup>With the same derivation as in Footnote 30, the right-hand-side can be written as

$$\begin{aligned} &\sum_{k=1}^{n+1} \frac{(n + 1)! (k - 1)!}{(n - k + 1)! (-a - n)_k} z^{n-k+1} - z^{n+1} M(a + n + 1, n + 2; z) \ln z \\ &- z^{n+1} \sum_{k=0}^{\infty} \frac{(a + n + 1)_k}{(n + 2)_k} \frac{z^k}{k!} (\psi(a + n + k + 1) - \psi(1 + k) - \psi(n + k + 2)). \end{aligned} \quad (\text{D.14})$$

**Proposition 31.** Consider a bounded region  $\Omega$  with  $\mathcal{C}^2$  boundary and  $\Omega \subset \mathbb{B}_{(0,\mathfrak{r})}$ . We have

$$\partial_{r(x)} \int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy = \int_{\mathbb{R}^3} \partial_{r(x)} \Phi_{\mathbf{k}_0}^+(x, y) f(y) dy \quad , \quad f \in L_c^2(\mathbb{R}^3). \quad (\text{E.1})$$

*Proof.* Recall the notation

$$\partial_{r(x)} h(x) = \lim_{\delta \rightarrow 0^+} \frac{h(x + \delta \frac{x}{|x|}) - h(x)}{\delta} \quad ; \quad \partial_{r(x)} h(x) = \frac{x}{|x|} \cdot \nabla_x h.$$

For  $\mathbf{k}_0$ , we work with compactly supported function  $f$ . Denote by  $\Omega$  the support of function  $f$  in this case (i.e. without attenuation). Also define the product domains

$$\begin{aligned} \mathfrak{R} &:= (\mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})})_x \times \Omega_y ; \\ \tilde{\mathfrak{R}} &:= (\mathbb{B}_{(0,\tilde{\mathfrak{r}})} \setminus \mathbb{B}_{(0,\mathfrak{r})})_x \times \Omega_y . \end{aligned}$$

**Step 0 :** We first rewrite the problem in order to apply dominated convergence theorem. In spherical coordinates based at  $x$ ,

$$r_x := |y - x| \quad , \quad \varpi_x = \frac{y - x}{|x - y|}.$$

we write

$$\int_{\mathbb{R}^3} \Phi_{\mathbf{k}_0}^+(x, y) dy = \int_0^\infty \int \Phi_{\mathbf{k}_0}^+(x, x + r_x \varpi_x) r_x^2 dr_x d\varpi_x.$$

Define

$$\begin{aligned} h_\delta &:= \frac{\Phi_{\mathbf{k}_0}^+(x + \delta \frac{x}{|x|}, x + r_x \varpi_x) - \Phi_{\mathbf{k}_0}^+(x, x + r_x \varpi_x)}{\delta} f(x + r_x \varpi_x) r_x^2 ; \\ h &:= \left( \partial_{r(x)} \Phi_{\mathbf{k}_0}^+ \Big|_{x, x+r_x \varpi_x} \right) f(x + r_x \varpi_x) r_x^2 . \end{aligned}$$

By definition of direction limit,

$$\lim_{\delta \rightarrow 0^+} h_\delta = \partial_{r(x)} \Phi_{\mathbf{k}_0}^+(x, y).$$

In terms of the  $h$  and  $h_\delta$ , what we want to justify is now of the form

$$\lim_{\delta \rightarrow 0^+} \int_0^\infty \int_{\mathbb{S}_{(0,1)}} h_\delta dr_x d\varpi_x = \int_0^\infty \int_{\mathbb{S}_{(0,1)}} \lim_{\delta \rightarrow 0^+} h dr_x d\varpi_x .$$

**Step 1 :** Since  $\Phi_{\mathbf{k}_0}^+(x, y) r_x^2$  is continuous in  $x$  and  $y$ ,  $h_\delta$  and  $h$  are measurable function. What remains to show that : there exists  $\delta > 0$  and an integrable function  $\mathfrak{g}(y)$  such that

$$|h_\delta| \leq \mathfrak{g}(y) \quad , \quad \forall \delta < \delta_0.$$

Define the function

$$s \mapsto \phi(s) := \Phi_{\mathbf{k}_0}^+(x + s \frac{x}{|x|}, y).$$

We have

$$\frac{d}{ds} \phi(s) = \partial_{r(x)} \Phi_{\mathbf{k}_0}^+ \Big|_{(x+s \frac{x}{|x|}, y)}.$$

and

$$\Phi_{\mathbf{k}_0}^+(x + \delta \frac{x}{|x|}, y) - \Phi_{\mathbf{k}_0}^+(x, y) = \int_0^\delta \frac{d}{ds} \phi(s) ds.$$

We obtain the bound

$$r_x^2 |f(y)| \frac{|\Phi_{k_0}^+(x + \delta \frac{x}{|x|}, y) - \Phi_{k_0}^+(x, y)|}{\delta} \leq \|f(y) r_x^2 \phi'(s)\|.$$

And

$$|h_\delta| \leq \left\| r_x^2 f(y) \nabla_x \Phi_{k_0}^+ \right\|_{L^\infty(\mathfrak{R})} \mathbf{1}_\Omega(y) \quad , \quad (x, y) \in \tilde{\mathfrak{R}}. \quad (\text{E.2})$$

On the other hand, from (F.32) in Appendix F.7, we have

$$|x - y|^2 |\nabla_x \Phi_{k_0}^+| \leq \mathfrak{c} |G_0^+(x, y)| + 2 \mathfrak{c} |x - y| (|\partial_s H_0^+| + |\partial_t H_0^+|).$$

From Remark 33 in Appendix F.6, exists  $C > 0, \tilde{C}$  depending on  $\Omega$ , and  $\tilde{C} > 0$  depending on  $\Omega, \mathfrak{r}, \tilde{\mathfrak{r}}$ , so that

$$|G_0^+(x, y)| < C \quad , \quad \text{for } x \in \mathbb{R}^3, y \in \Omega;$$

$$\text{and } \partial_t H_0^+, \text{ for } \partial_s H_0^+ < \tilde{C} \quad , \quad (x, y) \in \mathfrak{R}.$$

Thus there exists  $C' > 0$  depending on  $\Omega, \mathfrak{r}$  and  $\tilde{\mathfrak{r}}$  such that

$$|x - y|^2 |\nabla_x \Phi_{k_0}^+| \leq C' \quad , \quad \text{for } (x, y) \in \tilde{\mathfrak{R}}.$$

Combining with (E.2), we obtain: there exists  $C'' > 0$  depending on  $\Omega, \mathfrak{r}$  and  $\tilde{\mathfrak{r}}$

$$|h_\delta| \leq C'' \mathbf{1}_\Omega(y) \quad , \quad (x, y) \in \tilde{\mathfrak{R}}.$$

After this, we can apply Dominated Convergence Theorem to obtain

$$\lim_{\delta \rightarrow 0^+} \int_0^\infty \int_{\mathbb{S}_{(0,1)}} h_\delta dr_x d\varpi_x = \int_0^\infty \int_{\mathbb{S}_{(0,1)}} \lim_{\delta \rightarrow 0^+} h dr_x d\varpi_x.$$

□

**Remark 31.** If we show differentiability for  $x$  away from the region of integration in the variable  $y$ , then we can work directly with

$$h := \partial_{r(x)} \Phi_{k_0} \quad , \quad h_\delta := \frac{\Phi_{k_0}^+(x + \delta \frac{x}{|x|}, y) - \Phi_{k_0}^+(x, y)}{\delta}.$$

In particular, we assume

$$\Omega \subset \mathbb{B}_{(0,\mathfrak{r})},$$

and

$$\mathfrak{R} := (\mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})})_x \times (\partial\Omega)_y,$$

then Remark 33, in particular, (F.29) in Appendix F, gives  $C > 0$  such that

$$\sup_{(x,y) \in \mathfrak{R}} \Phi_{k_0}^+(x, y) \quad , \quad \sup_{(x,y) \in \mathfrak{R}} \partial_{r(x)} \Phi_{k_0}^+(x, y) < C < \infty.$$

As a result, the sequence  $\{h_\delta\}$  is bounded by an integrable function on  $\partial\Omega$  (for statement 1) or  $\mathbb{S}_{(0,\mathfrak{r})}$  (for statement 2). In addition, both  $h$  and  $h_\delta$  are continuous on region (E.5) or (E.6), and are thus measurable there. We then apply dominated convergence theorem to obtain: for  $(x, y) \in \mathbb{R}^3 \setminus \mathbb{B}_{(0,\tilde{\mathfrak{r}})} \times \partial\Omega$ ,  $\phi \in L^\infty(\partial\Omega)$

$$\partial_{r(x)} \int_{\mathbb{R}^3} f(y) \Phi_{k_0}^+(x, y) dy = \int_{\mathbb{R}^3} f(y) \partial_{r(x)} \Phi_{k_0}^+(x, y) dy \quad , \quad f \in L_c^2(\mathbb{R}^3). \quad \triangle$$

## E.2 Surface integral

Since our purpose for differentiating the integral is to obtain the asymptotic expansion as  $|x| \rightarrow \infty$ , we will only justify a weaker statement and assume  $x$  away from the domain of integration in variable  $y$ .

**Proposition 32.** • Consider a bounded region  $\Omega$  with  $\mathcal{C}^2$  boundary and  $\Omega \subset \mathbb{B}_{(0,\mathfrak{r})}$ . For  $(x, y) \in \mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})} \times \partial\Omega$ ,  $\phi \in L^\infty(\partial\Omega)$ , we have

$$\partial_{r(x)} \int_{\partial\Omega} \phi(y) \Phi_{\mathbf{k}}(x, y) d\sigma(y) = \int_{\partial\Omega} \phi(y) \partial_{r(x)} \Phi_{\mathbf{k}}(x, y) d\sigma(y). \quad (\text{E.3})$$

• With  $\tilde{\mathfrak{r}} > \mathfrak{r} > 0$ , For  $(x, y) \in \mathbb{R}^3 \setminus \mathbb{B}_{(0,\tilde{\mathfrak{r}})} \times \mathbb{S}_{(0,\mathfrak{r})}$ ,  $\phi \in L^\infty(\mathbb{S}_{(0,\mathfrak{r})})$ , we have

$$\partial_{r(x)} \int_{\mathbb{S}_{(0,\mathfrak{r})}} \phi(y) \partial_{r(y)} \Phi_{\mathbf{k}}(x, y) d\sigma(y) = \int_{\mathbb{S}_{(0,\mathfrak{r})}} \phi(y) \partial_{r(x)} \partial_{r(y)} \Phi_{\mathbf{k}}(x, y) d\sigma(y). \quad (\text{E.4})$$

*Proof.* For

$$(x, y) \in (\mathbb{R}^3 \setminus \Omega)_x \times \partial\Omega, \quad \text{with } \Omega \subset \mathbb{B}_{(0,\mathfrak{r})}, \quad (\text{E.5})$$

or

$$(x, y) \in (\mathbb{R}^3 \setminus \mathbb{B}_{(0,\tilde{\mathfrak{r}})})_x \times \mathbb{S}_{(0,\mathfrak{r})}, \quad (\text{E.6})$$

we can use Remark 33, in particular, (F.29) and (F.30) of Appendix F, for there exists  $C > 0$  such that

$$\sup_{(x,y) \in \mathfrak{R}} \Phi_{\mathbf{k}_0}^+(x, y), \quad \sup_{(x,y) \in \mathfrak{R}} \partial_{r(y)} \Phi_{\mathbf{k}_0}^+(x, y), \quad \sup_{(x,y) \in \mathfrak{R}} \partial_{r(x)} \partial_{r(y)} \Phi_{\mathbf{k}_0}^+(x, y) < C < \infty.$$

To justify (E.3), we use

$$h := \partial_{r(x)} \Phi_{\mathbf{k}_0}, \quad h_\delta := \frac{\Phi_{\mathbf{k}_0}^+\left(x + \delta \frac{x}{|x|}, y\right) - \Phi_{\mathbf{k}_0}^+(x, y)}{\delta},$$

while for (E.4), we work with

$$h := \partial_{r(x)} \partial_{r(y)} \Phi_{\mathbf{k}_0},$$

and

$$h_\delta := \frac{\partial_{r(y)} \Phi_{\mathbf{k}_0}^+\left(x + \delta \frac{x}{|x|}, y\right) - \partial_{r(y)} \Phi_{\mathbf{k}_0}^+(x, y)}{\delta}.$$

With the constant  $C$  introduced, we have the boundedness

$$|h|, \quad |h_\delta| < C.$$

As a result, the sequence  $\{h_\delta\}$  is bounded by an integrable function on  $\partial\Omega$  (for statement 1) or  $\mathbb{S}_{(0,\mathfrak{r})}$  (for statement 2). In addition, both  $h$  and  $h_\delta$  are continuous on region (E.5) or (E.6), and are thus measurable there. The proof is finished by applying dominated convergence theorem.  $\square$

## F Gradient and asymptotics

### F.1 Gradients and asymptotic of functions involving the distance function

**Notations** : Write  $x = (x_1, x_2, x_3)$  and  $y = (y_1, y_2, y_3)$ . Also denote

$$\partial_{r(x)} := \frac{x}{|x|} \cdot \nabla_x; \quad \partial_{r(y)} := \frac{y}{|y|} \cdot \nabla_y. \quad (\text{F.1})$$

Denote by  $(|x|, \theta_x, \phi_x)$ , and  $(|y|, \theta_y, \phi_y)$  the spherical coordinates of  $x$  and  $y$  with  $0 \leq \theta \leq \pi$  and  $0 \leq \phi \leq 2\pi$ . We have

$$x \cdot y = |x| |y| \frac{x}{|x|} \cdot \frac{y}{|y|}$$

and we define the bounded quantity  $\mathfrak{d}_{x,y}$ ,

$$\mathfrak{d}_{x,y} := \frac{x}{|x|} \cdot \frac{y}{|y|} = \cos \theta_x \cos \theta_y + \sin \theta_x \sin \theta_y \cos(\phi_x - \phi_y). \quad (\text{F.2})$$

We write

$$x \cdot y = |x| |y| \mathfrak{d}_{x,y}. \quad (\text{F.3})$$

In two dimension, this simplifies to

$$\frac{x}{|x|} \cdot \frac{y}{|y|} = \mathfrak{d}_{x,y}.$$

## F.2 Asymptotics involving the distance function

For  $y$  in compact set and as  $|x| \rightarrow \infty$ , using (F.3), we have the following expansion,

$$|x - y| = \left( |x|^2 - 2|x||y|\mathfrak{d}_{x,y} + |y|^2 \right)^{1/2} \quad (\text{F.4a})$$

$$= |x| \left( 1 - 2 \frac{|y|}{|x|} \mathfrak{d}_{x,y} + \frac{|y|^2}{|x|^2} \right)^{1/2} \quad (\text{F.4b})$$

$$= |x| \left( 1 - \frac{|y|}{|x|} \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-2}) \right). \quad (\text{F.4c})$$

For the version in 2Dcf. [9, p.64]. The above expansion gives, for  $y$  in compact set and as  $|x| \rightarrow \infty$ ,

$$|x - y| = |x| - |y| \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}); \quad (\text{F.5a})$$

$$\frac{1}{|x - y|} = \frac{1}{|x|} \left( 1 + \mathcal{O}(|x|^{-1}) \right); \quad (\text{F.5b})$$

Using the above expression, we next obtain

$$\begin{aligned} \frac{x \cdot (x - y)}{|x||x - y|} &= \frac{1}{|x|} \left( |x|^2 - |x||y|\mathfrak{d}_{x,y} \right) \frac{1}{|x|} \left( 1 + \mathcal{O}(|x|^{-1}) \right) \\ &= \left( 1 - \frac{|y|}{|x|} \mathfrak{d}_{x,y} \right) \left( 1 + \mathcal{O}(|x|^{-1}) \right) \end{aligned} \quad (\text{F.6a})$$

$$= 1 + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1); \quad (\text{F.6b})$$

$$\begin{aligned} \frac{y \cdot (x - y)}{|y||x - y|} &= \left( -|y| + |x|\mathfrak{d}_{x,y} \right) \frac{1}{|x|} \left( 1 + \mathcal{O}(|x|^{-1}) \right) \\ &= \left( -\frac{|y|}{|x|} + \mathfrak{d}_{x,y} \right) \left( 1 + \mathcal{O}(|x|^{-1}) \right) \end{aligned} \quad (\text{F.6c})$$

$$= \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1). \quad (\text{F.6d})$$

and

$$s = 2|x| + |y| \left( 1 - \mathfrak{d}_{x,y} \right) + \mathcal{O}(|x|^{-1}); \quad (\text{F.7a})$$

$$t = |y| \left( 1 + \mathfrak{d}_{x,y} \right) + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1). \quad (\text{F.7b})$$

## F.3 Gradients and normal gradients of the distance functions

$$\nabla_x |x| = \nabla_x \sqrt{x_1^2 + x_2^2 + x_3^2} = \frac{x}{|x|} \quad ; \quad \nabla_x |x|^{-1} = -\frac{x}{|x|^3}. \quad (\text{F.8})$$

$$\nabla_x |x - y| = \nabla_x ((x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2)^{1/2} = \frac{x - y}{|x - y|}; \quad (\text{F.9a})$$

$$\nabla_y |x - y| = \frac{y - x}{|x - y|}. \quad (\text{F.9b})$$

and

$$\nabla_x \frac{1}{|x - y|} = \nabla_x ((x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2)^{-1/2} = -\frac{x - y}{|x - y|^3}; \quad (\text{F.10a})$$

$$\nabla_y \frac{1}{|x - y|} = \frac{x - y}{|x - y|^3}. \quad (\text{F.10b})$$

We next consider the normal gradients

$$\partial_{r(y)} \frac{1}{|x - y|} = \frac{y}{|y|} \cdot \frac{x - y}{|x - y|^3} \quad ; \quad \partial_{r(x)} \frac{1}{|x - y|} = -\frac{x}{|x|} \cdot \frac{x - y}{|x - y|^3}; \quad (\text{F.11a})$$

$$\begin{aligned} \partial_{r(x)} \partial_{r(y)} \frac{1}{|x - y|} &= \frac{y}{|y|} \cdot \left( \frac{x}{|x|} \cdot \nabla_x \right) \frac{x - y}{|x - y|^3} \\ &= \frac{y}{|y|} \cdot \left( \frac{x}{|x||x - y|^3} \nabla_x (x - y) + (x - y) \partial_{r(x)} \frac{1}{|x - y|^3} \right) \\ &= \frac{y}{|y|} \cdot \left( \frac{x}{|x|} + 3 \frac{x - y}{|x - y|} \frac{x}{|x|} \cdot \frac{x - y}{|x - y|} \right) \frac{1}{|x - y|^3}. \end{aligned} \quad (\text{F.11b})$$

As a result of this, for  $y$  in compact set and  $|x| \rightarrow \infty$ , we have

$$\begin{aligned} \partial_{r(x)} |x - y|^{-1} &= \mathcal{O}(|x|^{-2}) \quad ; \quad \partial_{r(y)} |x - y|^{-1} = \mathcal{O}(|x|^{-2}); \\ \partial_{r(x)} \partial_{r(y)} |x - y|^{-1} &= \mathcal{O}(|x|^{-3}). \end{aligned} \quad (\text{F.12})$$

**Gradients and normal gradients of the functions  $s$  and  $t$**

$$\nabla_x s = \nabla_x (|x| + |y| + |x - y|) = \frac{x}{|x|} + \frac{x - y}{|x - y|}; \quad (\text{F.13a})$$

$$\nabla_y s = \frac{y}{|y|} + \frac{x - y}{|y - x|}; \quad (\text{F.13b})$$

$$\nabla_x t = \frac{x}{|x|} - \frac{x - y}{|x - y|} \quad ; \quad \nabla_y t = \frac{y}{|y|} - \frac{y - x}{|x - y|}. \quad (\text{F.13c})$$

We compute the normal gradients.

$$\partial_{r(y)} s = 1 + \frac{y}{|y|} \cdot \frac{y - x}{|x - y|} \quad ; \quad \partial_{r(y)} t = 1 - \frac{y}{|y|} \cdot \frac{y - x}{|x - y|}; \quad (\text{F.14a})$$

$$\partial_{r(x)} s = 1 + \frac{x}{|x|} \cdot \frac{x - y}{|x - y|} \quad ; \quad \partial_{r(x)} t = 1 - \frac{x}{|x|} \cdot \frac{x - y}{|x - y|}. \quad (\text{F.14b})$$

As a result of this, for  $y$  in compact set and  $|x| \rightarrow \infty$ , we have

$$\partial_{r(x)} s \stackrel{F.6b}{=} 1 + (1 + \mathcal{O}(|x|^{-1})) = 2 + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1); \quad (\text{F.15a})$$

$$\partial_{r(y)} s \stackrel{F.6d}{=} 1 + (\mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1})) = 1 + \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1). \quad (\text{F.15b})$$

and

$$\partial_{r(x)} t \stackrel{F.6b}{=} 1 - (1 + \mathcal{O}(|x|^{-1})) = \mathcal{O}(|x|^{-1}) = \mathcal{O}(1); \quad (\text{F.16a})$$

$$\partial_{r(y)} t \stackrel{F.6d}{=} 1 - (\mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1})) = 1 - \mathfrak{d}_{x,y} + \mathcal{O}(|x|^{-1}) = \mathcal{O}(1). \quad (\text{F.16b})$$

Using  $\partial_{r(x)}(x - y) = \frac{x}{|x|}$  to obtain the second order normal gradients

$$\begin{aligned}\partial_{r(x)}\partial_{r(y)}s &= \frac{y}{|y|} \cdot \partial_{r(x)} \frac{y - x}{|x - y|} \\ &= \frac{y}{|y|} \cdot \left( -\frac{x}{|x|} \frac{1}{|x - y|} + (y - x) \frac{x}{|x|} \cdot \frac{x - y}{|x - y|^3} \right); \end{aligned} \quad (\text{F.17a})$$

$$\partial_{r(x)}\partial_{r(y)}t = -\partial_{r(x)}\partial_{r(y)}s. \quad (\text{F.17b})$$

For  $y$  in compact set and  $|x| \rightarrow \infty$ , we have

$$\partial_{r(x)}\partial_{r(y)}s = -\partial_{r(x)}\partial_{r(y)}s = O(|x|^{-1}). \quad (\text{F.18})$$

#### F.4 Other identities with the distance function

We have

$$\begin{aligned}|y||x - y| - y \cdot (y - x) &= |y||x - y| - |y|^2 + y \cdot x \\ &= |y|(|x - y| - |y| - |x| + |x|(1 + \mathfrak{d}_{x,y})); \\ \Rightarrow 1 - \frac{y \cdot (y - x)}{|y||y - x|} &= \frac{-t + |x|(1 + \mathfrak{d}_{x,y})}{|x - y|}; \\ \Rightarrow \frac{\partial_{r(y)}t}{t} &= \frac{1}{t} \left( 1 - \frac{y \cdot (y - x)}{|y||y - x|} \right) = \frac{1}{|x - y|} (-1 + |x| \frac{1 + \mathfrak{d}_{x,y}}{t}). \end{aligned}$$

On the other hand, since

$$\begin{aligned}|x - y|^2 &= |x|^2 + |y|^2 - 2|x||y|\mathfrak{d}_{x,y} \\ \Rightarrow (|x| + |y|)^2 - |x - y|^2 &= 2|x||y|(1 + \mathfrak{d}_{x,y}); \end{aligned}$$

and

$$\begin{aligned}\frac{1}{t} &= \frac{1}{|x| + |y| - |x - y|} = \frac{|x| + |y| + |x - y|}{(|x| + |y|)^2 - |x - y|^2} = \frac{s}{2|x||y|(1 + \mathfrak{d}_{x,y})}; \\ \Rightarrow |x| \frac{1 + \mathfrak{d}_{x,y}}{t} &= |x| \frac{1 + \mathfrak{d}_{x,y}}{1} \frac{s}{2|x||y|(1 + \mathfrak{d}_{x,y})} = \frac{s}{2|y|}, \end{aligned}$$

we can write

$$\boxed{\frac{\partial_{r(y)}t}{t} = \frac{1}{|x - y|} \left( -1 + \frac{s}{2|y|} \right)}. \quad (\text{F.19})$$

Similarly, switching the role of  $x$  and  $y$ , we obtain

$$\frac{\partial_{r(x)}t}{t} = \frac{1}{t} \left( 1 - \frac{x \cdot (x - y)}{|x||x - y|} \right) = \frac{1}{|x - y|} \left( -1 + |y| \frac{1 + \mathfrak{d}_{x,y}}{t} \right).$$

After simplification, we have

$$\boxed{\frac{\partial_{r(x)}t}{t} = \frac{1}{|x - y|} \left( -1 + \frac{s}{2|x|} \right)}. \quad (\text{F.20})$$



## F.5 Partial derivatives of $H$

We calculate here  $\partial_s H$  and  $\partial_t H$ . Recall

$$H(s, t) = \begin{vmatrix} W_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix}.$$

We have

$$\partial_s \begin{vmatrix} W_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix} = - \begin{vmatrix} ikW'_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ ikW''_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix}.$$

Since  $W_{-\chi, 1/2}(-z)$  satisfies the ODE (4.67),

$$\partial_z^2 W + \left(-\frac{1}{4} + \frac{\chi}{z}\right) W = 0,$$

we can write

$$W''_{-\chi, 1/2}(-iks) = \left(\frac{1}{4} + \frac{\chi}{iks}\right) W_{-\chi, 1/2}(-iks). \quad (\text{F.21})$$

Replace this in the previous expression to obtain,

$$\begin{aligned} \partial_s H &= -ik \begin{vmatrix} W'_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ \left(\frac{1}{4} + \frac{\chi}{iks}\right) W_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix} \\ &= -ik \left( W'_{-\chi, 1/2}(-iks) M'_{-\chi, 1/2}(-ikt) - \frac{1}{4} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) \right) \\ &\quad + \frac{\chi}{s} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt). \end{aligned} \quad (\text{F.22})$$

Similarly, we have

$$\begin{aligned} \partial_t H &= -ik \begin{vmatrix} W_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \\ W'_{-\chi, 1/2}(-iks) & \left(\frac{1}{4} + \frac{\chi}{ikt}\right) M_{-\chi, 1/2}(-ikt) \end{vmatrix} \\ &= -ik \left( \frac{1}{4} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt) - W'_{-\chi, 1/2}(-iks) M'_{-\chi, 1/2}(-ikt) \right) \\ &\quad - \frac{\chi}{t} W_{-\chi, 1/2}(-iks) M_{-\chi, 1/2}(-ikt). \end{aligned} \quad (\text{F.23})$$

We next calculate  $\partial_s^2 H$  and  $\partial_{st} H$ . We will also use (F.21) to replace  $W''$  by  $W$ ,

$$\begin{aligned} \partial_s^2 H &= -ik \begin{vmatrix} -ik W''_{-\chi, 1/2}(-iks) & M_{-\chi, 1/2}(-ikt) \\ -ik \left(\frac{1}{4} + \frac{\chi}{iks}\right) W'_{-\chi, 1/2}(-iks) - \frac{\chi}{iks^2} W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \end{vmatrix} \\ &= -k^2 \left( \frac{1}{4} + \frac{\chi}{iks} \right) H - \frac{\chi}{s^2} M_{-\chi, 1/2}(-ikt) W'_{-\chi, 1/2}(-iks). \end{aligned} \quad (\text{F.24})$$

In a similar way, we obtain

$$\begin{aligned} \partial_{st} H &= -k^2 \begin{vmatrix} W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \\ \left(\frac{1}{4} + \frac{\chi}{iks}\right) W_{-\chi, 1/2}(-iks) & \left(\frac{1}{4} + \frac{\chi}{ikt}\right) M_{-\chi, 1/2}(-ikt) \end{vmatrix} \\ &= \frac{1}{4} k^2 H + ik\chi \begin{vmatrix} W'_{-\chi, 1/2}(-iks) & M'_{-\chi, 1/2}(-ikt) \\ s^{-1} W_{-\chi, 1/2}(-iks) & t^{-1} M_{-\chi, 1/2}(-ikt) \end{vmatrix}, \end{aligned} \quad (\text{F.25})$$

and

$$\partial_t^2 H = -k^2 \left( \frac{1}{4} + \frac{\chi}{ikt} \right) \begin{vmatrix} W_{-\chi,1/2}(-iks) & M_{-\chi,1/2}(-ikt) \\ W'_{-\chi,1/2}(-iks) & M'_{-\chi,1/2}(-ikt) \end{vmatrix} = -k^2 \left( \frac{1}{4} + \frac{\chi}{ikt} \right) H. \quad (\text{F.26})$$

## F.6 Some remarks

**Remark 32.** From the above expressions (F.22)–(F.25), we see that  $H(=G)$ , its first order derivatives

$$\partial_t H, \partial_s H,$$

and second order derivatives

$$\partial_{st} H, \partial_s^2 H,$$

are sum of quantities of the form

$$W_{-\chi,1/2}^{(n)}(-iks) M_{-\chi,1/2}^{(m)}(-ikt), \text{ where } n, m \in \{0, 1\} \quad (\text{F.27})$$

times factors of the form

$$\text{constant} \times s^{-\alpha} \text{ or } t^{-\beta}, \quad 0 \leq \alpha, \beta \leq 2.$$

Here  $n$  and  $m$  denote the order of the partial derivative in  $s$  for  $W_{-\chi,1/2}$  and in  $t$  for  $M_{-\chi,1/2}$ . In fact, since  $W$  and  $M$  satisfy an ODE of order two, all higher order derivatives of these functions can be expressed in terms of the zero-th order and first order derivatives. As a result, any derivative of  $H$   $\partial_s^\alpha \partial_t^\beta$  for  $\alpha, \beta \in \mathbb{N}$  are sum of quantities of the form (F.27) and the factor

$$\text{constant} \times s^k, \text{ or } t^{\tilde{k}}, \quad 0 \leq k, \quad \text{with } \tilde{k} \leq \max\{\tilde{\beta}, \beta\}. \quad \triangle$$

**Remark 33** (Boundedness). Consider  $x \in \mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})}$  with  $\mathfrak{r} > 0$  and  $y \in \Omega$  with  $\Omega$  bounded. Also define the product region

$$\mathfrak{R} := (\mathbb{R}^3 \setminus \mathbb{B}_{(0,\mathfrak{r})})_x \times \Omega_y.$$

In this region  $\mathfrak{R}$ ,

$$s = |x| + |y| + |x - y| > \mathfrak{r} > 0,$$

while  $t = |x| + |y| - |x - y|$  is bounded but can attain zero.

- From Prop 29 in Appendix C.1,  $M$  and  $M'$  are both defined at zero,

$$M'_{-\chi,1/2}(0) = 1, \quad M_{-\chi,1/2}(0) = 0.$$

While  $t$  can take on value zero, the limit at  $z = 0$  exists,

$$\lim_{t \rightarrow 0} \frac{M_{-\chi,1/2}(-2ikt)}{t} = -2ik.$$

On the other hand, by (F.7b), for  $y$  in compact set,  $t = O(|x|^{-1})$  as  $|x| \rightarrow \infty$ , i.e.  $t$  is bounded. As a result of this,

$$\sup_{(x,y) \in \mathfrak{R}} M_{-\chi,1/2}(-2ikt), \quad \sup_{(x,y) \in \mathfrak{R}} M'_{-\chi,1/2}(-2ikt), \quad \sup_{(x,y) \in \mathfrak{R}} \frac{M_{-\chi,1/2}(-2ikt)}{t} < \infty.$$

- From Prop 30 in Appendix C.1,

$$W_{\chi, \frac{1}{2}}(z) = \frac{1}{\Gamma(1-\chi)} + O(z \ln z), \quad z \rightarrow 0,$$

$$W'_{\chi, \frac{1}{2}}(z) = \frac{\ln z + \psi(\frac{1}{2}-\chi) + 2\gamma}{\Gamma(\frac{1}{2}-\chi)} + \frac{1}{\Gamma(1-\chi)} + O(z \ln z), \quad z \rightarrow 0.$$

On the other hand, from the asymptotic expansion at infinity of Whittaker  $W$ , cf. Prop C.4 in Appendix C,

$$\begin{aligned} W_{\chi, \frac{1}{2}}(z) &= e^{-\frac{1}{2}z} z^\chi \left(1 + O(|z|^{-1})\right), \quad |\operatorname{Arg} z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty, \\ W'_{\chi, \frac{1}{2}}(z) &= e^{-\frac{1}{2}z} z^\chi \left(\frac{1}{2} + O(|z|^{-1})\right), \quad |\operatorname{Arg} z| \leq \frac{3}{2}\pi - \delta, \quad z \rightarrow \infty, \end{aligned}$$

we have

$$\begin{aligned} W_{-\chi, \frac{1}{2}}(e^{-i\pi} i k s) &= e^{\frac{1}{2} i k s} (e^{-i\pi} i k s)^{-\chi} \left(\frac{1}{2} + O(|s|^{-1})\right), \quad \text{as } s \rightarrow \infty; \\ W'_{-\chi, \frac{1}{2}}(e^{-i\pi} i k s) &= e^{\frac{1}{2} i k s} (e^{-i\pi} i k s)^{-\chi} \left(\frac{1}{2} + O(|s|^{-1})\right), \quad \text{as } s \rightarrow \infty. \end{aligned} \quad (\text{F.28})$$

We have  $W_{-\chi, 1/2}(-2iks)$  and  $W'_{-\chi, 1/2}(-2iks)$  decay for  $k \in \mathbb{C}$  with  $\operatorname{Im} k = 0$ , or but stay bounded for  $k_0 > 0$ , cf. subsection 4.2.3. Putting together the behavior at zero and infinity, we have

$$\sup_{(x,y) \in \mathfrak{R}} W_{-\chi, \frac{1}{2}}(-2i k s), \quad \sup_{(x,y) \in \mathfrak{R}} W'_{-\chi, \frac{1}{2}}(-2i k s) < \infty.$$

Under the current assumption  $s > \mathfrak{r}$ , using the expression of its partial derivatives given in (F.22) and (F.23), and the above observation, we obtain the bounded of the partial derivatives of  $H$ ,

$$\sup_{(x,y) \in \mathfrak{R}} \partial_s^n H, n \in \{0, 1, 2\}, \quad \sup_{(x,y) \in \mathfrak{R}} \partial_t H, \quad \sup_{(x,y) \in \mathfrak{R}} \partial_s \partial_t H < \infty. \quad (\text{F.29})$$

On the other hand, from expression (F.26) for  $\partial_t^2 H$ , we see that  $\partial_t^2 H$  is not bounded due to the factor  $t^{-1}$  (which is not couple with  $M$  but  $H$ , and the latter is bounded but not zero at  $t = 0$ ). However, using either (F.19) or (F.20), we have the boundedness of

$$\sup_{(x,y) \in \mathfrak{R}} (\partial_{r(y)} t) \partial_t^2 H, \quad \sup_{(x,y) \in \mathfrak{R}} (\partial_{r(x)} t) \partial_t^2 H < \infty. \quad (\text{F.30})$$

△

**Remark 34** (Asymptotic expansion). Following from the same reasoning in Remark 33, we obtain readily the asymptotics expansion of  $\partial_s^n \partial_t^m H$ ,  $n, m \in \{0, 1\}$ . In particular, since variable  $t$  is bounded,

$$M_{-\chi, 1/2}(-2ik|t|), \quad M'_{-\chi, 1/2}(-2ik|t|), \quad \frac{M_{-\chi, 1/2}(-2ik|t|)}{t},$$

contribute as bounded terms. On the other hand, variable  $s = |x|(1 + O(|x|^{-1}))$ , the final asymptotic expansion follows from that of  $W_{-\chi, 1/2}(-2ik|t|)$  and  $W'_{-\chi, 1/2}(-2ik|t|)$  in (F.28). As a result, for  $n, m \in \mathbb{N}$ , we have

$$\partial_s^n \partial_t^m H = e^{\frac{1}{2} i k s} (e^{-i\pi} i k s)^{-\chi} \left(c(y) + O(|s|^{-1})\right), \quad \text{as } |x| \rightarrow \infty,$$

for  $y$  in compact as  $|x| \rightarrow \infty$ . Here,  $c(y)$  is a bounded and continuous function depending on  $y$ . △

## F.7 Gradient of $\Phi_k$

$y = 0$  Recall from (4.80), we have

$$\Phi_k(x, 0) = \mathfrak{c} \frac{G(x, 0)}{|x|}, \quad \text{with } G(x, 0) = W_{-\chi, 1/2}(-2ik|x|).$$

By chain rule,

$$\nabla_x \frac{1}{\mathfrak{c}} \Phi_k(x, 0) = G(x, 0) \nabla_x |x|^{-1} + \frac{1}{|x|} \nabla_x G(x, 0).$$

We next substitute in the identities

$$\nabla_x |x|^{-1} \stackrel{\text{(F.8)}}{=} -\frac{x}{|x|^3};$$

$$\nabla_x G(x, 0) = -2ik W'_{-\chi, 1/2}(-2ik|x|) \nabla_x |x| \stackrel{\text{(F.8)}}{=} -2ik W'_{-\chi, 1/2}(-2ik|x|) \frac{x}{|x|},$$

to obtain

$$\nabla_x \Phi_k(x, 0) = -c G(x, 0) \frac{x}{|x|^3} - 2c k W'_{-\chi, 1/2}(-2ik|x|) \frac{x}{|x|^2}. \quad (\text{F.31})$$

$y \neq 0$  By chain rule, we have

$$\nabla_x \Phi_k(x, y) = c G(x, y) \nabla_x \frac{1}{|x-y|} + \frac{c}{|x-y|} \nabla_x G(x, y).$$

From the calculation in Appendix F, we have

$$\nabla_x \frac{1}{|x-y|} \stackrel{\text{(F.10a)}}{=} -\frac{x-y}{|x-y|^3},$$

and

$$\nabla_x G = (\nabla_x s) \partial_s H + (\nabla_x t) \partial_t H;$$

$$\text{with } \nabla_x s \stackrel{\text{(F.13a)}}{=} \frac{x}{|x|} + \frac{x-y}{|x-y|} \quad ; \quad \nabla_x t \stackrel{\text{(F.13c)}}{=} \frac{x}{|x|} - \frac{x-y}{|x-y|}.$$

Hence

$$\nabla_x \Phi_k(x, y) = -c G(x, y) \frac{(x-y)}{|x-y|^3} + \frac{c}{|x-y|} \left( \frac{x}{|x|} (\partial_s + \partial_t) H + \frac{x-y}{|x-y|} (\partial_s - \partial_t) H \right). \quad (\text{F.32})$$

The partial derivatives of  $H$  are given in (F.23) and (F.22).

We next consider the normal derivatives. We have

$$\partial_{r(y)} \frac{1}{c} \Phi_k = G \partial_{r(y)} |x-y|^{-1} + \frac{\partial_{r(y)} s}{|x-y|} \partial_s H + \frac{\partial_{r(y)} t}{|x-y|} \partial_t H. \quad (\text{F.33})$$

And,

$$\begin{aligned} & \partial_{r(x)} \partial_{r(y)} \frac{\Phi_k}{c} \\ &= \left( \partial_{r(x)} \partial_{r(y)} |x-y|^{-1} \right) G + \left( \partial_{r(y)} |x-y|^{-1} \right) \partial_{r(x)} s \partial_s H + \left( \partial_{r(y)} |x-y|^{-1} \right) \partial_{r(x)} t \partial_t H \\ &+ \left( \partial_{r(x)} \frac{\partial_{r(y)} s}{|x-y|} \right) \partial_s H + \left( \frac{\partial_{r(y)} s}{|x-y|} \partial_{r(x)} s \right) \partial_s^2 H + \left( \frac{\partial_{r(y)} s}{|x-y|} \partial_{r(x)} t \right) \partial_{ts} H \\ &+ \left( \partial_{r(x)} \frac{\partial_{r(y)} t}{|x-y|} \right) \partial_t H + \left( \frac{\partial_{r(y)} t}{|x-y|} \partial_{r(x)} s \right) \partial_{st} H + \left( \frac{\partial_{r(y)} t}{|x-y|} \partial_{r(x)} t \right) \partial_t^2 H. \end{aligned} \quad (\text{F.34})$$

## G Incoming/outgoing convention

In this discussion, we assume that

$$k_0, \omega_0 > 0, \quad r > 0, \quad t > 0$$

The notion of incoming and outgoing are based on the direction of propagation in time. In particular, with  $t > 0$  and  $r > 0$ ,

- outgoing corresponds to as  $t \nearrow \infty$ ,  $r$  increases (wave expanding to  $\infty$ ),
- while oncoming to as  $t \nearrow \infty$ ,  $r$  decreases (wave retracting to 0).

Starting from the above notion of direction of propagation, the definition of incoming and outgoing solution in time-harmonic regime depends on the convention of the time-harmonic part.

**Convention 1 :** Time-harmonic part is given by  $e^{-i\omega_0 t}$ . This is equivalent to the Fourier transformation convention

$$(\mathcal{F}f)(\omega_0) := \int e^{i\omega_0 t} f(t) dt \quad , \quad (\mathcal{F}^{-1}f)(t) = c \int e^{-i\omega_0 t} f(\omega_0) d\omega_0. \quad (\text{G.1})$$

This is the convention used in [15, (4)]. In this case, based on the above notion of incoming/outgoing,

$$e^{ik_0 r} e^{-i\omega_0 t} = e^{i(k_0 r - \omega_0 t)} \text{ is outgoing ;}$$

$$e^{-ik_0 r} e^{-i\omega_0 t} = e^{-i(k_0 r + \omega_0 t)} \text{ is incoming .}$$

Thus, in this time-harmonic regime convention

$$e^{ik_0 r} \text{ is outgoing } , \quad \text{while} \quad e^{-ik_0 r} \text{ is incoming .}$$

This is the convention in [12], [21, p.26], which results in the sommerfeld radiation condition for Helmholtz

$$\partial_r u - ik_0 u = o(r^{-1}) , \quad r \rightarrow \infty.$$

**Convention 2 :** Time harmonic part is given by  $e^{i\omega_0 t}$ . This is equivalent to the Fourier transformation convention

$$(\mathcal{F}f)(\omega_0) := \int e^{-i\omega_0 t} f(t) dt \quad , \quad (\mathcal{F}^{-1}f)(t) = c \int e^{i\omega_0 t} f(\omega_0) d\omega_0. \quad (\text{G.2})$$

In this case, the sign is switched compared to Convention 1, i.e.

$$e^{ik_0 r} e^{i\omega_0 t} = e^{i(k_0 r + \omega_0 t)} \text{ is incoming ;}$$

$$e^{-ik_0 r} e^{i\omega_0 t} = e^{i(-k_0 r + \omega_0 t)} \text{ is outgoing .}$$

Thus, in this time-harmonic regime convention

$$e^{ik_0 r} \text{ is incoming } , \quad \text{while} \quad e^{-ik_0 r} \text{ is outgoing .}$$

## H Verification fundamental solution for $y = 0$

We show that  $\Phi_\omega$  as constructed is a fundamental solution (or equivalently that  $\Phi_\omega$  is a distributional solution to (4.131)). In the process, we will retrieve the constant  $\mathfrak{c}$ . The proof is adapted from [38, Prop. 4.9] for the Laplacian and from [35, Prop. 2.1] for the Helmholtz operator.

For arbitrary  $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^3)$ , we have to show that

$$\left\langle \left( -\Delta_x - k^2 + \frac{\alpha}{|x|} \right) \Phi_\omega , \phi \right\rangle = \phi(y) , \text{ or equivalently } \left\langle \Phi_\omega , \left( -\Delta_x - k^2 + \frac{\alpha}{|x|} \right) \phi \right\rangle = \phi(y) .$$

Here  $\langle \cdot, \cdot \rangle$  is the distributional pairing  $\mathcal{D}'(\mathbb{R}^3) \times \mathcal{D}(\mathbb{R}^3)$ . It suffices to investigate for  $y = 0$ . We have

$$\Phi_\omega(0, y) = \mathfrak{c} G(y) = \mathfrak{c} \frac{g(y)}{|y|} , \quad g(y) = W_{-\chi, 1/2}(-2i k y) .$$

We will show that

$$\lim_{\epsilon \rightarrow 0} \int_{\Omega_{(y, \epsilon)}} \mathfrak{c} G(y) \left( -\Delta_y - k^2 + \frac{\alpha}{|y|} \right) \phi(y) dy = \phi(0) ,$$

where

$$\Omega_{(y,\epsilon)} := \mathbb{R}^3 \setminus B_\epsilon \quad , \quad B_\epsilon = \{y \in \mathbb{R}^3 : |y| \leq \epsilon\}.$$

Since  $\Phi_k(x, y)$  satisfies

$$\left(-\Delta_x - k^2 + \frac{\alpha}{|x|}\right) \Phi_k(x, y) = 0 \quad , \quad \text{on } \Omega_{(y,\epsilon)} \quad , \quad \epsilon > 0,$$

we apply the second Green's formula,

$$\int_{\Omega} \left( (\Delta w) v - w (\Delta v) \right) dx = \int_{\partial\Omega} \left( v \partial_n w - w \partial_n v \right) d\sigma(x) \quad , \quad w, v \in \mathcal{C}^2(\Omega), \quad (\text{H.1})$$

to obtain

$$\begin{aligned} & \int_{\Omega_{(y,\epsilon)}} \left[ (-\Delta - k^2 + \frac{\alpha}{|x|}) \phi(x) \right] \Phi_k(x, y) dx \\ &= \int_{\Omega_{(y,\epsilon)}} \left[ \left( -\Delta - k^2 + \frac{\alpha}{|x|} \right) \phi(x) \right] \Phi_k(x, y) dx - \int_{\Omega_{(y,\epsilon)}} \phi(x) \left( -\Delta - k^2 + \frac{\alpha}{|x|} \right) \Phi_k(x, y) dx \\ &= \int_{\Omega_{(y,\epsilon)}} (-\Delta \phi) \Phi_k(x, y) dx - \int_{\Omega_{(y,\epsilon)}} \phi(x) (-\Delta \Phi_k(x, y)) dx \\ &= - \int_{\partial\Omega_{(y,\epsilon)}} \left( \Phi_k(x, y) (\partial_n \phi)(x) - \phi(x) (\partial_n \Phi_k)(x) \right) d\sigma(x) \\ &= G(\epsilon) \int_{\mathbb{S}(0,\epsilon)} \partial_n \phi d\sigma(x) - G'(\epsilon) \int_{\mathbb{S}(0,\epsilon)} \phi(x) d\sigma(x) \\ &= \underbrace{\epsilon^2 G(\epsilon) \int_{\mathbb{S}(0,1)} (\partial_n \phi)(\epsilon \varpi) d\sigma(\varpi)}_{:= \mathbb{I}_1} - \underbrace{\epsilon^2 G'(\epsilon) \int_{\mathbb{S}(0,\epsilon)} \phi(\epsilon \varpi) d\sigma(\varpi)}_{:= \mathbb{I}_2}. \end{aligned}$$

A change of variable  $x = \epsilon \varpi$  was done to obtain the last equality. We next consider the limits of each integral as  $\epsilon \rightarrow 0^+$ .

Consider first integral  $\mathbb{I}_1$ . Recall that  $G(r) = \frac{g(r)}{r}$ . Using the limiting form of  $W_{-\chi, 1/2}(\bullet)$  around 0, cf. (4.38) in Appendix C, we have

$$\begin{aligned} g(r) &= W_{-\chi, \frac{1}{2}}(-2ik_\gamma r) = \frac{1}{\Gamma(1+\chi)} + O\left((-2ik_\gamma r) \ln(-2ik_\gamma r)\right) \quad , \quad r \rightarrow 0 \\ &= \frac{1}{\Gamma(1+\chi)} + O(r \ln r) \quad , \quad r \rightarrow 0. \end{aligned}$$

This means

$$\lim_{r \rightarrow 0} g = \frac{1}{\Gamma(1+\chi)} \quad \text{and} \quad G(r) \in L^1(0, 1). \quad (\text{H.2})$$

As a result, with  $\sigma(\mathbb{S}(0, 1))$  denoting the surface area of  $\mathbb{S}(0, 1)$ ,

$$\mathbb{I}_1 = \epsilon g(\epsilon) \int_{\mathbb{S}(0,1)} (\partial_n \phi)(\epsilon \varpi) d\sigma(\varpi) \leq \epsilon \sigma(\mathbb{S}(0, 1)) |g(\epsilon)| \|\phi\|_{C^1} \Rightarrow \lim_{\epsilon \rightarrow 0^+} \mathbb{I}_1 = 0. \quad (\text{H.3})$$

Consider second integral  $\mathbb{I}_2$ . We first consider the limit of the factor in  $\epsilon^2 G'(\epsilon)$ . We have

$$G'(r) = \frac{g'(r)}{|x|} - \frac{g}{|x|^2} \Rightarrow r^2 G'(r) = r g'(r) - g(r).$$

Using the asymptotic of  $g$  at 0, cf. (C.11)

$$\begin{aligned} g'(r) &= -2ik_\gamma W'_{-\chi, \frac{1}{2}}(-2ik_\gamma r) \\ &= -2ik_\gamma \left( \frac{\ln(-2ik_\gamma r) + \psi(\frac{1}{2} + \chi) + 2\gamma}{\Gamma(\frac{1}{2} + \chi)} + \frac{1}{\Gamma(1+\chi)} \right) + O(z \ln z) \quad , \quad z \rightarrow 0. \end{aligned}$$

As a result,

$$\lim_{r \rightarrow 0^+} r g'(r) = 0 \quad \text{and} \quad \lim_{r \rightarrow 0^+} r^2 G'(r) = -\frac{1}{\Gamma(1 + \chi)}. \quad (\text{H.4})$$

The limit of the integral is obtained by using dominated convergence to pass the limit inside the integral

$$\lim_{\epsilon \rightarrow 0} \int_{\mathbb{S}(0,1)} \phi(\epsilon \varpi) d\sigma(\varpi) = \int_{\mathbb{S}(0,1)} \phi(0) d\sigma(\varpi) = \phi(0) \sigma(\mathbb{S}(0,1)) = 4\pi \phi(0).$$

As a result,

$$\lim_{\epsilon \rightarrow 0^+} \mathbb{I}_2 = -\frac{4\pi}{\Gamma(1 + \chi)} \phi(0). \quad (\text{H.5})$$

Putting together (H.3) and (H.5), we have

$$\lim_{\epsilon \rightarrow 0^+} \int_{\Omega(y, \epsilon)} \left[ (-\Delta - k^2 + \frac{\alpha}{|x|}) \phi(x) \right] \Phi_k(x, y) dx = \lim_{\epsilon \rightarrow 0^+} (\mathbb{I}_1 - \mathbb{I}_2) = \frac{4\pi}{\Gamma(1 + \chi)} \phi(0).$$

This means the normalizing constant  $\mathfrak{c} = \frac{\Gamma(1 + \chi)}{4\pi}$ .

## I Miscellaneous calculation

We compute  $|e^{ik_\gamma r - i\eta_\gamma \log(2k_\gamma r)}|$ . Start by rewriting,

$$\begin{aligned} \eta_\gamma \log(2k_\gamma r) &= \eta_\gamma (\ln|2k_\gamma r| + i \operatorname{Arg}(k_\gamma)) \\ \Rightarrow i\eta_\gamma \log(2k_\gamma r) &= i \operatorname{Re} \eta_\gamma \ln|2k_\gamma r| - \operatorname{Im} \eta_\gamma \ln|2k_\gamma r| - \eta_\gamma \operatorname{Arg}(k_\gamma) \\ \Rightarrow e^{-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r)} &= e^{2r \operatorname{Im} k_\gamma - (\operatorname{Im} \eta_\gamma) \ln|2k_\gamma r|} e^{i(2r \operatorname{Re} k_\gamma + (\operatorname{Re} \eta_\gamma) \ln|2k_\gamma r|)} e^{-\eta_\gamma \operatorname{Arg}(k_\gamma)} \\ \Rightarrow |e^{-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r)}| &= e^{2r \operatorname{Im} k_\gamma - (\operatorname{Im} \eta_\gamma) \ln|2k_\gamma r|} |e^{-\eta_\gamma \operatorname{Arg}(k_\gamma)}|. \end{aligned}$$

Note that the last factor is a constant i.e. does not depend on  $r$ . We focus on the first factor. By definition

$$\begin{aligned} \eta_\gamma &= \frac{\alpha}{2} |k_\gamma|^2 (\operatorname{Re} k_\gamma - i \operatorname{Im} k_\gamma) \\ \Rightarrow 2r \operatorname{Im} k_\gamma - \operatorname{Im} \eta_\gamma \ln|2k_\gamma r| &= 2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln|2k_\gamma r| \right) \\ &= 2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln r \right) - \operatorname{Im} k_\gamma \frac{\alpha \ln|2k_\gamma|}{2|k_\gamma|^2}. \end{aligned}$$

Thus we can write

$$\begin{aligned} |e^{-ik_\gamma r + i\eta_\gamma \log(2k_\gamma r)}| &= e^{2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln r \right)} \left| e^{-\operatorname{Im} k_\gamma \frac{\alpha \ln|2k_\gamma|}{2|k_\gamma|^2} - \eta_\gamma \operatorname{Arg}(k_\gamma)} \right|; \\ |e^{ik_\gamma r - i\eta_\gamma \log(2k_\gamma r)}| &= e^{-2 \operatorname{Im} k_\gamma \left( r - \frac{\alpha}{4|k_\gamma|^2} \ln r \right)} \left| e^{\operatorname{Im} k_\gamma \frac{\alpha \ln|2k_\gamma|}{2|k_\gamma|^2} + \eta_\gamma \operatorname{Arg}(k_\gamma)} \right|. \end{aligned}$$

## J Remarks and calculation involving square root branch

We work with the following branch of argument

$$\operatorname{Arg}_1 : \mathbb{C} \longrightarrow (-\pi, \pi] \quad , \quad \operatorname{Arg}_2 : \mathbb{C} \longrightarrow [0, 2\pi).$$

Note that  $\operatorname{Arg}_1$  is the usual principal branch, cf. [27]. We have also introduced in subsection 4.1 the two branches of square root  $\mathfrak{g}_1$  and  $\mathfrak{g}_2$  associated with the above arguments,

$$\mathfrak{g}_1(z) = |z|^{1/2} e^{\frac{1}{2}i \operatorname{Arg}_1(z)} \quad , \quad \mathfrak{g}_2(z) = |z|^{1/2} e^{\frac{1}{2}i \operatorname{Arg}_2(z)}. \quad (\text{J.1})$$

## J.1 Comparison between the two branches

We distinguish the following cases

- For  $\operatorname{Re} z < 0$  and  $\operatorname{Im} z < 0$

$$\operatorname{Arg}_1(z) + 2\pi = \operatorname{Arg}_2(z) \quad \Rightarrow \quad \mathfrak{g}_2(z) = \mathfrak{g}_1(z)e^{i\pi} = -\mathfrak{g}_1(z).$$

In this case

$$\operatorname{Re} \mathfrak{g}_1(z) > 0, \operatorname{Im} \mathfrak{g}_1(z) < 0 \quad \text{and} \quad \operatorname{Re} \mathfrak{g}_2(z) < 0, \operatorname{Im} \mathfrak{g}_2(z) > 0.$$

- When  $\operatorname{Re} z > 0$  and  $\operatorname{Im} z > 0$

$$\operatorname{Arg}_1(z) = \operatorname{Arg}_2(z) \quad \Rightarrow \quad \mathfrak{g}_1(z) = \mathfrak{g}_2(z);$$

$$\operatorname{Re} \mathfrak{g}_1(z) = \operatorname{Re} \mathfrak{g}_2(z) > 0; \operatorname{Im} \mathfrak{g}_1(z) = \operatorname{Im} \mathfrak{g}_2(z) > 0.$$

And

$$\operatorname{Arg}_1(-z) = \operatorname{Arg}_1(z) - \pi \quad \Rightarrow \quad \mathfrak{g}_1(-z) = \mathfrak{g}_1(z)e^{-i\frac{\pi}{2}} = -i\mathfrak{g}_1(z);$$

$$\operatorname{Arg}_2(-z) = \operatorname{Arg}_2(z) + \pi \Rightarrow \mathfrak{g}_2(-z) = \mathfrak{g}_2(z)e^{i\frac{\pi}{2}} = i\mathfrak{g}_2(z).$$

- When  $\operatorname{Re} z < 0$  and  $\operatorname{Im} z > 0$

$$\mathfrak{g}_1(z) = \mathfrak{g}_2(z) \quad , \quad \operatorname{Re} \mathfrak{g}_1(z) > 0 \quad , \quad \operatorname{Im} \mathfrak{g}_1(z) > 0,$$

and

$$\operatorname{Arg}_1(-z) = \operatorname{Arg}_1(z) - \pi \quad \Rightarrow \quad \mathfrak{g}_1(-z) = -i\mathfrak{g}_1(z);$$

$$\operatorname{Arg}_2(-z) = \operatorname{Arg}_2(z) + \pi \quad \Rightarrow \quad \mathfrak{g}_2(-z) = i\mathfrak{g}_2(z);$$

$$\text{and} \quad \mathfrak{g}_1(-z) = -\mathfrak{g}_2(-z).$$

## J.2 Square root of product

**Proposition 33.** • Consider  $z, w \in \mathbb{C} \setminus \{0\}$  satisfying

$$0 \leq \operatorname{Arg}_1(z), \operatorname{Arg}_1(w) \leq \pi \quad \text{such that} \quad (\operatorname{Arg}_1 w, \operatorname{Arg}_1 z) \neq (0, \pi), \quad (\text{J.2})$$

or

$$-\pi < \operatorname{Arg}_1(z), \operatorname{Arg}_1(w) < 0. \quad (\text{J.3})$$

Then  $w$  and  $z$  satisfies

$$-\pi < \operatorname{Arg}_1(w) - \operatorname{Arg}_1(z) \leq \pi. \quad (\text{J.4})$$

- If  $w, z \in \mathbb{C}$  satisfy (J.4), then

$$\operatorname{Arg}_1\left(\frac{w}{z}\right) = \operatorname{Arg}_1(w) - \operatorname{Arg}_1(z), \quad (\text{J.5})$$

and

$$\mathfrak{g}_1\left(\frac{w}{z}\right) = \frac{\mathfrak{g}_1(w)}{\mathfrak{g}_1(z)}. \quad (\text{J.6})$$

*Proof.* **First statement** Consider  $z, w \in \mathbb{C} \setminus \{0\}$  with  $\operatorname{Im} z \geq 0$  and  $\operatorname{Im} w \geq 0$ . We have

$$\begin{aligned} 0 &\leq \operatorname{Arg}_1(z) \leq \pi, \quad 0 \leq \operatorname{Arg}_1(w) \leq \pi \\ \Rightarrow \quad -\pi &\leq \operatorname{Arg}_1(w) - \operatorname{Arg}_1(z) \leq \pi. \end{aligned}$$



Note that the only case when the difference between two angles is  $-\pi$  is when  $\text{Arg}_1(w) = 0$  and  $\text{Arg}_1(z) = \pi$  ie  $w > 0$  and  $z < 0$ . This case is ruled out by the assumption for this case that

$$(\text{Arg}_1 w, \text{Arg}_1 z) \neq (0, \pi).$$

Thus  $w$  and  $z$  satisfies (J.4). Similarly, in the second case with hypothesis (J.3),  $z, w \in \mathbb{C} \setminus \{0\}$  with  $\text{Im } z < 0$  and  $\text{Im } w < 0$ . And (J.4) follows automatically.

**Second statement** To obtain (J.5), we write  $\frac{w}{z}$

$$\frac{w}{z} = \left| \frac{w}{z} \right| \exp(i \text{Arg}_1(\frac{w}{z})) = \frac{|w|}{|z|} \exp\left(i \text{Arg}_1(\frac{w}{z})\right),$$

as

$$\frac{w}{z} = \frac{|w|}{|z|} \exp[i(\text{Arg}_1(w) - \text{Arg}_1(z))].$$

Property (J.5) now follows from (J.4) and the two equivalent representations of  $\frac{w}{z}$ .

We next show (J.6), given (J.5). This is true because

$$\begin{aligned} \mathfrak{g}_1\left(\frac{w}{z}\right) &= \sqrt{\frac{|w|}{|z|}} \exp\left(\frac{1}{2}i \text{Arg}_1\left(\frac{w}{z}\right)\right) = \sqrt{\frac{|w|}{|z|}} \exp\left(\frac{1}{2}i(\text{Arg}_1(w) - \text{Arg}_1(z))\right) \\ &= \frac{\sqrt{|w|} \exp(\frac{1}{2}i \text{Arg}_1(w))}{\sqrt{|z|} \exp(\frac{1}{2}i \text{Arg}_1(z))} = \frac{\mathfrak{g}_1(w)}{\mathfrak{g}_1(z)}. \end{aligned}$$

□

We apply the above theorem to following particular case.

**Corollary 34.** For  $k \in \mathbb{C} \setminus \{0\}$  with  $0 \leq \text{Arg}_1 k < \pi$ , consider  $w$  and  $z$  with

$$w = 1 - \frac{1}{k^2} \left( \frac{\alpha}{r} + \frac{\ell(\ell+1)}{r^2} \right) \quad \text{and} \quad z = 1 - \frac{1}{k^2} \frac{\alpha}{r}.$$

Then their argument in the branch  $\text{Arg}_1$  satisfies (J.4) i.e.

$$-\pi < \text{Arg}_1 w - \text{Arg}_1 z \leq \pi.$$

As a result of this,

$$\mathfrak{g}_1 \left( 1 - \frac{1}{k^2} \left( \frac{\alpha}{r} + \frac{\ell(\ell+1)}{r^2} \right) \right) = \mathfrak{g}_1 \left( 1 - \frac{1}{k^2} \frac{\alpha}{r} \right) \mathfrak{g}_1 \left( 1 - \frac{\frac{\ell(\ell+1)}{r^2}}{1 - \frac{1}{k^2} \frac{\alpha}{r}} \right).$$

*Proof.* It suffices to verify that  $w$  and  $z$  satisfy condition (J.4). We consider the following cases.

- $\text{Arg}_1 k = 0$ , i.e.  $k > 0$ . Write

$$-k^{-2} = -\frac{1}{a^2} \Rightarrow \text{Arg}_1(-k^{-2}) = \pi.$$

In this case, we distinguish further the following situations.

$$\begin{aligned} z > 0, w > 0 : \text{Arg}_1 z = \text{Arg}_1 w = 0 &\Rightarrow \text{Arg}_1 w - \text{Arg}_1 z = 0; \\ z > 0, w < 0 : \text{Arg}_1 w = \pi, \text{Arg}_1 z = 0 &\Rightarrow \text{Arg}_1 w - \text{Arg}_1 z = \pi; \\ z < 0, w < 0 : \text{Arg}_1 w = \text{Arg}_1 z = \pi &\Rightarrow \text{Arg}_1 w - \text{Arg}_1 z = 0. \end{aligned}$$

Note that under the current assumption that  $k > 0$   $z > w$ , it cannot happen that  $z < 0$  and  $w > 0$ .

- $0 < \text{Arg}_1 k < \frac{\pi}{2}$ , then

$$0 < \text{Arg}_1 k^2 < \pi \quad \Rightarrow \quad -\pi < \text{Arg}_1 k^{-2} < 0 \quad \Rightarrow \quad 0 < \text{Arg}_1(-k^{-2}) < \pi.$$

In this case,

$$0 < \text{Arg}_1(w), \text{Arg}_1(z) < \pi, \quad -\pi < \text{Arg}_1 w - \text{Arg}_1 z < \pi.$$

- $\text{Arg}_1 k = \frac{\pi}{2}$ , i.e.  $k = ia$  where  $a > 0$ , then

$$-k^{-2} = \frac{1}{a} \quad \Rightarrow \quad \text{Arg}_1(-k^{-2}) = 0.$$

In this case,

$$\text{Arg}_1(w) = \text{Arg}_1(z) = 0, \quad \text{Arg}_1 w - \text{Arg}_1 z = 0.$$

- $\frac{\pi}{2} < \text{Arg}_1 k < \pi$ , we have

$$-\pi < \text{Arg}_1(k^2) < 0 \quad \Rightarrow \quad 0 < \text{Arg}_1 k^{-2} < \pi \quad \Rightarrow \quad -\pi < \text{Arg}_1 k^{-2} < 0.$$

In this case

$$-\pi < \text{Arg}_1(w), \text{Arg}_1(z) < 0, \quad -\pi < \text{Arg}_1 w - \text{Arg}_1 z < \pi.$$

□

### J.3 Power series expansion

For  $x \mapsto \sqrt{x+1}$  is real-analytic on  $-1 < x < 1$ , with Taylor expansion around  $x = 0$ ,

$$\begin{aligned} \sqrt{x+1} &= \sum_{k=0}^{\infty} \binom{1/2}{k} x^k = 1 + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k 2^{2k-1}} \binom{2k-2}{k-1} x^k \\ &= 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 - \frac{5}{128}x^4 + \dots, \quad -1 < x < 1. \end{aligned} \tag{J.7}$$

We denote the translated disc by

$$\mathbb{B}_1 := \{z-1 \mid |z| < 1\}, \quad \mathbb{B}_{-1} := \{z+1 \mid |z| < 1\}.$$

Since the branch cut of  $\mathbf{g}_1$  is  $\mathbb{R}^-$  and  $\mathbb{B}_1 \cap \mathbb{R}_{\leq 0} = \emptyset$  thus on  $\mathbb{B}_1$ ,  $z \mapsto \mathbf{g}_1(z+1)$  is analytic for  $|z| < 1$ , and restricts to a real-analytic function on  $\mathbb{B}_1 \cap \mathbb{R}_{>0} = (0, 1)$ . On the other hand, restricted to the real axis,  $z \mapsto \mathbf{g}_1(z+1)$  gives the usual (real) square root since

$$z = x, \quad 0 < x < 1, \quad \text{Arg}_1(x+1) = 0, \quad \mathbf{g}_1(z+1) = \mathbf{g}_1(x+1) = \sqrt{x+1}.$$

The latter function is real-analytic and with Taylor series (J.7). By analytic continuation, we then have

$$\begin{aligned} \mathbf{g}_1(z+1) &= \sum_{k=0}^{\infty} \binom{1/2}{k} z^k = 1 + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k 2^{2k-1}} \binom{2k-2}{k-1} z^k \\ &= 1 + \frac{1}{2}z - \frac{1}{8}z^2 + \frac{1}{16}z^3 - \frac{5}{128}z^4 + \dots, \quad |z| < 1, \end{aligned} \tag{J.8}$$

and

$$\begin{aligned} \mathbf{g}_1(-z+1) &= \sum_{k=0}^{\infty} \binom{1/2}{k} (-z)^k = 1 + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k 2^{2k-1}} \binom{2k-2}{k-1} (-z)^k \\ &= 1 - \frac{1}{2}z + \frac{1}{8}z^2 - \frac{1}{16}z^3 + \frac{5}{128}z^4 + \dots, \quad |z| < 1. \end{aligned} \tag{J.9}$$

Similarly, the branch cut of  $\mathbf{g}_2$  is  $\mathbb{R}_{\geq 0}$  and  $\mathbb{B}_{-1} \cap \mathbb{R}_{\geq 0} = \emptyset$ ,  $z \mapsto \mathbf{g}_2(z-1)$  is analytic on  $\mathbb{B}_{-1}$ . At the same time  $\mathbb{B}_{-1} \cap \mathbb{R}_{<0} = (-1, 0)$ , thus the function restricts to the real negative axis gives a real-analytic function. When  $z = -x$ ,  $0 < x < 1$ , by definition of  $\mathbf{g}_2$ , we have

$$\text{Arg}_2(-x-1) = \pi, \quad \mathbf{g}_2(-x-1) = \sqrt{x+1} e^{i\frac{\pi}{2}} = i\sqrt{x+1}.$$

As a result of this,

$$\begin{aligned}
 \mathfrak{g}_2(z-1) &= i \sum_{k=0}^{\infty} \binom{1/2}{k} (-z)^k = i + i \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k 2^{2k-1}} \binom{2k-2}{k-1} (-z)^k \\
 &= i - i \frac{1}{2} z - i \frac{1}{8} z^2 - i \frac{1}{16} z^3 - i \frac{5}{128} z^4 + \dots, \quad |z| < 1.
 \end{aligned} \tag{J.10}$$

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