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# Solving time-harmonic scattering problems based on the pole condition: Theory

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Summary The pole condition is a general concept for the theoretical analysis and the numerical solution of a variety of wave propagation problems. It says that the Laplace transform of the physical solution in radial direction has no poles in the lower complex halfplane. In the present paper we show that for the Helmholtz equation with a radially symmetric potential the pole condition is equivalent to Sommerfeld's radiation condition. Moreover, a new representation formula based on the pole condition is derived and used to prove existence, uniqueness and asymptotic properties of solutions. This lays the foundations of a promising new algorithm to solve time-harmonic scattering problems numerically and provides a new approach for analyzing existing algorithms such as the Perfectly Matched Layer (PML) method and the Bayliss-Gunzburger-Turkel (BGT) algorithm.

**Key words** transparent boundary conditions, Laplace transform, Sommerfeld radiation condition

#### 1 Introduction

Differential equations of Helmholtz type arise in acoustic, electromagnetic and quantum scattering theory. Such equations have an infinite number of bounded solutions satisfying a given condition on the boundary of the scatterer. To make the solution unique, we have

to impose the additional condition that the solution be an "outgoing" wave. The standard condition in this context is Sommerfeld's radiation condition (cf. [15,16]). The pole condition, which has briefly been described in the abstract, is an alternative and more general condition. It is shown that for the Helmholtz equation both conditions are equivalent. In the context of acoustic and two-dimensional electromagnetic as well as quantum scattering problems, both conditions imply that energy is transported away from the origin.

The aim of this paper is not only to give a new proof of existence, uniqueness and asymptotic properties of solutions to scattering problems based on the pole condition, but also to lay the foundations of a new efficient numerical algorithm. In this paper we derive a set of equations, which can be solved numerically. Algorithms for the solution of these equations and numerical results will be reported in [7]. Our method has the remarkable feature that the far field pattern (or scattering amplitude) of the solution is computed automatically even if the user is only interested in the behavior of the solution on a bounded domain. In many situations, e.g. for inverse scattering problems, the far field pattern is the main quantity of interest, and in this case our method has an important advantage, in particular if Green's function is not known explicitly.

Besides giving rise to a new algorithm, our analysis also sheds new light on existing methods. In [6] we show that the approximate solutions obtained by the PML method converge exponentially to the true solution as the thickness of the sponge layer tends to infinity. Moreover, we analyze the BGT method for the general situation considered in this paper. A brief overview on existing numerical methods will also be given in [6].

The pole condition has first been considered for problems with one space-like and one time-like variable. In [12,13] the time-discretized Schrödinger equation is interpreted as a sequence of inhomogeneous Helmholtz problems. One-way wide angle Helmholtz equations, ranging between the Schrödinger and the Helmholtz equation, have been studied in [14]. With the results below, we hope to be able to carry over the analysis of these papers to problems with arbitrary space dimensions.

#### 2 Main results and outline of the paper

We consider partial differential equations of the form

$$\Delta u + \left(1 + p(|x|) + \frac{1}{|x|^2} q\left(\frac{x}{|x|}\right)\right) \kappa^2 u = 0 \tag{1}$$

with real-valued functions p, q in some exterior domain  $\Omega \subset \{x \in \mathbb{R}^d : |x| > a_u\}$ ,  $a_u > 0$ . p is assumed to be analytic of the form  $p(t) = \sum_{j=2}^{\infty} p_j t^{-j}$ , and  $q \in C^{\infty}(S^{d-1})$  where  $S^d := \{x \in \mathbb{R}^d : |x| = 1\}$ . p describes either a radially symmetric potential or a variation of the refractive index. The function q allows to treat problems in hyperbolic-elliptic coordinates (cf. Section 4). This is advantageous for numerical computations with elongated obstacles.

Let us first motivate the pole condition for the simplest case d=1, p=0 and  $a_u=1$ . Here (1) reduces to the ordinary differential equation  $u''+\kappa^2 u=0$  with the general solution

$$u(1+r) = C_1 e^{i\kappa r} + C_2 e^{-i\kappa r}, \qquad r > 0.$$

The term  $C_1 e^{i\kappa r}$  corresponds to an outgoing wave, and  $C_2 e^{-i\kappa r}$  to an incoming wave. The Laplace transform  $\hat{u}_1(s) := \int_0^\infty e^{-sr} u(1+r) dr$  of  $u(1+\cdot)$ , Re s>0, is given by

$$\hat{u}_1(s) = \frac{C_1}{s - i\kappa} + \frac{C_2}{s + i\kappa}.$$

This function, which has a holomorphic extension to  $\mathbb{C} \setminus \{i\kappa, -i\kappa\}$ , satisfies  $\operatorname{res}_{i\kappa} \hat{u}_1 = C_1$  and  $\operatorname{res}_{-i\kappa} \hat{u}_1 = C_2$ . We define the residual of a function  $f: U \subset \mathbb{C} \to \mathbb{C}$  at a point  $\sigma \in \overline{U}$  by  $\operatorname{res}_{\sigma} f:=\lim_{s \to \sigma, s \in U} (s - \sigma) f(s)$  if the limit exists. u is outgoing if and only if  $\hat{u}_1$  has no pole at  $-i\kappa$ , i.e. if and only if  $\operatorname{res}_{-i\kappa} \hat{u}_1 = 0$ .

In order to formulate a similar condition for  $d \geq 2$ , we introduce the function

$$U(\rho, \hat{x}) := \rho^{\frac{d-1}{2}} u(\rho \hat{x}) \tag{2}$$

for  $\rho > a_u, \ \hat{x} \in S^{d-1}$  and its (shifted) Laplace transform

$$\hat{U}_a(s,\hat{x}) := \int_0^\infty e^{-sr} U(r+a,\hat{x}) \, \mathrm{d}r, \tag{3}$$

for Re s>0,  $\hat{x}\in S^{d-1}$ , and  $a\geq a_u$ . Note that U is defined such that  $\|U(\rho,\cdot)\|_{L^2(S^{d-1})}=\|u\|_{L^2(\rho S^{d-1})}$  for all  $\rho>a_u$ .

**Definition 1 (pole condition)** A bounded function  $u: \{x \in \mathbb{R}^d : |x| > a_u\} \to \mathbb{C}$  satisfies the pole condition if for some  $a \geq a_u$  the function  $\hat{U}_a(\cdot,\hat{x})$  defined by (2) and (3) has a holomorphic extension to the lower complex half-plane  $\mathbb{C}^- := \{s \in \mathbb{C} : \operatorname{Im} s < 0\}$  for all  $\hat{x} \in S^{d-1}$  such that the function  $s \mapsto \int_{S^{d-1}} |\frac{\partial \hat{U}_a}{\partial s}(s,\hat{x})|^2 ds(\hat{x})$  is bounded on compact subsets of  $\mathbb{C}^-$ .

**Remark 2** If the pole condition is satisfied for one  $a \geq a_u$ , it is satisfied for all  $a \geq a_u$ . This follows from the identity

$$\int_{0}^{\infty} e^{-sr} U(a+r,\hat{x}) dr = \int_{0}^{b-a} e^{-sr} U(a+r,\hat{x}) dr$$

$$+e^{-s(b-a)} \int_{0}^{\infty} e^{-sr} U(b+r,\hat{x}) dr$$
(4)

and the fact the both  $s\mapsto \int_0^{b-a}e^{-sr}U(a+r,\hat x)\,\mathrm{d} r$  and  $s\mapsto e^{-s(b-a)}$  are entire functions. Hence, the pole condition is a condition concerning the behavior of u at infinity, but not the behavior of u on any compact set.

A similar condition without the scaling (2) has been considered in [11]. We will show that a solution u to the differential equation (1) satisfies the pole condition if and only if it satisfies the Sommerfeld's radiation condition

$$\lim_{\rho \to \infty} \rho^{\frac{d-1}{2}} \left( \frac{\partial u}{\partial \rho} - i\kappa u \right) = 0, \qquad \rho = |x| \tag{5}$$

uniformly for all directions  $\frac{x}{|x|}$ .

The structure of the singularity is more complicated in general than in the simple example above. If a solution to (1) satisfies the pole condition, then  $U(\cdot,\hat{x})$  has an analytic extension not only to  $\mathbb{C}_{-}$ , but even to  $\mathbb{C}\setminus\{i\kappa-t:t\geq 0\}$ , i.e. we do not have an isolated pole, but pole with a branch cut. The functions

$$u_{\infty}(\hat{x}) = e^{-i\kappa a} \operatorname{res}_{i\kappa} \hat{U}_a(\cdot, \hat{x}), \tag{6a}$$

$$\Psi_a(t,\hat{x}) = \frac{e^{-i\kappa a}}{2\pi i} \lim_{\epsilon \to 0} \left( \hat{U}_a(i\kappa - t - i\epsilon, \hat{x}) - \hat{U}_a(i\kappa - t + i\epsilon) \right)$$
(6b)

are well defined for  $\hat{x} \in S^{d-1}$ , t > 0, and a sufficiently large. It is a crucial result of our analysis that these functions determine the solution U completely via the representation formula

$$U(a+r,\hat{x}) = e^{i\kappa(a+r)} \left( u_{\infty}(\hat{x}) + \int_0^\infty e^{-tr} \Psi_a(t,\hat{x}) \, \mathrm{d}t \right), \quad r \ge 0. \quad (7)$$

Let  $\Delta_{S^{d-1}}$  denote the Laplace-Beltrami operator on  $S^{d-1}$  and define

$$A_q \varphi := \Delta_{S^{d-1}} \varphi + \left( \frac{(d-1)(3-d)}{4} + q \right) \varphi \tag{8}$$

for  $\varphi \in C^2(S^{d-1})$ . Then  $u_{\infty}$  and  $\Psi_a$  satisfy the Volterra integrodifferential equation

$$\left\{ \check{p}_{a}(t) + te^{-at} A_{q} \right\} u_{\infty}(\hat{x}) + t(t - 2i\kappa) \Psi_{a}(t, \hat{x})$$

$$+ \int_{0}^{t} \left\{ \check{p}_{a}(t - t_{1}) + (t - t_{1})e^{-a(t - t_{1})} A_{q} \right\} \Psi_{a}(t_{1}, \hat{x}) dt_{1} = 0.$$
(9)

Here  $\check{p}_a$  is the inverse Laplace transform of  $p(a+\cdot)$  (cf. Lemma 4). If p=0, then (9) can be converted to a differential equation by multiplying by  $e^{at}$  and differentiating twice with respect to t.

Given boundary data  $f(\hat{x}) = U(a, \hat{x})$ , eq. (7) implies

$$u_{\infty}(\hat{x}) + \int_0^{\infty} \Psi_a(t, \hat{x}) dt = e^{-i\kappa a} f(\hat{x}).$$
 (10)

We show that the system (9), (10) has a unique solution  $(u_{\infty}, \Psi_a)$ . The numerical solution of these equations, which are typically coupled with a finite element method inside of the artificial boundary  $\Gamma_a := \{x : |x| = a\}$ , is studied in [7]. Other boundary conditions can easily be taken care of by differentiating (7). It suffices to to compute  $\Psi_a(t, \hat{x})$  on a small interval  $t \in [0, T]$  since  $\Psi_a(t, \hat{x})$  decays exponentially as  $t \to \infty$ . Once  $u_{\infty}$  and  $\Psi_a$  are known,  $U(\rho, \hat{x})$  can be evaluated for  $\rho \geq a$  using (7).

The plan of this paper is as follows:

In Section 3 we introduce the Dirichlet-to-Neumann map on  $\Gamma_a$  and prove an existence and uniqueness theorem based on properties of this operator. In Section 4 we derive an ordinary differential equation for the Fourier coefficients of  $U(r,\cdot)$  and a corresponding Volterra integral equation for the Laplace transform of these functions. The unique solvability of these integral equations is established in Section 5. In the following section the main results of this paper are proved for single Fourier modes. As a simple consequence of a representation formula corresponding to (7) we derive asymptotic formulas for (generalized) Hankel functions for large arguments. In Section 8 we construct the Dirichlet-to-Neumann map using Fourier series and show that it satisfies the assumptions of the existence and uniqueness theorem in Section 3. Then, in Section 9, we establish the formulas (7) and (9) and show the equivalence of the pole condition and Sommerfeld's radiation condition.

#### 3 The Dirichlet-to-Neumann map on the artificial boundary

For simplicity, we assume that  $\Omega$  is the complement of some sufficiently smooth compact set K contained in  $\{x: |x| < a\}$  such that

p(|x|) is well defined and finite for  $x \in \Omega$ . Moreover, we assume that u satisfies the Neumann boundary conditions  $\frac{\partial u}{\partial \nu} = f$  on the boundary  $\partial K$ . We could easily accommodate for more complicated situations, e.g. different boundary conditions or inhomogeneities in the interior of  $\Gamma_a$ .

From now on we assume w.r.o.g. that  $\kappa=1$ . Since a and p are arbitrary, this can be achieved by the following rescaling:  $\tilde{x}=\kappa^{-1}x$ ,  $\tilde{\rho}=\kappa^{-1}\rho$ ,  $\tilde{a}=\kappa^{-1}a$ ,  $\tilde{t}=\kappa t$ ,  $\tilde{s}=\kappa s$ ,  $\tilde{p}(\tilde{\rho})=p(\rho)$ ,  $\tilde{\tilde{p}}(\tilde{t})=\kappa^{-1}\tilde{p}(t)$ ,  $\tilde{u}(\tilde{x})=u(x)$ ,  $\tilde{U}(\tilde{\rho},\hat{x})=\kappa^{-\frac{d-1}{2}}U(\rho,\hat{x})$ ,  $\tilde{U}(\tilde{s},\hat{x})=\kappa^{-\frac{d+1}{2}}\hat{U}(s,\hat{x})$ ,  $\tilde{u}_{\infty}(\hat{x})=\kappa^{-\frac{d-1}{2}}u_{\infty}(\hat{x})$ ,  $\tilde{\Psi}(\tilde{t},\hat{x})=\kappa^{-\frac{d+1}{2}}\Psi(t,\hat{x})$ .

To arrive at a weak formulation, we multiply (1) by a function  $-\overline{v}$  and integrate over  $\Omega_a := \{x \in \Omega : |x| < a\}$ . Formally applying Green's Theorem yields

$$\int_{\Omega_c} \left( \nabla u \nabla \overline{v} - \left( 1 + p(|x|) + \frac{q(\hat{x})}{|x|^2} \right) u \overline{v} \right) dx - \int_{\Gamma_c \cup \partial K} \frac{\partial u}{\partial \nu} \overline{v} ds = 0$$

where the unit normal vector  $\nu$  points to the exterior of  $\Omega_a$ . Now we introduce a so-called Dirichlet-to-Neumann map  $L: H^{1/2}(\Gamma_a) \to H^{-1/2}(\Gamma_a)$  which maps the Dirichlet data  $u|_{\Gamma_a}$  of a solution u satisfying (1) and (5) to its Neumann data  $\frac{\partial u}{\partial \nu}|_{\Gamma_a}$ . Existence and uniqueness of such solutions in  $\{x: |x| > a\}$  will be proved later. With the sesquilinear form  $a: H^1(\Omega_a) \times H^1(\Omega_a) \to \mathbb{C}$ ,

$$a(u,v) := \int_{arOmega_a} \left( 
abla u 
abla \overline{v} - \left( 1 + p(|x|) + rac{q(\hat{x})}{|x|^2} 
ight) u \overline{v} 
ight) \, \mathrm{d}x - \int_{arGamma_a} L u \overline{v} \, \mathrm{d}s$$

and the continuous anti-linear functional  $F: H^1(\Omega_a) \to \mathbb{C}$ ,

$$F(v) := \int_{\partial K} f \overline{v} \, \mathrm{d}s,$$

the variational problem reads

$$a(u,v) = F(v)$$
 for all  $v \in H^1(\Omega_a)$ . (11)

**Proposition 3** Let L be an operator with the following properties:

- 1.  $L: H^{1/2}(\Gamma_a) \to H^{-1/2}(\Gamma_a)$  is linear and bounded.
- 2. There exists a compact operator  $\tilde{L}: H^{1/2}(\Gamma_a) \to H^{-1/2}(\Gamma_a)$  such that  $\operatorname{Re} \int_{\Gamma_a} (-L + \tilde{L}) \varphi \, \overline{\varphi} \, \mathrm{d} s \geq 0$  for all  $\varphi \in H^{1/2}(\Gamma_a)$ .
- 3. Im  $\int_{\Gamma_a} L\varphi \overline{\varphi} \, ds > 0$  for all  $\varphi \in H^{1/2}(\Gamma_a), \varphi \neq 0$ .

Then the variational problem (11) has a unique solution u for all right hand sides F, and u depends continuously on F.

*Proof* As the proof is rather standard (cf., e.g., [1, Theorem 5.7] for a similar proof), we only give a brief sketch. Condition 1 ensures that the sesquilinear form a is well-defined. Condition 2 is used to establish the Gårding inequality

Re 
$$a(u, u) + c_2 ||u||_{L^2(\Omega_a)}^2 + \left\langle \tilde{L} \operatorname{Tr} u, \operatorname{Tr} u \right\rangle_{L^2(\Gamma_a)} \ge c_1 ||u||_{H^1(\Omega_a)}^2$$

for all  $u \in H^1(\Omega_a)$  with constants  $c_1, c_2 > 0$  and the trace operator  $\operatorname{Tr}: H^1(\Omega_a) \to H^{1/2}(\Gamma_a)$ . Since the embedding operator  $H^1(\Omega_a) \hookrightarrow (H^1(\Omega_a))'$  and the operator  $\operatorname{Tr}' \tilde{L} \operatorname{Tr}: H^1(\Omega_a) \to H^1(\Omega_1)$  are compact, it can be shown by the Lax-Milgram Lemma and Riesz theory that the operator induced by the sesquilinear form a is Fredholm with index 0, i.e. uniquess implies existence and stability. Let  $u \in H^1(\Omega_a)$  satisfy a(u,v)=0 for all  $v \in H^1(\Omega_a)$ . Taking the imaginary part of this equation and using Condition 3, it follows that u has vanishing Cauchy data on  $\Gamma_a$ . Hence, by virtue of the Cauchy-Kowalewskaya Theorem and elliptic regularity results, u must vanish everywhere.

Usually the properties of L required in the previous proposition are proved using special properties of the Hankel functions (cf. [1,8]). In the following we present a more systematic approach which also works for  $p \neq 0$ .

## 4 The Laplace transform of the separated differential equation

We first show how the two-dimensional Helmholtz equation in elliptic coordinates can be transformed to the form (1). An analogous transform exists for prolate spheroidal coordinates in  $\mathbb{R}^3$ . Let f > 0 and consider the coordinate transforms

$$\varUpsilon\left(\frac{\xi}{\theta}\right) := e^{\xi} \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}, \qquad \varPhi_f \begin{pmatrix} \xi \\ \theta \end{pmatrix} := f \begin{pmatrix} \cosh \xi \cos \theta \\ \sinh \xi \sin \theta \end{pmatrix}.$$

Note that  $\Gamma_a:=\Upsilon(\{\ln a\}\times[0,2\pi])$  is the circle with radius a centered at the origin, and that  $\tilde{\varGamma}_a:=\Phi_f(\{\ln a\}\times[0,2\pi])$  is the ellipse with foci located at (f,0) and (-f,0) and eccentricity  $\frac{2}{a+a^{-1}}$ . Let  $\tilde{u}$  satisfy the Helmholtz equation  $\Delta \tilde{u}+\tilde{\kappa}^2 u=0$  in the exterior of  $\tilde{\varGamma}_a$ . Then  $u(x):=\tilde{u}(\Phi_f(\Upsilon^{-1}(x)))$  is defined in the exterior of  $\varGamma_a$ . A computation shows that the Gramian matrix  $G=D(\Phi_f\circ\Upsilon^{-1})^TD(\Phi_f\circ\Upsilon^{-1})$  is given by  $G(x)=\frac{f^2}{4}(1+p(|x|)+|x|^{-2}q(\hat{x}))I$  where

$$p(\rho) = \rho^{-4}$$
 and  $q\left(\begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}\right) = -2\cos 2\theta.$  (12)

Therefore, by the formula for the Laplacian in general coordinates (cf. [17, Sec. 2.4]),  $\Delta \tilde{u} = \frac{4}{f^2} \left(1 + p(|x|) + |x|^{-2} q(\hat{x})\right)^{-1} \Delta u$ . This shows that u satisfies the differential equation (1) with  $\kappa = \tilde{\kappa} \frac{f}{2}$  and p, q given by (12).

Let  $\{(\varphi_j, \lambda_j) : j \in \mathbb{N}\}$  be a complete orthonormal system of eigenfunctions and eigenvalues of the operator  $A_q$  defined in (8). The existence of such a system follows from the fact that  $A_q$  is self-adjoint and has a compact resolvent for  $q \in C^{\infty}(S^{d-1})$  (cf. [17, Sec. 8.2]). If q = 0, then  $\varphi_j$  may be chosen as trigonometric monomials for d = 2 and spherical harmonics for d = 3. In the example above the functions  $\varphi_j$  will be Matthieu's functions. Let  $U_j(r) := \int_{S^1} U(r, \cdot) \overline{\varphi_j} \, \mathrm{d}s$  denote the Fourier coefficients of U. Using the formula

$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{d-1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \Delta_{S^{d-1}}$$

it follows after some simple computations that the Fourier coefficients  $U_i(r)$  satisfy the differential equations

$$U_j''(\rho) + (1 + p(\rho) + \lambda_j \rho^{-2}) U_j(\rho) = 0.$$
 (13)

Note that there is no term involving  $U'_j$  due to the scaling factor  $\rho^{(d-1)/2}$ .

Let  $(\mathcal{L}f)(s) := \int_0^\infty e^{-s\rho} f(\rho) \,\mathrm{d}\rho$ , Re s > 0 denote the Laplace transform of a function f. In order to derive an equation for  $\hat{U}_{j,a} := \mathcal{L}U_j(\cdot + a)$  we need the following lemma:

**Lemma 4** Assume that the convergence radius of the series  $p(t^{-1}) = \sum_{m=1}^{\infty} p_m t^m$  is greater than  $\frac{1}{a_p}$ ,  $a_p \in (0, \infty)$  and let  $a > a_p$ . Let

$$\check{p}_a(s) := e^{-as} \sum_{m=1}^{\infty} \frac{p_m}{(m-1)!} s^{m-1}$$
(14)

be the inverse Laplace transform of  $p(\cdot + a)$  (i.e.  $(\mathcal{L}\check{p}_a)(r) = p(r + a)$ ), and let  $u \in C([0, \infty))$  be a bounded function. Then

$$\mathcal{L}\left(p(\cdot+a)u\right)(s) = \int_{s}^{\infty} \check{p}_{a}(s_{1}-s)(\mathcal{L}u)(s_{1}) \,\mathrm{d}s_{1} \tag{15}$$

for Re s>0. Here  $\int_s^\infty f(s_1) ds_1 := \int_0^\infty f(s+t) dt$ . For all  $k=0,1,\ldots$  there exists a constant C>0 such that

$$|\check{p}_a^{(k)}(s)| \le Ce^{-a\operatorname{Re} s + a_p|s|}$$
 (16a)

for all  $s \in \mathbb{C}$ . If  $p_1 = 0$  then also

$$|\check{p}_a(s)| \le C|s|e^{-a\operatorname{Re} s + a_p|s|}.$$
(16b)

Proof We first prove by induction in  $m \in \mathbb{N}$  that (15) is true for  $p(t^{-1}) = t^m$ . To show this for m = 1 we consider the function  $f(t) := (t+a)^{-1}u(t)$ . A simple computation shows that  $\lim_{s\to\infty} \mathcal{L}f(s) = 0$  and

$$(\mathcal{L}u)(s) = (\mathcal{L}((\cdot + a)f))(s) = a(\mathcal{L}f)(s) - (\mathcal{L}f)'(s).$$

On the other hand, the right hand side of (15) with  $\check{p}_a(s) = e^{-as}$  is the unique solution of this differential equation vanishing at  $\infty$ . Now assume that (15) holds true for  $p(t^{-1}) = t^m$  with  $m \leq j, j \in \mathbb{N}$ . Then

$$\mathcal{L}\left(\frac{u}{(\cdot+a)^{j+1}}\right)(s) = \int_{s}^{\infty} \frac{e^{a(s-s_1)}(s_1-s)^{j-1}}{(j-1)!} \left(\mathcal{L}\left(\frac{u}{\cdot+a}\right)\right)(s_1) \, \mathrm{d}s_1$$

$$= \int_{s}^{\infty} \frac{e^{a(s-s_1)}(s_1-s)^{j-1}}{(j-1)!} \int_{s_1}^{\infty} e^{a(s_1-s_2)}(\mathcal{L}u)(s_2) \, \mathrm{d}s_2 \, \mathrm{d}s_1$$

$$= \int_{s}^{\infty} e^{a(s-s_2)}(\mathcal{L}u)(s_2) \int_{s}^{s_2} \frac{(s_1-s)^{j-1}}{(j-1)!} \, \mathrm{d}s_1 \, \mathrm{d}s_2$$

$$= \int_{s}^{\infty} \frac{e^{a(s-s_2)}(s_2-s)^{j}}{j!} (\mathcal{L}u)(s_2) \, \mathrm{d}s_2.$$

So far we have proved (15) if  $t \mapsto p(t^{-1})$  is a polynomial. It remains to consider the case that p is given by an infinite series. It follows from the definition of  $a_p$  that  $C := \sup_{m>0} |p_{m+1}| a_p^{-m} < \infty$ . Hence,

$$|\check{p}_a(s)| \le e^{-a\operatorname{Re} s} \sum_{m=0}^{\infty} \frac{|p_{m+1}||s|^m}{m!} \le Ce^{-a\operatorname{Re} s} \sum_{m=0}^{\infty} \frac{a_p^m |s|^m}{m!}$$
  
 $\le Ce^{-a\operatorname{Re} s + a_p |s|}.$ 

The other estimates in (16) are derived in a similar manner. Since all partial sums in the definition of  $p_a$  are bounded by the right hand side of the previous inequality and since the series p(t) converges uniformly for  $|t| \geq a$ , it can be shown by Lebesgue's Dominated Convergence Theorem that

$$\int_{0}^{\infty} e^{-sr} p(r+a)u(r) dr = \lim_{M \to \infty} \int_{0}^{\infty} e^{-sr} \sum_{m=1}^{M} \frac{p_{m}}{(r+a)^{m}} u(r) dr$$

$$= \lim_{M \to \infty} \int_{s}^{\infty} e^{a(s-s_{1})} \sum_{m=1}^{M} \frac{p_{m}(s-s_{1})^{m-1}}{(m-1)!} (\mathcal{L}u)(s_{1}) ds_{1}$$

$$= \int_{s}^{\infty} \check{p}_{a}(s_{1}-s) (\mathcal{L}u)(s_{1}) ds_{1}.$$

It follows from (13) and Lemma 4 that

$$\int_{s}^{\infty} \left( \check{p}_{a}(s_{1} - s) + e^{-a(s_{1} - s)}(s_{1} - s)\lambda_{j} \right) \hat{U}_{j,a}(s_{1}) ds_{1}$$

$$+ (s^{2} + 1)\hat{U}_{j,a}(s) = s U_{j}(a) + U'_{j}(a), \qquad \text{Re } s > 0.$$
 (17)

#### 5 The integral equation in the Laplace domain

In this and the following two sections we consider differential equations of the form

$$U''(a+r) + (1 + (\mathcal{L}P)(r)) U(a+r) = 0, \qquad r > 0$$
 (18)

with an analytic function P of the form (14) with  $p_1 = 0$  which satisfies the estimates (16). The equations (13) are of this form. The dependence of the solution on  $\lambda_j$  will be discussed later. For studying the integral equation in the Laplace domain, it is useful to factor out the singularities of  $\hat{U}$  at  $\pm i$ , i.e. to look at the function

$$w(s) = \hat{U}(s)(s^2 + 1). \tag{19}$$

Here and in the following we often omit the index a in  $\hat{U}_a$ . Due to Lemma 4 the function w satisfies the Volterra integral equation

$$w(s) + Jw(s) = sU(a) + U'(a)$$
 (20)

with

$$(Jw)(s) := \int_{s}^{\infty} P(s_1 - s) \frac{w(s_1)}{s_1^2 + 1} \, \mathrm{d}s_1. \tag{21}$$

Let us introduce the cuts  $S_{\pm i} := \{\pm i + t : t < 0\}$  and  $V := \mathbb{C} \setminus (S_i \cup S_{-i})$  (cf. Fig. 1a)). We define the metric on V by  $d(s_1, s_2) := \sqrt{|s_1 - s_2|^2 + |\varphi(s_1) - \varphi(s_2)|^2}$  with the function  $\varphi : V \to \mathbb{R}$  given by  $\varphi(s) := -\operatorname{Re} s$  if  $\operatorname{Re} s \leq 0$  and  $|\operatorname{Im} s| < 1$ ,  $\varphi(s) := 0$  else. This metric is defined such that points on opposite sides of the cuts are far away from each other. Let  $(\overline{V}, \overline{d})$  denote the completion of the metric space (V, d). Then  $\overline{V}$  is the union of V and the set of points  $s_{\pm} := \lim_{\epsilon \to 0, \epsilon > 0} s \pm i\epsilon$  with  $s \in S_i \cup S_{-i}$ . For a continuous function  $v : \overline{V} \to \mathbb{C}$  we can define a "jump function"  $[v] : S_i \cup S_{-i} \to \mathbb{C}$  by

$$[v](s) := v(s_{-}) - v(s_{+}), \qquad s \in S_i \cup S_{-i}.$$
 (22)

Note that [v] is continuous on  $S_i \cup S_{-i}$  with respect to the topology induced by the usual norm of  $\mathbb{C}$ .

We introduce the norm

$$||w||_X := \sup_{s \in \overline{V}} \frac{|w(s)|}{|s|^2 + 1}$$

and denote by X the space of all  $w \in C(\overline{V})$  which are holomorphic in V and satisfy  $w(s) = o(|s|^2)$  uniformly for  $|s| \to \infty$ . X is equipped with the norm  $\|\cdot\|_X$ .

In the following we use the notation  $|s|_1 := |\operatorname{Re} s| + |\operatorname{Im} s|$  for  $s \in \mathbb{C}$ . Moreover, we define the diamond shaped domains  $D_{\pm} := \{s \in \overline{V} : |s \mp i|_1 < \frac{1}{2}\}.$ 

In order not to interrupt the flow of the argument, the proofs of the following two lemmas will be given in the appendix.

**Lemma 5** Let  $0 < \alpha < 1$ . Then there exists a constant c such that for all  $w \in X$ 

$$|(Jw)(s)| \leq c \left( \sup_{\operatorname{Re} s_1 \geq \operatorname{Re} s} \frac{|w(s_1)|}{|s_1|^2 + 1} \right), \ s \in \overline{V} \setminus (D_+ \cup D_-), (23a)$$

$$|(Jw)'(s)| \leq c \left( \sup_{\operatorname{Re} s_1 \geq \operatorname{Re} s} \frac{|w(s_1)|}{|s_1|^2 + 1} \right), \ s \in \overline{V} \setminus (D_+ \cup D_-), (23b)$$

$$|(Jw)(s) - (Jw)(\sigma)| \leq c ||w||_X d(s, \sigma)^{\alpha}, \ s, \sigma \in D_{\pm}, \tag{23c}$$

$$|(Jw)(s)| \leq c ||w||_X, \ s \in \overline{V}. \tag{23d}$$

**Lemma 6** The operator J is compact from X to X.

**Proposition 7** The integral equation (20) has a unique solution in X for all  $U(a), U'(a) \in \mathbb{C}$ .

Proof Let  $w \in X$  satisfy the homogeneous equation w + Jw = 0. If we can show that w = 0, then the assertion follows from Riesz theory and Lemma 6. (23d) implies that  $||w||_{\infty} < \infty$ . Hence, there exists  $s^* \in \mathbb{C}$  with  $|\operatorname{Re} s^*| \geq \sigma := 2\sqrt{c/a^2}$  such that  $|w(s)| \leq 2|w(s^*)|$  for all  $s \in \mathbb{C}$  with  $|\operatorname{Re} s| \geq \sigma$ . It follows from (23a) that

$$|w(s^*)| = |(Jw)(s^*)| \le \sup_{\text{Re } s_1 \ge \sigma} \frac{c}{a^2(|s_1^2| + 1)} |w(s_1)|$$

$$< \frac{1}{4} \sup_{\text{Re } s_1 \ge \sigma} |w(s_1)| \le \frac{1}{2} |w(s^*)|,$$

i.e.  $w(s^*) = 0$ . This, however, implies that w(s) = 0 for all  $s \in \mathbb{C}$  with Re  $s \geq \sigma$ , and since w is holomorphic in V and continuous in  $\overline{V}$ , w(s) = 0 for all  $s \in \overline{V}$ .  $\square$ 

#### 6 The cut functions

In this section we study the cut functions

$$\psi_{a,\pm}(t) := \frac{[\hat{U}_a](\pm i - t)}{2\pi i \operatorname{res}_{+i} \hat{U}_a}, \qquad t > 0$$
 (24)

(cf. (22)). Note that  $\operatorname{res}_{\pm i} \hat{U}_a = \pm 2iw(\pm i)$ . Again, we will often drop the index a. In the next lemma we derive Volterra integral equations for  $\psi_{\pm}$ , which are uniquely solvable. This shows that  $\psi_{\pm}$  can be defined without the assumption  $\operatorname{res}_i \hat{U}_a \neq 0$  and that, in fact,  $\psi_{\pm}$  only depends on P, but not on U.

**Lemma 8** If  $\operatorname{res}_{\pm i} \hat{U} \neq 0$ , the cut functions  $\psi_{\pm}(t)$  defined by (24) for t > 0 satisfy the integral equations

$$\psi_{+}(t) + \int_{0}^{t} \frac{P(t-t_{1})}{t(t-2i)} \psi_{+}(t_{1}) dt_{1} = -\frac{P(t)}{t(t-2i)},$$
 (25a)

$$\psi_{-}(t) + \int_{0}^{t} \frac{P(t-t_{1})}{t(t+2i)} \psi_{-}(t_{1}) dt_{1} = -\frac{P(t)}{t(t+2i)}.$$
 (25b)

*Proof* We will only prove (25a) since the proof of (25b) is analogous. Due to (20) and (19) we have

$$(s_{\pm}^2 + 1)\hat{U}(s_{\pm}) + \int_{\gamma_{\pm}^{\epsilon}} P(s_1 - s_{\pm})\hat{U}(s_1) \, \mathrm{d}s_1 = s_{\pm}U(a) + U'(a)$$

for  $s=i-t\in S_i$  and  $\epsilon>0$ . The paths  $\gamma_+^{\epsilon}$  and  $\gamma_-^{\epsilon}$  are shown in Fig. 1. Subtracting the equation with the + sign from the equation with the - sign yields

$$t(t-2i)[\hat{U}](i-t) + \int_{-t}^{-\epsilon} P(t+t_1)[\hat{U}](i+t_1) dt_1$$
$$+ \int_{0}^{2\pi} P(t-\epsilon e^{-i\varphi}) \frac{w(i-\epsilon e^{i\varphi})}{(-\epsilon e^{i\varphi})(2i-\epsilon e^{i\varphi})} (-i\epsilon) e^{i\varphi} d\varphi = 0.$$

Since w is continuous at i, the last integral converges to  $\pi P(t)w(i) = 2\pi i P(t) \operatorname{res}_i \hat{U}$  as  $\epsilon \to 0$ . Dividing by  $2\pi i (\operatorname{res}_i \hat{U})t(t-2i)$  establishes (25a).  $\square$ 

Since both the kernel of the integral operators and the right hand sides are bounded due to our assumptions on P, the Volterra integral equations (25) are uniquely solvable (cf.,e.g.,[9, Theorem 10.15]). From these integral equations we can deduce the following two lemmas concerning the behavior of  $\psi_{\pm}$  near 0 and near  $\infty$ . Since

$$\psi_{-}(t) = \overline{\psi_{+}(t)} \tag{26}$$

the first lemma is only formulated for  $\psi_+$ .

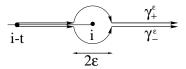


Fig. 1. Integration path in the proof of Lemma 8

**Lemma 9** The function  $\psi_+$  defined in (24) belongs to  $C^{\infty}([0,\infty))$ , and the derivatives of  $\psi_+$  at 0 can be computed recursively as follows:

$$\psi_{+}(0) = -\lim_{t \to 0} \frac{P(t)}{t(t-2i)},\tag{27a}$$

$$\psi_{+}^{(k+1)}(0) = -\lim_{t \to 0} \frac{d^{k+1}}{dt^{k+1}} \left\{ \frac{P(t)}{t(t-2i)} \right\}$$
 (27b)

$$+\frac{(k+1)!}{2i}\sum_{j=0}^{k+1}\frac{1}{(2i)^{k+1-j}(j+2)!}\sum_{n=1}^{j}P^{(n)}(0)\psi_{+}^{(j-n)}(0).$$

The proof will be given in the appendix. Since the first term on the right hand side of (the analog of) (4) does not contribute to  $\operatorname{res}_{\pm i} \hat{U}_a$  and  $\psi_{a,\pm}$ , the quantities

$$U_{\infty}^{\pm} := e^{\pm ia} \operatorname{res}_{\pm i} \hat{U}_a \tag{28}$$

are independent of a, and

$$\psi_{a,\pm}(t) = e^{(b-a)t} \psi_{b,\pm}(t). \tag{29}$$

for  $b \geq a$ . The last identity can be used to define  $\psi_{\lambda,\pm}$  for all  $\lambda \in \mathbb{R}$ .

**Lemma 10** For all  $a \in \mathbb{R}$  and  $\epsilon > 0$  the cut functions satisfy

$$|\psi_{a,\pm}(t)| = \mathcal{O}\left(e^{-(a-a_p-\epsilon)t}\right), \qquad t \to \infty.$$
 (30)

*Proof* Due to (29) it suffices to prove the lemma for  $a = a_p$ . It follows from (16a) with k = 0 and (25) that

$$|\psi_{a_p,\pm}(t)| \le rac{C}{|t(t-2i)|} \left(1 + \int_0^t |\psi_{a_p,\pm}(t_1)| \, \mathrm{d}t_1 \right)$$

for all t > 0. Choosing  $t_*$  such that  $\frac{C}{|t_*(t_*-2i)|} \le \epsilon$ , it follows that

$$|\psi_{a_p,\pm}(t)| \leq \Gamma + \int_t^t \epsilon |\psi_{a_p,\pm}(t_1)| \,\mathrm{d}t_1, \qquad t > t_*,$$

where  $\Gamma:=\epsilon(1+\int_0^{t_*}|\psi_{a_p,\pm}(t_1)|\,\mathrm{d}t_1)$ . Now Gronwall's lemma (cf. [2, Sec. 3.1]) implies  $|\psi_{a_p,\pm}(t)|\leq \Gamma e^{\epsilon(t-t_*)}$  for  $t>t_*$ .  $\square$ 

**Theorem 11** The function U has a holomorphic extension to  $\{z \in \mathbb{C} : \operatorname{Re} z > a\}$ , and U and  $U^{(k)}$   $(k \geq 1)$  satisfy the representation formulas

$$U(z+a) = U_{\infty}^{+} e^{i(z+a)} \left( 1 + \int_{0}^{\infty} e^{-tz} \psi_{a,+}(t) dt \right)$$

$$+ U_{\infty}^{-} e^{-i(z+a)} \left( 1 + \int_{0}^{\infty} e^{-tz} \psi_{a,-}(t) dt \right),$$

$$U^{(k)}(z+a) = U_{\infty}^{+} e^{i(z+a)} \left( i^{k} + \int_{0}^{\infty} (i-t)^{k} e^{-tz} \psi_{a,+}(t) dt \right)$$

$$+ U_{\infty}^{-} e^{-i(z+a)} \left( (-i)^{k} + \int_{0}^{\infty} (-i-t)^{k} e^{-tz} \psi_{a,-}(t) dt \right)$$

$$(31a)$$

for Re(z) > 0 and  $a \ge a_p$ .

Proof Let  $\gamma_1^R(t) := 1 + it, -R \le t \le R$  (cf. Fig. 2a)). Then

$$U(a+r) = \lim_{R \to \infty} \frac{1}{2\pi i} \int_{\gamma_1^R} e^{rs} \hat{U}_a(s) \, \mathrm{d}s$$

for  $a>a_p$  and  $r\geq 0$  by the inversion theorem for the Fourier transform. Now

$$\frac{1}{2\pi i} \int_{\gamma_1^R} e^{rs} \hat{U}_a(s) \, ds = -\frac{1}{2\pi i} \int_{\gamma_2^R} e^{rs} \hat{U}_a(s) \, ds$$

due to Cauchy's integral theorem. Due to (19), (20) and (23d) the function  $\hat{U}$  decays of order  $|\hat{U}_a(s)| = \mathcal{O}(|s|^{-1})$  as  $|s| \to \infty$  uniformly for all directions. Using this and the exponential decay of the integrand as  $\text{Re } s \to -\infty$ , it can be shown that the integrals from B to C, from C to D and from D to A vanish as  $R \to \infty$ . A computation similar to that in the proof of Lemma 8 shows that the integrals around  $\pm i$  converge to  $\text{res}_{\pm i} \hat{U}_a e^{\pm ir}$  as  $R \to \infty$ . The integrals along  $S_{\pm i}$  converge to  $\text{res}_{\pm i} \hat{U}_a \int_0^\infty e^{r(\pm i-t)} \psi_{a,\pm}(t) \, dt$  as  $R \to \infty$ . This yields (31a) for  $z \geq 0$ . Differentiating (31a) and changing the order of differentiation and integration, which is possible by Lebesgue's Dominated Convergence Theorem and (30), we obtain (31b). It is obvious that (31a) defines a holomorphic extension of U.  $\square$ 

Equation (31a) provides a decomposition of any Fourier mode U satisfying eq. (18) into an outgoing part and an incoming part. For a solution u to the full partial differential equation (1) a corresponding decomposition is not always possible. For example, the solution  $u(x) = e^{i\kappa x_1}$  for p = q = 0 does not decay like  $\mathcal{O}(\rho^{-(d-1)/2})$ . Since the Sommerfeld radiation condition implies such a behavior (cf. [1,

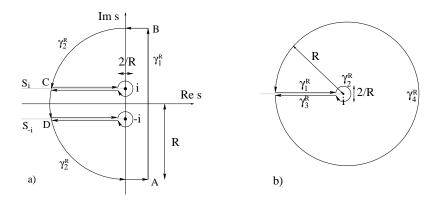


Fig. 2. Integration paths in the proofs of Theorem 11 and Proposition 13.

Sec. 2.2]) and since incoming solutions are complex conjugates of outgoing solutions, u cannot be decomposed into an outgoing and an incoming part. The reason that Theorem 11 does not carry over in full extent to the partial differential equation (1) is concerned with the fact that the condition numbers of the matrices  $L_a$  in the next corollary increase exponentially with  $|\lambda_i|$ .

Corollary 12 The matrix  $L_a$  defined by

$$\begin{pmatrix} U(a) \\ U'(a) \end{pmatrix} = L_a \begin{pmatrix} U_{\infty}^+ \\ U_{\infty}^- \end{pmatrix}$$

via (31a) and (31b) is regular. Hence, there exists  $(U(a), U'(a)) \neq 0$  such that  $\operatorname{res}_{-i} \hat{U}_a = 0$ . In this case  $\hat{U}_a$  satisfies the pole condition.

Proof Let  $L_a(U_\infty^+, U_\infty^-)^T = 0$ . Since U solves a linear second order differential equation, U(r) = U'(r) = 0 implies that  $U \equiv 0$ , and hence  $U_\infty^+ = U_\infty^- = 0$ . Hence,  $L_a$  is regular. If  $\operatorname{res}_{-i} \hat{U}_a = 0$ , then  $[U_a](-i-t) = 0$ , and therefore [w](-i-t) = 0 for all t > 0, i.e. w is continuous in the lower half-plane. Using Morera's Theorem and a contour deformation around the cut  $S_{-i}$  it can be shown that w is holomorphic in the lower half-plane. As w(-i) = 0,  $\hat{U}_a$  is also holomorphic in the lower half-plane.  $\square$ 

Finally, we need a representation formula for  $U_a$  in terms of the cut function.

**Proposition 13** Let  $\operatorname{res}_{-i} \hat{U}_a = 0$ . Then  $\hat{U}_a(s)$  satisfies the representation formula

$$\hat{U}_a(s) = -\frac{\operatorname{res}_i \hat{U}_a}{i - s} - \int_0^\infty \frac{\operatorname{res}_i \hat{U}_a \psi_{a,+}(t)}{i - t - s} \, \mathrm{d}t, \quad s \in \mathbb{C} \backslash S_i.$$
 (32)

*Proof* Due to Corollary 12 the assumption  $\operatorname{res}_{-i} \hat{U}_a = 0$  implies that  $\hat{U}_a$  is holomorphic in  $\mathbb{C}\setminus (S_i \cup \{i\})$ . Therefore, Cauchy's formula

$$\hat{U}_a(s) = \frac{1}{2\pi i} \int_{\gamma_i^R + \gamma_i^R + \gamma_i^R + \gamma_i^R} \frac{\hat{U}_a(s_1) \, \mathrm{d}s_1}{s_1 - s}$$

with the contour shown in Fig. 2b) holds true. The integral over  $\gamma_2^R$  converges to the first term on the right hand side of (32). Recall from the proof of Theorem 11 that  $\hat{U}_a(s) = \mathcal{O}(|s|^{-1})$  as  $|s| \to \infty$  uniformly for all directions. Hence, the integral over  $\gamma_4^R$  tends to 0 as  $R \to \infty$  since the integrand is of order  $\mathcal{O}(|s|^{-2})$ . Finally, the integrals over  $\gamma_1^R$  and  $\gamma_3^R$  yield the integral term in (32).  $\square$ 

#### 7 Asymptotic expansion of the far field

**Theorem 14** Let  $m \in \{0,1,2,\ldots\}$ , and assume that  $U_{\infty}^+ = 0$  or  $U_{\infty}^- = 0$ , respectively. Then U and U' satisfy the asymptotic formulas

$$U(z) = U_{\infty}^{\pm} e^{\pm iz} \left( 1 + \sum_{l=0}^{m-1} \frac{\psi_{0,\pm}^{(l)}(0)}{z^{l+1}} + \mathcal{O}\left(\frac{1}{|z|^{m+1}}\right) \right), \tag{33}$$

$$U'(z) = U_{\infty}^{\pm} e^{\pm iz} \left( \pm i + \sum_{l=0}^{m-1} \frac{\pm i \psi_{0,\pm}^{(l)}(0) - l \psi_{0,\pm}^{(l-1)}(0)}{z^{l+1}} + \mathcal{O}\left(\frac{1}{|z|^{m+1}}\right) \right)$$

respectively, for  $z \to \infty$  such that  $|\arg z| \le \varphi < \frac{\pi}{2}$ . Here  $0 \cdot \psi_{0,\pm}^{(-1)}(0) := 0$ 

*Proof* Note that the integral term in (31a) is the Laplace transform of  $\psi_{a,\pm}$ . Due to (29) we may choose a=0. Using the asymptotic formula

$$(\mathcal{L}f)(z) = \sum_{l=0}^{m-1} \frac{f^{(l)}(0)}{z^{l+1}} + \mathcal{O}(|z|^{-m-1}), \qquad (34)$$

 $z \to \infty, |\arg z| \le \varphi < \pi/2$ , which holds for bounded functions  $f \in C^m([0,\infty))$  (cf. [3, p.47]), (31a) and Lemma 9 we immediately obtain (33). The asymptotic formula for U' follows analogously from (31b) and the identity  $\frac{d^l}{dt^l} \left( (\pm i - t) \psi_{0,\pm}(t) \right) \Big|_{t=0} = \pm i \psi_{0,\pm}^{(l)}(0) - l \psi_{0,\pm}^{(l-1)}(0)$ .

As a special case of the previous theorem we reproduce the asymptotic formula for the Hankel functions for large arguments (cf. [18]).

Corollary 15 The Hankel functions  $H_j^{(1)}$  of the first kind of order j satisfy

$$H_{j}^{(1)}(z) = \sqrt{rac{2}{\pi z}} e^{i(z - rac{j\pi}{2} - rac{\pi}{4})} \Big( \sum_{k=0}^{m} \left\{ \prod_{l=1}^{k} rac{j^2 - (l - rac{1}{2})^2}{-2ilz} 
ight\} + \mathcal{O}ig(|z|^{-m-1}ig) \Big)$$

for  $z \to \infty$  such that  $|\arg z| \le \varphi < \frac{\pi}{2}$   $(m \ge 0)$ .

Proof With  $P(t) = e^{-at}t(\frac{1}{4} - j^2)$ ,  $U_{\infty}^+ = \sqrt{\frac{2}{\pi}} \exp\left(-i\frac{j\pi}{2} - i\frac{\pi}{4}\right)$  we get  $H_j^{(1)}(\rho) = \rho^{-1/2}U(\rho)$ . Using the identity  $\frac{1}{t(t-2i)} = \frac{1}{-2it}\sum_{l=0}^{\infty}t^l(2i)^{-l}$  and (27) we obtain

$$\psi_{0,+}(0) = \frac{j^2 - \frac{1}{4}}{-2i},$$

$$\psi_{0,+}^{(k+1)}(0) = \left(\frac{k+1}{2i} + \frac{1}{2i(k+2)} \left(\frac{1}{4} - j^2\right)\right) \psi_{0,+}^{(k)}(0)$$

$$= \frac{1}{-2i(k+2)} \left(j^2 - \left(k - \frac{3}{2}\right)^2\right) \psi_{0,+}^{(k)}(0).$$

Now the assertion follows from (33).  $\square$ 

#### 8 Spectral properties of the Dirichlet-to-Neumann map

Let  $\mathcal{H}_j$  denote the solution to (13) with  $U_{\infty}^+ = 1$  and  $U_{\infty}^- = 0$ . For the Helmholtz equation in  $\mathbb{R}^2$  we have  $H_j^{(1)}(\rho) = \sqrt{\frac{2}{\pi\rho}} \exp(-i\frac{j\pi}{2} - i\frac{\pi}{4})\mathcal{H}_{2j}(\rho)$ . A complete orthonormal system in  $L^2(\Gamma_a)$  is given by  $\varphi_j^a(a\hat{x}) := a^{-\frac{d-1}{2}}\varphi_j(\hat{x})$ . We expect the solution to (1) satisfying the pole condition and the boundary condition  $\operatorname{Tr}_{\Gamma_a} u = f\left(f \in H^{1/2}(\Gamma_a)\right)$  to be

$$u(\rho \hat{x}) = \sum_{j=1}^{\infty} \langle f, \varphi_j^a \rangle \rho^{-\frac{d-1}{2}} \frac{\mathcal{H}_j(\rho)}{\mathcal{H}_j(a)} \varphi_j(\hat{x})$$
 (35)

for  $\rho \geq a$  and  $\hat{x} \in S^{d-1}$ . Since the Dirichlet-to-Neumann map L satisfies  $(Lf)(\hat{x}) = \frac{\partial}{\partial \rho} u(\rho \hat{x})|_{\rho=a}$ , this leads to the definition

$$(Lf)(\hat{x}) := \sum_{j=1}^{\infty} \operatorname{DtN}(\lambda_j, a) \langle f, \varphi_j \rangle \varphi_j(\hat{x})$$
(36)

with the eigenvalues

$$DtN(\lambda_{j}, a) = \frac{\left(\rho^{-\frac{d-1}{2}} \mathcal{H}_{j}(\rho)\right)'|_{\rho=a}}{a^{-\frac{d-1}{2}} \mathcal{H}_{j}(a)} = \frac{\mathcal{H}'_{j}(a)}{\mathcal{H}_{j}(a)} - \frac{d-1}{2a}.$$
 (37)

The Sobolev norm on  $\Gamma_a$  of index  $s \in \mathbb{R}$  is defined by  $\|f\|_{H^s(\Gamma_a)} := \|\Lambda_0^s f\|_{L^2(\Gamma_a)}$  where  $\Lambda_0 := \sqrt{I - \Delta_{\Gamma_a}}$  (cf., e.g., [17, Chapter 4]). We show that an equivalent norm is obtained if  $\Lambda_0$  is replaced by  $\Lambda_q := \sqrt{c_q I - A_q}$  with  $c_q := 1 + \frac{1}{4}(d-1)(3-d) + \|q\|_{\infty}$ .

**Lemma 16** For all  $s \in \mathbb{R}$  there exist a constant  $\gamma > 0$  such that for all  $f \in C^{\infty}(\Gamma_a)$ 

$$\frac{1}{\gamma} \|\Lambda_0^s f\|_{L^2} \le \|\Lambda_q^s f\|_{L^2} \le \gamma \|\Lambda_0^s f\|_{L^2}. \tag{38}$$

*Proof* The operator  $c_q I - A_q$  is strictly positive since

$$\langle (c_q I - A_q) f, f \rangle_{L^2} = \|\nabla f\|_{L^2}^2 + \langle (1 - q + \|q\|_{\infty}) f, f \rangle_{L^2} \ge \|f\|_{L^2}^2.$$
(39)

Here  $\nabla f$  is the surface gradient of f. Hence,  $\Lambda_q$  is well defined. Since  $\Lambda_0^{2k}-\Lambda_q^{2k}$  is a differential operator of order 2(k-1) for  $k\in\mathbb{N}$ , it follows that  $\|(\Lambda_0^{2k}-\Lambda_q^{2k})f\|_{L^2}\leq c\|f\|_{H^{2(k-1)}}$ . Ehrling's lemma (cf. [10, Sec. 6.4]) and the compactness of the embedding of  $H^{2k}(\Gamma_a)$  in  $H^{2(k-1)}(\Gamma_a)$  imply that  $\|f\|_{H^{2(k-1)}}\leq \epsilon\|f\|_{H^{2k}}+C(\epsilon)\|f\|_{L^2}$  for all  $\epsilon>0$ . Together with (39) and the triangle inequality this yields  $\|\Lambda_0^{2k}f\|\leq (1+C(\epsilon))\|\Lambda_\rho^{2k}f\|+\epsilon\|\Lambda_0^{2k}f\|$ . Choosing  $\epsilon=\frac{1}{2}$ , we obtain the first inequality in (38). With this result, it follows analogously that  $\|\Lambda_\rho^{2k}f\|\leq (1+C(\epsilon))\|\Lambda_0^{2k}f\|+\epsilon\gamma\|\Lambda_\rho^{2k}f\|$ . Setting  $\epsilon=\frac{1}{2\gamma}$  yields the second inequality in (38), possibly with a larger  $\gamma$ . Hence, we have proved (38) for s=2k. Then (38) for  $s\in(0,2k)$  follows from the Heinz inequality.  $\square$ 

As a consequence, an equivalent norm is given by  $||f||_{H^s(\Gamma_a)}^2 \sim \sum_{j=1}^{\infty} (c_q - \lambda_j)^s |\langle f, \varphi_j^a \rangle|^2$  for all  $s \in \mathbb{R}$ . Hence, the properties 1-3 in Proposition 3 are equivalent to

$$|\mathrm{DtN}(\lambda_j, a)| = \mathcal{O}\left(\sqrt{|\lambda_j|}\right), \qquad j \to \infty,$$
 (40a)

$$\operatorname{DtN}(\lambda_j,a) + l_j \leq 0 ext{ for some sequence } |l_j| = \operatorname{o}\!\left(\sqrt{|\lambda_j|}\right), (40\mathrm{b})$$

Im 
$$DtN(\lambda_j, a) > 0$$
 for all  $j$ . (40c)

**Lemma 17** Let U satisfy the assumptions of Sections 5-7, and let  $U_{\infty}^-=0$ . Then

$$\operatorname{Im} U'(\rho)\overline{U(\rho)} = \left|U_{\infty}^{+}\right|^{2} \qquad \text{for all } \rho \ge a. \tag{41}$$

*Proof* Taking the imaginary part of

$$0 = \int_{a}^{\rho} \left( U'' + (1+p)U \right) \overline{U} \, \mathrm{d}\rho_{1}$$
$$= U'(\rho)\overline{U(\rho)} - U'(a)\overline{U(a)} + \int_{a}^{\rho} \left( -|U'|^{2} + (1+p)|U|^{2} \right) \, \mathrm{d}\rho_{1}$$

yields  $\operatorname{Im} U'(\rho)\overline{U(\rho)} = \operatorname{Im} U'(a)\overline{U(a)} = const.$  The constant can be evaluated using Theorem 14 by taking the limit  $\rho \to \infty$ .  $\square$ 

Eq. (41) with  $\rho = a$  implies (40c) after dividing by  $|U(a)|^2$ . The next corollary shows that no division by 0 can occur in (35) and (37).

Corollary 18 Under the assumptions of Lemma 17,  $U(\rho) = 0$  for some  $\rho \geq a$  implies U = 0. Furthermore, there exists at most one solution to (1) satisfying the pole condition and the boundary condition  $\operatorname{Tr} u = f$  for  $f \in H^{1/2}(\Gamma_a)$ .

Proof If  $U(\rho)=$ , then  $U_{\infty}^+=0$  due to (41). Since  $U_{\infty}^-=0$  by assumption, (31a) implies U=0. It suffices to prove uniqueness for f=0. Under the given assumptions all Fourier modes of u satisfy  $\operatorname{res}_{-i}\hat{U}_{j,a}=0$  and  $U_{j,a}(a)=0$ . This implies  $U_{j,a}=0$ , and hence u=0.  $\square$ 

Next, we will prove (40a) and (40b). Let  $\nu_j = \sqrt{-\lambda_j}$ , and let  $\psi_{\nu,a,+}$  denote the solution to (25a) with  $P(t) = \check{p}_a(t) - \nu_j^2 t e^{-at}$ . Since  $\lambda_j \to -\infty$  as  $j \to \infty$ , it follows that  $\nu_j \to \infty$ . For looking at this limit process, we may assume w.r.o.g. that  $p_2 = \check{p}'_a(0) = 0$  by setting  $\nu_j = \sqrt{-p_2 - \lambda_j}$ . Multiplying (25a) by t(t-2i), applying the Laplace transform and using the identity  $\mathcal{L}(\int_0^t f(t-t_1)g(t_1) dt_1) = (\mathcal{L}f) \cdot (\mathcal{L}g)$  yields the ordinary differential equation

$$\left(\partial_z^2 + 2i\partial_z + p(z) - \nu_j^2 z^{-2}\right) v(z; \nu_j) = 0$$
 (42)

for  $v(z; \nu_j) := 1 + (\mathcal{L}\psi_{\nu,0,+})(z)$ . Here and in the following we use the variables  $z = \rho + i\sigma$  with  $\rho, \sigma \in \mathbb{R}$ . Since

$$\mathcal{H}_j(\rho) = e^{i\rho} v(\rho; \nu_j) \tag{43}$$

due to (31a), eq. (42) can alternatively be derived immediately from (13).

In this section f' denotes the usual derivative of a holomorphic function f whereas  $\dot{f}$  denotes the partial derivative of f with respect

to  $\sigma$ . By the chain rule,  $\dot{f}=if'$ , so  $-\ddot{v}+2\dot{v}+(p-\nu^2z^{-2})v=0$  where the argument (z) of p and the arguments  $(z,\nu)$  of v have been omitted. Hence, the logarithmic derivative  $\chi(z;\nu):=\frac{\dot{v}(z;\nu)}{v(z;\nu)}$  satisfies the Riccati differential equation

$$\dot{\chi}(z;\nu) + \chi^2(z;\nu) - 2\chi(z;\nu) = p(z) - \nu^2 z^{-2}.$$
 (44)

It follows from Plancherel's Theorem and (30) that

$$\int_{-\infty}^{\infty} |v(\rho + i\sigma; \nu) - 1|^2 d\sigma = \frac{1}{2\pi} \|\psi_{\nu,\rho,+}\|_{L^2}^2 < \infty \quad \text{and}$$
$$\int_{-\infty}^{\infty} |\dot{v}(\rho + i\sigma; \nu)|^2 d\sigma = \frac{1}{2\pi} \|it\psi_{\nu,\rho,+}\|_{L^2}^2 < \infty.$$

Therefore, the Lebesgue measure of the sets  $A_{\epsilon}(\rho, \nu) := \{\sigma : |v(\rho + i\sigma) - 1| > \epsilon \text{ or } |\dot{v}(\rho + i\sigma)| > \epsilon\} < \infty \text{ is finite for all } \epsilon > 0.$  Hence, for all  $\rho \geq a$  and all  $\nu \geq 0$  there exists a sequence  $\sigma_l$  such that  $\sigma_l \notin A_{1/l}(\rho, \nu)$  and  $\sigma_l > l$ . This implies

$$\lim_{l \to \infty} \chi(\rho + i\sigma_l; \nu) = 0. \tag{45}$$

We now construct an approximation to  $\chi(\rho + i\sigma; \nu)$  for  $\sigma \geq 0$  by formal computations and then prove its validity. We rewrite (44) as  $\dot{\chi} = -(\chi - 1 + \gamma_1)(\chi - 1 - \gamma_1)$  with  $\gamma_1(z; \nu) := \sqrt{1 + p(z) - \nu^2 z^{-2}}$ . Here and in the following we choose the negative real axis as branch cut of the square root function. Neglecting the term  $\dot{\chi}$  yields the two possible approximations  $1 + \gamma_1$  and  $1 - \gamma_1$ . Only the latter of these approximations has the right behavior as  $\sigma \to \infty$ . The "error function"  $\Delta_1 := \chi - 1 + \gamma_1$  satisfies the differential equation

$$\dot{\Delta}_1 = \dot{\gamma}_1 - (\Delta_1 - 2\gamma_1)\Delta_1. \tag{46}$$

Since this equation has the same structure as (44), we can apply the same procedure as above to (46) and hopefully get a better approximation to  $\chi$ . This process may be repeated recursively as follows: Set  $\gamma_0 := 1$  and assume we have constructed a function  $\gamma_j$  (j = 1, 2, ...) such that

$$\chi = 1 - \gamma_j + \Delta_j,\tag{47}$$

where  $\Delta_j$  satisfies the differential equation

$$\dot{\Delta}_{j} = -(\Delta_{j} - 2\gamma_{j})\Delta_{j} + \dot{\gamma}_{j} - \dot{\gamma}_{j-1}. \tag{48}$$

This equation can be rewritten as  $\dot{\Delta}_j = -(\Delta_j - \gamma_j - \gamma_{j+1})(\Delta_j - \gamma_j + \gamma_{j+1})$  with

$$\gamma_{j+1} := \sqrt{\gamma_j^2 + \dot{\gamma}_j - \dot{\gamma}_{j-1}}.\tag{49}$$

The function  $\Delta_{j+1} := \Delta_j - \gamma_j + \gamma_{j+1}$  satisfies (47) and (48) with j replaced by j+1.

It turns turns out that the approximation of order j=2 is the lowest which is sufficient for our purposes. In the appendix we establish the following bounds on  $\Delta_2 = \chi - 1 + \gamma_2$ :

**Lemma 19** Given  $0 < a < A < \infty$  there exist constants  $\Gamma, N > 0$  such that for all  $\rho \in [a, A]$  and all  $\nu \geq N$ 

$$|\Delta_2(\rho + i\sigma; \nu)| \le \begin{cases} 2, & 0 \le \sigma < \Gamma/\nu, \\ \Gamma(\sigma\nu)^{-1}, & \Gamma/\nu \le \sigma < \nu, \\ \Gamma/\sigma^{-2}, & \nu \le \sigma. \end{cases}$$
(50)

It follows from (43) that  $\frac{\mathcal{H}_j'(\rho)}{\mathcal{H}_j(\rho)} = i + \frac{v'(\rho;\nu_j)}{v(\rho;\nu_j)} = i(1-\chi(\rho;\nu_j))$ . A simple computation shows that  $\gamma_2(\rho,\nu) = i\nu/\rho + \mathcal{O}(1)$  as  $\nu \to \infty$ . Using (47) and (50) we obtain

$$\frac{\mathcal{H}_j'(\rho)}{\mathcal{H}_j(\rho)} = i(\gamma_2(\rho; \nu_j) - \Delta_2(\rho; \nu_j)) = -\frac{\nu_j}{\rho} + \mathcal{O}(1). \tag{51}$$

This implies (40a) and (40b). Thus, we have proved existence and uniqueness of the variational problem (11) with L defined in (36).

**Corollary 20** 1. Given  $a < R_1 < R_2 < \infty$ , there exists constants C, N > 0 such that

$$\left| \mathcal{H}_{j}^{(l)}(\rho) \right| \le C \mathcal{H}_{j}(a) \left( \frac{\nu_{j}}{\rho} \right)^{l} \left( \frac{a}{\rho} \right)^{\nu} \tag{52}$$

for all  $\nu_j \geq N$ ,  $R_1 < \rho < R_2$  and l = 0, 1, 2.

2. u defined in (35) is a solution to (1) with corresponding Dirichlet-to-Neumann map (36), and the series in (35) and all its term-by-term derivatives of order  $\leq 2$  converge uniformly on compact subsets of  $\{x: |x| > a\}$ .

*Proof* It follows from (51) that

$$\mathcal{H}_{j}(\rho) = \exp\left(\int_{a}^{\rho} \frac{\mathcal{H}'_{j}(\rho_{1})}{\mathcal{H}_{j}(\rho_{1})} d\rho_{1}\right) \mathcal{H}_{j}(a) = \left(\frac{a}{\rho} + \mathcal{O}\left(\frac{1}{\nu}\right)\right)^{\nu}.$$

This implies (52) for l = 0. Together with (51) with obtain (52) for l = 1. The case l = 2 follows from differential equation (13).

Now the second part follows from the estimates

$$\|\varphi_{j}\|_{C^{l}} \leq C \|\varphi_{j}\|_{H^{l+d/2}} \leq C\Gamma \|\Lambda_{q}^{l+d/2}\varphi_{j}\|_{L^{2}} = C\Gamma \sqrt{c_{q} - \lambda_{j}}^{l+d/2}$$
(53)

 $(l=0,1,\dots)$  on the eigenfunctions  $\varphi_j$ . Here we have used Sobolev's Embedding Theorem on  $S^{d-1}$  (cf. [17, Sec. 4.3]) and Lemma 16.  $\square$ 

Corollary 21 For any  $a > a_p$  we have

$$|\mathcal{H}_j(a)| = \exp\left(\nu_j \ln \frac{2\nu_j}{ea} + \mathcal{O}(\ln \nu_j)\right), \qquad j \to \infty.$$
 (54)

*Proof* It follows from the definition of  $\chi$  and  $\sigma_l$  before (45) that

$$1 = \lim_{l \to \infty} |v(a + i\sigma_l; \nu_j)| = \exp\left(\operatorname{Re} \int_0^\infty \chi(a + i\sigma; \nu_j) \, d\sigma\right) |v(a; \nu_j)|,$$

i.e.  $|\mathcal{H}_{j}(a)| = \exp(-\operatorname{Re} \int_{0}^{\infty} \chi(a+i\sigma;\nu_{j}) d\sigma)$ . By virtue of Lemma 19,  $\operatorname{Re} \int_{0}^{\infty} \Delta_{2}(a+i\sigma;\nu) d\sigma = \mathcal{O}(\nu^{-1} \ln \nu)$  as  $\nu \to \infty$ . It can be seen from eq. (79) that there exists a constant C > 0 such that  $1 - \operatorname{Re} \gamma_{2}(a+i\sigma;\nu) \leq 0$  and  $1 - \operatorname{Re} \gamma_{2} = (1 - \operatorname{Re} \sqrt{1 - (\nu/z)^{2}})(1 + \mathcal{O}(\nu^{-1}))$  uniformly for  $\sigma \geq C/\nu$  as  $\nu \to \infty$ . Moreover,  $\int_{0}^{C/\nu} \operatorname{Re} |\gamma_{2}(a+i\sigma;\nu)| d\sigma = \mathcal{O}(1)$ . Hence,

$$\int_0^\infty \operatorname{Re} \chi(a + i\sigma; \nu) d\sigma$$

$$= \int_{C/\nu}^\infty \left( 1 - \operatorname{Re} \sqrt{1 - \frac{\nu^2}{(a + i\sigma)^2}} \right) d\sigma \left( 1 + \mathcal{O}\left(\frac{1}{\nu}\right) \right) + \mathcal{O}(1).$$

Finally,

$$\int_{C/\nu}^{\infty} (1 - \operatorname{Re} \sqrt{1 - \frac{\nu^2}{(a + i\sigma)^2}}) \, d\sigma = \operatorname{Re} \int_{a + iC/\nu}^{a + i\infty} (1 - \sqrt{1 - \frac{\nu^2}{z^2}}) \frac{dz}{i}$$

$$= \operatorname{Re} \left( iz \left( -1 + \sqrt{1 - \frac{\nu^2}{z^2}} \right) + \nu \ln \left( \frac{\nu}{z} - i\sqrt{1 - \frac{\nu^2}{z^2}} \right) \right) \Big|_{z = a + iC/\nu}^{z = a + iC/\nu}$$

$$= \nu - \nu \ln \frac{2\nu}{a} + \mathcal{O}(1), \qquad \nu \to \infty.$$

This completes the proof.  $\Box$ 

For the special case of Hankel functions, eq. (54) agrees with a well-known formula, which can be derived from the series representation of the Hankel functions (cf. [1,18]).

#### 9 Equivalence to Sommerfeld's radiation condition

A crucial tool in the proofs of this section are the following uniform estimates of the cut functions.

**Lemma 22** There exists a constants  $C, N \geq 0$  such that the estimates

$$|\psi_{\nu,a,+}(t)| \le C\nu^2 e^{-t(a-a_p)} \left(\frac{|\sqrt{t}+\sqrt{t-2i}|}{\sqrt{2}}\right)^{2\nu},$$
 (55a)

$$|\psi'_{\nu,a,+}(t)| \le C \frac{\nu^3 e^{-t(a-a_p)}}{\sqrt{t|t-2i|}} \left(\frac{|\sqrt{t}+\sqrt{t-2i}|}{\sqrt{2}}\right)^{2\nu}$$
 (55b)

hold true for all all t > 0 and all  $\nu \ge N$ . If p = 0 then (55) is valid with  $a_p = 0$ ,  $C = \frac{1}{2}$  and  $N = \sqrt{2}$ .

Proof Due to (29) it suffices to prove (55) for a = 0. Set  $\check{p}_0(t) := e^{at}\check{p}_a(t)$  and recall that we have assumed w.r.o.g. that  $\check{p}'_0(0) = 0$ . Multiplying (25a) by t(t-2i), differentiating twice and dividing by t(t-2i) yields the integro-differential equation

$$\psi_{\nu,0,+}''(t) = \frac{\nu^2 - 2}{t(t - 2i)} \psi_{\nu,0,+}(t) - 4 \frac{t - i}{t(t - 2i)} \psi_{\nu,0,+}'(t) - \int_0^t \frac{\check{p}_0''(t - t_1)}{t(t - 2i)} \psi_{\nu,0,+}(t_1) dt_1 - \frac{\check{p}_0''(t)}{t(t - 2i)}.$$
 (56)

Here  $P(t) = -\nu^2 t + \check{p}_0(t)$  in (25a). We will derive bounds on the function

$$y(t) := \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix} = \begin{pmatrix} \psi_{\nu,0,+}(t) \\ \zeta_{\nu}(t)^{-1} \psi'_{\nu,0,+}(t) \end{pmatrix}$$

where  $\zeta_{\nu}(t) := \frac{\sqrt{\nu^2 - 2}}{\sqrt{t(t - 2i)}}$ . The function  $\zeta_{\nu}$  is chosen such that both components of y have approximately the same size, i.e. such that  $\zeta_{\nu}$  approximates the logarithmic derivative  $\psi'_{\nu,0,+}/\psi_{\nu,0,+}$ . Using (56) and  $\operatorname{Re}(\psi_{\nu,0,+}\overline{\psi'_{\nu,0,+}}) = \operatorname{Re}(\overline{\psi_{\nu,0,+}}\psi'_{\nu,0,+})$  we get

$$\frac{1}{2} \frac{d}{dt} |y(t)|^2 = \operatorname{Re} \left( y_1' \overline{y_1} + y_2' \overline{y_2} \right)$$

$$= \operatorname{Re} \left( \left( 1 + \frac{\zeta_{\nu}^2}{|\zeta_{\nu}|^2} \right) \psi_{\nu,0,+} \overline{\psi_{\nu,0,+}'} - 3 \frac{t - i}{t(t - 2i)} \frac{|\psi_{\nu,0,+}'|^2}{|\zeta_{\nu}|^2} \right)$$

$$- \operatorname{Re} \left( \frac{\check{p}_0''(t)}{t(t - 2i)} \frac{\overline{\psi_{\nu,0,+}'}}{|\zeta_{\nu}|^2} + \int_0^t \frac{\check{p}_0''(t - t_1)}{t(t - 2i)} \psi_{\nu,0,+}(t_1) \, \mathrm{d}t_1 \frac{\overline{\psi_{\nu,0,+}'}}{|\zeta_{\nu}|^2} \right).$$
(57)

Using the identity  $|1+z^2|=2\operatorname{Re} z$  with  $z=\zeta_\nu/|\zeta_\nu|$  and the inequalities  $2|ab|\leq |a|^2+|b|^2$  and  $\operatorname{Re}\zeta_\nu>0$  we obtain

$$\left|1 + \frac{\zeta_{\nu}^{2}}{|\zeta_{\nu}|^{2}}\right| \cdot \left|\psi_{\nu,0,+}\overline{\psi'_{\nu,0,+}}\right| \le \operatorname{Re}(\zeta_{\nu}) \left(|y_{1}|^{2} + |y_{2}|^{2}\right).$$

Moreover, note that  $\operatorname{Re} \frac{t-i}{t(t-2i)} = \frac{2+t^2}{t(t^2+4)} > 0$ . If p = 0, this implies  $\frac{1}{2} \frac{d}{dt} |y(t)|^2 \leq \operatorname{Re}(\zeta_{\nu}(t))|y(t)|^2$  and hence, by Gronwall's lemma

$$|y(t)|^2 \le \exp\left(2\int_0^t \operatorname{Re}\zeta_{\nu}(t_1) dt_1\right) |y(0)|^2.$$

Here  $|y(0)| = |\psi_{\nu,0,+}(0)| = \frac{1}{2}\nu^2$  due to (27a). Using the indefinite integral  $\int (t(t-2i))^{-1/2} dt = 2\ln(\sqrt{t}+\sqrt{t-2i})$  and the estimate  $\sqrt{\nu^2-2} < \nu$  for  $\nu \ge \sqrt{2}$ , we obtain the assertion for the case p=0.

Next we are going to derive a bound on |y(t)| for  $t \le 1$  and general p. The inequality  $-x^2 + 2xy - y^2 \le 0$  for  $x, y \in \mathbb{R}$  yields

$$-3\frac{2+t^2}{\nu^2|t-2i|}|\psi_{\nu,0,+}'|^2+\frac{|\check{p}_0''(t)|}{\nu^2}|\psi_{\nu,0,+}'|\leq \frac{|t-2i|}{12(2+t^2)}\frac{|\check{p}_0''(t)|^2}{\nu^2}.$$

Moreover,  $\int_0^t |\frac{\check{p}_0''(t-t_1)}{t(t-2i)}\psi_{\nu,0,+}(t_1)| dt_1 \leq C \max_{0\leq t_1\leq t} |y_1(t_1)|$  for  $0\leq t\leq 1$ . Hence, (57) implies

$$\frac{1}{2}\frac{d}{dt}|y(t)|^2 < \text{Re}(\zeta_{\nu}(t))|y(t)|^2 + \frac{C}{\nu^2} + \frac{C}{\nu} \max_{0 \le t_1 \le t} |y(t_1)|^2$$
 (58)

with a constant C independent of  $\nu$ . Let  $\varphi(t)$  be the solution to the initial value problem

$$\frac{1}{2}\varphi'(t) = \left(\frac{C}{\nu} + \operatorname{Re}(\zeta_{\nu}(t))\right)\varphi(t) + \frac{C}{\nu^2}, \qquad \varphi(0) = |y(0)|^2, \qquad (59)$$

We claim that  $|y(t)|^2 < \varphi(t)$  for  $0 < t \le 1$ . Assume on the contrary that the set  $M := \{0 < t \le 1 : |y(t)|^2 \ge \varphi(t)\}$  is not empty, and let  $t_* := \inf M$ . Then  $t_* > 0$  since  $\frac{d}{dt}|y(0)|^2 < \varphi'(0)$ . Moreover, it follows from the definition of  $t_*$  that  $\varphi'(t_*) \le \frac{d}{dt}|y(t_*)|^2$ . On the other hand,  $\max_{0 \le t \le t_*} |y(t)|^2 \le \max_{0 \le t \le t_*} \varphi(t) = \varphi(t_*)$ . Hence,  $\frac{d}{dt}|y(t_*)|^2 < \varphi'(t_*)$  due to (58) and (59). This is a contradiction. Hence,  $|y(t)|^2 < \varphi(t)$  for  $0 < t \le 1$ . From the explicit solution

$$\varphi(t) = \exp\left(\int_0^t 2\left(\frac{C}{\nu} + \operatorname{Re}\zeta_{\nu}(t_2)\right) dt_2\right) |y(0)|^2 + \frac{2C}{\nu^2} \int_0^t \exp\left(\int_{t_1}^t 2\left(\frac{C}{\nu} + \operatorname{Re}\zeta_{\nu}(t_2)\right) dt_2\right) dt_1$$

it follows that  $\varphi(t) \leq C \nu^4 \exp\left(2ta_p + \int_0^t 2\operatorname{Re}\zeta_{\nu}(t_2)\,\mathrm{d}t_2\right)$ . This implies (55) for  $0 < t \leq 1$ .

Now we will prove (55) for  $t \geq 1$ . We may assume  $|y(t)| \neq 0$ . Otherwise (55) is trivially satisfied at t, and we have to apply the following argument separately on all intervals where |y| does not vanish. Dividing (57) by |y(t)| and using (16a) with k=2 we obtain

$$|y(t)|' = \frac{1}{2|y(t)|} \frac{d}{dt} |y(t)|^2 \le \operatorname{Re}(\zeta_{\nu}(t))|y(t)| + \frac{C}{t|(t-2i)\zeta_{\nu}(t)|} \eta(t)$$

with  $\eta(t) := e^{a_p t} (1 + \int_0^t e^{-a_p t_1} |y(t_1)| dt_1)$ . Inserting the identities

$$|y(t)| = e^{a_p t} \left\{ e^{-a_p t} \eta(t) \right\}' = \eta'(t) - a_p \eta(t),$$
 (60a)

$$|y(t)|' = \eta''(t) - a_p \eta'(t).$$
 (60b)

and using the estimate  $\frac{C}{t|(t-2i)\zeta_{\nu}(t)|} \leq a_p \operatorname{Re} \zeta_{\nu}(t)$ , which holds for all  $t \geq 1$  and  $\nu$  sufficiently large, we obtain  $\eta'' \leq (a_p + \operatorname{Re} \zeta_{\nu}) \eta'$ . This implies  $\eta'(t) \leq \eta'(1) \exp(a_p(t-1) + \int_1^t \operatorname{Re} \zeta_{\nu}(t_1) \, \mathrm{d}t_1)$  due to Gronwall's lemma. Now it follows from (60a) and (55) for t=1 that  $|y(t)| \leq Ce^{a_pt} \left(\frac{|1+\sqrt{1-2i}|}{\sqrt{2}}\right)^{2\nu}$  for t>1.  $\square$ 

**Corollary 23** For  $k \in \{0, 1, ...\}$  and  $m \in \{0, 1\}$  there exist constants  $C, \sigma > 0$  such that for all  $a > a_p$  and all  $\nu_j \geq N$ 

$$\frac{\|t^k \psi_{\nu_j, a, +}^{(m)}\|_{L^1}}{|\mathcal{H}_j(a)|} \le \frac{C}{(a - a_p)^{k+1-m}} \exp\left(\nu_j \left(\sigma + \ln \frac{a}{a - a_p}\right)\right). (61)$$

*Proof* We use the estimate

$$\frac{|\sqrt{t}+\sqrt{t-2i}|}{\sqrt{2}} \leq \left\{ \begin{array}{ll} \gamma\sqrt{t}, & & t \geq 1, \\ \gamma, & & 0 \leq t < 1 \end{array} \right.$$

with  $\gamma := \frac{1+\sqrt{5}}{\sqrt{2}}$ . Using Stirling's formula  $\Gamma(x+1) = \exp(x \ln \frac{x}{e} + \mathcal{O}(\ln x))$  as  $x \to \infty$ , we obtain

$$\int_{0}^{\infty} e^{-t(a-a_{p})} \left( \frac{|\sqrt{t} + \sqrt{t-2i}|}{\sqrt{2}} \right)^{2\nu} t^{k} dt 
\leq \gamma^{2\nu} \int_{0}^{\infty} e^{-(a-a_{p})t} t^{\nu+k} dt + \gamma^{2\nu} \int_{0}^{1} e^{-(a-a_{p})t} dt 
\leq \gamma^{2\nu} \left( (a-a_{p})^{-\nu-k-1} \Gamma(\nu+k+1) + 1 \right) 
\leq \frac{C}{(a-a_{p})^{k+1}} \exp\left( \nu \ln \gamma^{2} - \nu \ln(a-a_{p}) + \nu \ln \frac{\nu+k}{e} + \mathcal{O}(\ln \nu) \right).$$

Together with (55a) and (54) this implies (61) for m = 0. The case m = 1 follows analogously from (55b) using  $\sqrt{t|t - 2i|} \ge t$ .  $\square$ 

**Theorem 24** Assume that u satisfies (1) in  $\{x \in \mathbb{R}^d : |x| > a_u\}$ , that  $\operatorname{Tr} u \in H^{1/2}(\Gamma_{a_u} \text{ and that } \operatorname{res}_{-i} \hat{U}_{j,a_u} = 0 \text{ for all } j. \text{ Let } a \text{ be sufficiently large such that } \sigma + \ln \frac{a_u}{a-a_p} < 0.$  Then the following is true:

1. The functions

$$u_{\infty}(\hat{x}) := \sum_{j} \frac{U_{j}(a)}{\mathcal{H}_{j}(a)} \varphi_{j}(\hat{x}), \tag{62a}$$

$$\Psi_a(t,\hat{x}) := \sum_j \frac{U_j(a)}{\mathcal{H}_j(a)} \psi_{\nu_j,a,+}(t) \varphi_j(\hat{x})$$
 (62b)

are well defined for all  $t \geq 0$  and  $\hat{x} \in S^{d-1}$ . Moreover,

$$||u_{\infty}||_{C^{l}(S^{d-1})} < \infty, \tag{63a}$$

$$\int_0^\infty t^k \left\| \frac{\partial^m}{\partial t^m} \Psi_a(t, \cdot) \right\|_{C^l(S^{d-1})} \, \mathrm{d}t < \infty \tag{63b}$$

for  $m \in \{0,1\}$  and  $k,l \in \{0,1,\dots\}$ , and the series (62a) and (62b) converges with respect to all of these norms.

2. The formulas (7) and (9) hold true. Equation (7) may be differentiated any number of times both with respect to  $\rho$  and  $\hat{x}$ , and integration and differentiation may be interchanged.

*Proof* Due to (31a) the assumption  $\operatorname{res}_{-i} \hat{U}_{j,a_u} = 0$  implies that

$$U_j(\rho) = \frac{U_j(a_u)}{\mathcal{H}_j(a_u)} \mathcal{H}_j(\rho) \tag{64}$$

for all  $\rho \geq a_u$ . It follows from Corollary 20 and the boundedness of the Fourier coefficients  $U_j(a_u)$  that

$$|U_j(a)| = |U_j(a_u)| \left| \frac{\mathcal{H}_j(a)}{\mathcal{H}_j(a_u)} \right| \le C \left( \frac{a_u}{a} \right)^{\nu_j}. \tag{65}$$

Choose J such that  $\nu_j \geq N$  for  $j \geq J$ , N given in Lemma 22. Using Corollary 23 and the bound (53) we obtain

$$\sum_{j>J} |U_j(a)| \|\varphi_j\|_{C^l(S^{d-1})} \frac{\|t^k \psi_{\nu_j,a,+}^{(m)}\|_{L^1}}{|\mathcal{H}_j(a)|}$$
(66)

$$\leq C\sum_{j\geq J}\frac{(c_q+\nu_j^2)^{l/2+d/4}}{(a-a_p)^{k+1-m}}\exp\Big(\nu_j\Big(\sigma+\ln\frac{a}{a-a_p}+\ln\frac{a_u}{a}\Big)\Big).$$

Since  $N(\lambda) := \#\{\nu_j : \nu_j^2 \leq \lambda\}$  has the asymptotic behavior  $N(\lambda) \sim C\lambda^{(d-1)/2}$  (cf. [17, Sec. 8.3]), it follows from our assumption on a that the sum on the right hand side of (66) is finite. For j < J we use Lemma 10. This proves (63b). (63a) follows analogously from (53), (54) and (65).

To prove (7) for fixed  $\hat{x} \in S^{d-1}$ , we set  $\psi_{a,+} = \psi_{\nu_j,a,+}$  and  $U_{\infty}^+ = \frac{U_j(a)}{\mathcal{H}_j(a)}\varphi_j(\hat{x})$  in (31a). Then  $U(\rho) = U_j(\rho)\varphi_j(\hat{x})$  due to (64). Now the assertion follows by summing up over j and using (63). The differentiability properties of (7) are shown analogously using (31b) instead of (31a) and replacing  $\varphi_j(\hat{x})$  by a derivative of  $\varphi_j$  at  $\hat{x}$ . (9) follows in the same manner from (25a) multiplied by  $U_{\infty}^+$ .  $\square$ 

Note that  $u_{\infty}$  may be interpreted as a delta peak of the cut function  $\Psi_a$  at t=0. In other words, the formulas (7) and (9) remain valid if we formally replace  $\Psi_a(t,\hat{x})$  by  $\Psi_a(t,\hat{x}) + \delta_0(t)u_{\infty}(\hat{x})$  and then set  $u_{\infty}=0$ .

**Theorem 25** A bounded solution u to the differential equation (1) satisfies the Sommerfeld radiation condition (5) if and only if it satisfies the pole condition.

*Proof* Let us first assume that u satisfies the Sommerfeld radiation condition (5), and let U be defined by (2). Then

$$\frac{\partial}{\partial \rho} U(\rho, \hat{x}) - \left( i + \frac{d-1}{2\rho} \right) U(\rho, \hat{x}) = o(1), \qquad \rho \to \infty$$
 (67)

uniformly for  $\hat{x} \in S^{d-1}$ . Therefore, the Fourier coefficients  $U_j(\rho) := \langle U(\rho, \cdot), \varphi_j \rangle$  satisfy

$$U'_j(\rho) - \left(i + \frac{d-1}{2\rho}\right) U_j(\rho) = o(1), \qquad \rho \to \infty.$$

Due to Theorem 14 this is equivalent to  $\operatorname{res}_{-i} \hat{U}_{j,a} = 0$ . Hence,  $U_j(\rho) = U_j(a)\mathcal{H}_j(\rho)/\mathcal{H}_j(a)$ . Here a is chosen such that the assumption of Theorem 24 is satisfied. A comparison of Fourier coefficients shows that  $\hat{U}_a(s,\hat{x}) = \sum_j \frac{U_j(a)}{\mathcal{H}_j(a)} \varphi_j(\hat{x}) \hat{\mathcal{H}}_{j,a}(s)$  for  $\operatorname{Re} s > 0$  and  $\hat{x} \in S^{d-1}$ . We claim that for  $\hat{x} \in S^{d-1}$  a holomorphic extension of  $\hat{U}_a(\cdot,\hat{x})$  to  $\mathbb{C} \setminus S_i$  is given by the function

$$s \mapsto -e^{-ia} \left( \frac{u_{\infty}(\hat{x})}{i-s} + \int_0^{\infty} \frac{\Psi_a(t,\hat{x})}{i-t-s} \, \mathrm{d}t \right). \tag{68}$$

Due to the estimates (63) this function is well-defined and holomorphic in  $\mathbb{C}\backslash S_i$ . To show that it coincides with  $\hat{U}_a(s,\hat{x})$  for Re s>0,

we use Proposition 13 and the identity  $\operatorname{res}_i \hat{\mathcal{H}}_{j,a} = e^{-ia}$ , which follows from (28) and the definition of  $\mathcal{H}_j$ . The boundedness of  $s \mapsto \int_{S^{d-1}} |\frac{\partial}{\partial s} \hat{U}_a(s,\hat{x})|^2 d\hat{x}$  follows from (63b) using Cauchy's inequality.

Now assume that u satisfies the pole condition, and let  $\hat{U}_a(\cdot,\hat{x})$  be defined by (3). Using a standard corollary to Lebesgue's Dominated Convergence Theorem and the boundedness assumption in the pole condition, it follows that the Fourier coefficients  $\hat{U}_{j,a}(s) := \langle \hat{U}_a(s,\cdot), \varphi_j \rangle$  satisfy  $\operatorname{res}_{-i} \hat{U}_{j,a} = 0$ . Differentiating (7) once and using a partial integration we get

$$\begin{split} \frac{\partial}{\partial \rho} U(\rho, \hat{x}) - i U(\rho, \hat{x}) &= -\int_0^\infty e^{-t(\rho - a)} t \Psi_a(t, \hat{x}) \, \mathrm{d}t \\ &= -\frac{1}{\rho - a} \int_0^\infty e^{-t(\rho - a)} \frac{\partial}{\partial t} \left\{ t \Psi_a(t, \hat{x}) \right\} \, \mathrm{d}t. \end{split}$$

By virtue of (63b), the integral term on the right hand side of this equation is uniformly bounded for  $\hat{x} \in S^{d-1}$ . Since U is also uniformly bounded, this implies (67), which is equivalent to (5).  $\square$ 

We mention that (6) holds true with  $u_{\infty}$  and  $\Psi_a$  defined by (62). This follows from the Sokhotski-Plemelj formula (cf. [4]) and the fact that the function (68) coincides with  $\hat{U}_a(\cdot,\hat{x})$ .

We have constructed a solution  $(u_{\infty}, \Psi_a)$  to the system (9), (10) if  $f(\hat{x}) = U(a, \hat{x})$  and if the assumptions of Theorem 24 are satisfied. Uniqueness of this solution follows from the uniqueness of the corresponding system for each Fourier mode.

Remark 26 We have proved (9) for separable coordinates. In some interesting applications non-separable coordinate systems occur, e.g. optical components involving optical fibers or evanescent field microscopy, where the interaction between an optical fiber and a rough surface is investigated. Modeling optical components has actually been one of the motivations for our work. In many cases one can formally derive an equation similar to (9) where  $\check{p}(t) + te^{-at}A_q$  is replaced by a differential operator depending on t and  $\hat{x}$  in a more general way. The numerical algorithms are almost the same in this more general situation, and we are already using non-separable coordinate systems in our codes. A theoretical justification of these formulas and algorithms remains an interesting open problem for future research.

### Appendix

Proof of Lemma 5.

Part a) Since the operator J is defined by an integral over a holomorphic function (cf. (21)), we may deform the integration path in

order to facilitate the proof. Hence, we choose the path  $\gamma_s(t) := s + t$ ,  $t \ge 0$  if it does not intersect with  $D_+ \cup D_-$ . Otherwise we set

$$\gamma_s(t) := s + t + i\psi_s(t), \qquad t \ge 0 \tag{69}$$

with a real-valued function  $\psi_s$  as shown in Fig. 3(a).  $\psi_s$  is chosen such that  $\gamma_s$  does not intersect  $D_+ \cup D_- \cup S_i \cup S_{-i}$ ,  $\psi_s(0) = 0$ ,  $|\psi| \leq \frac{1}{2}$ ,  $|\psi'_s| \leq 1$ , meas(supp  $\psi_s$ )  $\leq 1$ , and  $\lim_{t\to\infty} \psi(t) = 0$ . We have

$$(Jw)(s) = \int_0^\infty P(t + i\psi_s(t)) \frac{|\gamma_s(t)|^2 + 1}{\gamma_s(t)^2 + 1} \frac{w(\gamma_s(t))}{|\gamma_s(t)|^2 + 1} \gamma_s'(t) dt$$
 (70)

Due to (16b) there exists a constant c > 0 such that for all  $t \ge 0$ 

$$\sup_{|\tau| \le \min(t, 1/2)} |P(t + i\tau)| \, \mathrm{d}t \le cte^{-(a - a_p)t/2}. \tag{71}$$

To see this, choose T such that  $-at+a_p\sqrt{t^2+1/4} \leq -(a-a_p)t/2$  for  $t\geq T$ . Then (71) holds for  $t\geq T$ . By a compactness argument it is also true  $t\leq T$ . Here and in the following, c is a generic constant. Moreover,  $\sup_{s\in \mathfrak{C}\setminus (\mathbb{D}_+\cup \mathbb{D}_-)}\frac{|s|^2+1}{|s^2+1|}<\infty$ . Hence,

$$\begin{aligned} |(Jw)(s)| & \leq c \left( \int_0^\infty t e^{-(a-a_p)t/2} \, \mathrm{d}t \right) \left( \sup_{\text{Re } s_1 \geq \text{Re } s} \frac{|w(s_1)|}{|s_1|^2 + 1} \right) \\ & = \frac{c}{((a-a_p)/2)^2} \left( \sup_{\text{Re } s_1 \geq \text{Re } s} \frac{|w(s_1)|}{|s_1|^2 + 1} \right). \end{aligned}$$

This implies (23a).

Part b) Differentiating (21) yields

$$(Jw)'(s) = \int_{s}^{\infty} P'(s_1 - s) \frac{w(s_1)}{s_1^2 + 1} ds_1$$
 (72)

since P(0) = 0. Now we use (16a) and estimate the integral term as above to establish (23b).

Part c) W.r.o.g. we may assume that  $s, \sigma \in D_+$  and that  $|s-i|_1 \ge |\sigma-i|_1$ . In this proof we say that s and  $\sigma$  are on opposite sides of  $S_i$  if Re s, Re  $\sigma < 0$  and Im(s-i) Im $(\sigma-i) < 0$  or if s and  $\sigma$  are the limit of a sequence of such points. We first assume that s and  $\sigma$  are not on opposite sides of  $S_i$ . Let  $\gamma_{\sigma s}$  be the shortest path from  $\sigma$  to s in  $D_+$  such that  $|s_1 - i|_1 \ge |\sigma - i|_1$  for all  $s_1 \in \gamma_{\sigma s}$  (cf. Fig. 3(b)). The length of this path can be estimated by  $l(\gamma_{\sigma s}) \le 3\delta$  where  $\delta := |s - \sigma|$ .

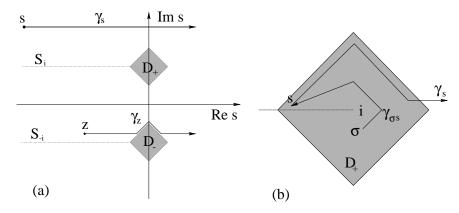


Fig. 3. Integration paths in the proof of Lemma 5

Moreover, we choose the path  $\gamma_s$  from s to  $\infty$  such that  $|s_1 - i|_1 \ge |s - i|_1$  for all  $s \in \gamma_s$  (cf. Fig. 3(b)). We have

$$(Jw)(\sigma) - (Jw)(s) = \int_{\gamma_{\sigma s}} \frac{P(s_1 - \sigma)}{s_1^2 + 1} w(s_1) \, \mathrm{d}s_1 + \int_{\gamma_s} \left( P(s_1 - \sigma) - P(s_1 - s) \right) \frac{w(s_1)}{s_1^2 + 1} \, \mathrm{d}s_1.$$

To estimate the integral over  $\gamma_{\sigma s}$ , we use the inequalities  $|s| \leq |s|_1 \leq \sqrt{2}|s|$  and (16b):

$$\left| \frac{P(s_1 - s)}{(s_1 + i)(s_1 - i)} \right| \le \sqrt{2} \left| \frac{1}{s_1 + i} \right| \cdot \left| \frac{P(s - s_1)}{s - s_1} \right| \le c.$$

Together with the bound on  $l(\gamma_{\sigma s})$  this yields  $\left| \int_{\gamma_{\sigma s}} \dots \right| \leq c\delta ||w||_X$ . The integral over  $\gamma_s$  is estimated by the mean value theorem:

$$\left| \int_{\gamma_s} \left( P(s_1 - \sigma) - P(s_1 - s) \right) \frac{w(s_1) \, \mathrm{d}s_1}{s_1^2 + 1} \right| \\ \leq \delta \int_{\gamma_s} \sup_{z \in [\sigma, s]} |P'(s_1 - z)| \frac{|w(s_1)| \, |\mathrm{d}s_1|}{|s_1^2 + 1|}$$

To bound the integrand for  $s_1 \in D_+ \cap \gamma_s$  we note that

$$|s_1 - i|_1 \ge |s_1 - s|_1 - |s - i|_1 \ge |s_1 - s|_1 - |s_1 - i|_1$$
 and  $2|s_1 - i|_1 \ge 2|s - i|_1 \ge |s - i|_1 + |\sigma - i|_1 \ge |s - \sigma|_1 \ge \delta$ 

due to the choice of  $\gamma_s$ . Adding these inequalities yields  $4|s_1 - i|_1 \ge |s_1 - s|_1 + \delta$ . Together with the estimates  $|s_1 - s|_1 \ge \text{Re}(s_1 - s)$  and

 $|s_1+i|_1 \ge 1$  we obtain  $|s_1^2+1| \ge \frac{1}{2}|s_1+i|_1|s_1-i|_1 \ge \frac{1}{8}$  (Re $(s_1-s)+\delta$ ). Outside of  $D_+$  the bound  $\left|\frac{w(s_1)}{s_1^2+1}\right| \le c\|w\|_X$  holds true. With (16a) and  $t^* := \sup\{t \ge 0: s+t \in D_+\}$  we obtain

$$\left| \int_{\gamma_s} \dots \right| \le c\delta \|w\|_X \left( \int_0^{t^*} \frac{\mathrm{d}t}{t+\delta} + \int_{t^*}^{\infty} e^{-(a-a_p)t/2} \, \mathrm{d}t \right)$$
$$\le c\delta \|w\|_X \left( \ln \Delta + \frac{(a-a_p)}{2} \right) \le c\delta^{\alpha} \|w\|_X.$$

Since  $\delta \leq d(s, \sigma)$ , we have proved (23c) if s and  $\sigma$  are not on opposite sides of  $S_i$ . Otherwise, we obtain from our previous estimates that

$$|(Jw)(\sigma) - (Jw)(s)| \le |(Jw)(\sigma) - (Jw)(i)| + |(Jw)(i) - Jw(s)|$$
  
 
$$\le c(|\sigma - i|^{\alpha} + |i - s|^{\alpha})$$

Using the inequalities

$$|\operatorname{Im}(\sigma - i)| + |\operatorname{Im}(i - s)| = |\operatorname{Im}(\sigma - s)| \le d(\sigma, s),$$
  

$$|\operatorname{Re}(s - i)| = |\operatorname{Re} s| \le |\operatorname{Re} \sigma| + |\operatorname{Re}(s - \sigma)| \le d(s, \sigma),$$
  

$$|\operatorname{Re}(\sigma - i)| = |\operatorname{Re} \sigma| \le d(s, \sigma),$$

we also obtain (23c).

Part d) (23d) follows easily from (23a) and (23c).  $\Box$ 

Proof of Lemma 6. It follows from eq. (72) that Jw is holomorphic in V for  $w \in X$  and from Lemma 5 that Jw is continuous in  $\overline{V}$ . Together with the estimate (23d) this shows that J maps X into X. To prove compactness, let  $(w_n)_{n\in\mathbb{N}}$  be a sequence in X with  $||w_n||_X \leq$ 1 for all  $n \in \mathbb{N}$ . We have to show that the sequence  $v_n := Jw_n$ ,  $n \in \mathbb{N}$  has a convergent subsequence in X. Let us first consider the restrictions of  $v_n$  to some compact subset  $K \subset \overline{V}$ . Due to (23b) and (23c), the sequence  $(v_n|_K)_{n\in\mathbb{N}}$  is equicontinuous on K with respect to the metric d. Hence, by the Arzelà-Ascoli Theorem, there exists a subsequence of  $(v_n)_{n\in\mathbb{N}}$  which converges with respect to the norm  $\|\varphi\|_{\infty,K} := \sup_{s \in K} |\varphi(s)|$ . In order to construct a subsequence which converges globally, we introduce the sets  $K_j := \{s \in V : |s| \leq j\}$  for  $j \in \mathbb{N}$ . It is easy to show that these sets are compact with respect to the metric d. By the argument above, there exists a subsequence  $(v_{n_1(l)})_l$  which converges with respect to  $\|\cdot\|_{\infty,K_1}$ . Applying the same argument again, we get a subsequence  $(v_{n_2(l)})_l$  which converges with respect to  $\|\cdot\|_{\infty,K_2}$ . Repeating this process of selecting subsequences, we arrive at an array  $v_{n_i(l)}$  with the property that each row is a subsequence of the previous row. The diagonal subsequence  $v_{n(l)} :=$ 

 $v_{n_l(l)}$  converges to some function v with respect to the supremum norm on each  $K_j$ . In particular,  $\lim_{l\to\infty}v_{n(l)}(s)=v(s)$  for all  $s\in\overline{V}$ . It remains to show that  $\|v_{n(l)}-v\|_X\to 0$ . Let  $\epsilon>0$ . By virtue of Lemma 5(b) there exists a constant C>0 such  $|v_{n(l)}(s)|\leq C$  for all  $s\in\overline{V}$  and  $l\in\mathbb{N}$ . Therefore,

$$\frac{|v(s) - v_{n(l)}(s)|}{1 + |s|^2} \le \epsilon \quad \text{for all } l \in \mathbb{N} \text{ and } |s| \ge \sqrt{\frac{2C}{\epsilon}}. \tag{73}$$

Let  $J \geq \sqrt{2C/\epsilon}$ ,  $J \in \mathbb{N}$ . Since  $v_{n(l)}$  converges to v with respect to  $\|\cdot\|_{\infty,K_J}$ , there exists  $L \in \mathbb{N}$  such that

$$\sup_{s \in K_J} \frac{\left| v(s) - v_{n(l)}(s) \right|}{|s^2| + 1} \le \|v(s) - v_{n(l)}\|_{\infty, K_J} \le \epsilon \tag{74}$$

for  $l \geq L$ . Putting (73) and (74) together yields  $||v - v_{n(l)}||_X \leq \epsilon$  for  $l \geq L$ .  $\square$ 

*Proof of Lemma 9.* Introducing  $(Kv)(t) := \int_0^t \frac{P(t-t_1)}{t(t-2i)} v(t_1) dt_1$ , eq. (25a) can be written as

$$\psi_{+}(t) + (K\psi_{+})(t) = -\frac{P(t)}{t(t-2i)}, \qquad t > 0.$$
 (75)

By repeated partial integration we obtain

$$\int_0^t P(t-t_1) \frac{t_1^j}{j!} dt_1 = \sum_{l=1}^\infty P^{(l)}(0) \int_0^t \frac{(t-t_1)^l}{l!} \frac{t_1^j}{j!} dt_1 = \sum_{l=1}^\infty \frac{P^{(l)}(0)t^{l+j+1}}{(l+j+1)!}.$$

Changing the order of integration and summation in the first equality is justified because the Taylor series of P converges uniformly. The right hand side of the last equation is an analytic function in t. If  $v(t) = \sum_{j=0}^{\infty} \frac{v^{(j)}(0)}{j!} t^j$  is a polynomial, then

$$(Kv)(t) = \frac{1}{t(t-2i)} \int_0^t P(t-t_1) \sum_{j=0}^\infty \frac{v^{(j)}(0)}{j!} t_1^j dt_1$$
$$= \frac{1}{t-2i} \sum_{l=1}^\infty \sum_{j=0}^\infty P^{(l)}(0) v^{(j)}(0) \frac{t^{l+j}}{(l+j+1)!}.$$

Expanding  $(t-2i)^{-1}$  in a power series and using the Cauchy product twice yields

$$(Kv)(t) = \frac{1}{-2i} \sum_{r=0}^{\infty} \left(\frac{t}{2i}\right)^r \sum_{m=1}^{\infty} \frac{t^m}{(m+1)!} \sum_{n=1}^m P^{(n)}(0)v^{(m-n)}(0)$$
(76)  
$$= \frac{1}{-2i} \sum_{l=1}^{\infty} t^l \sum_{j=0}^l \left(\frac{1}{2i}\right)^{l-j} \frac{1}{(j+2)!} \sum_{n=1}^j P^{(n)}(0)v^{(j-n)}(0).$$

In particular, it can be seen that Kv is analytic at t = 0.

We prove by induction that  $\psi_+ \in C^n([0,\infty))$  for  $n \in \mathbb{N}$ . Let us start with the case n=0. Note that the right hand side of (75) can be continuously extended to a function in  $C^{\infty}([0,\infty))$ . We know from Lemma 5 that  $|\psi_+(t)| = \mathcal{O}(t^{\alpha-1})$  as  $t \to 0$ . Moreover,  $P(t) = \mathcal{O}(t)$ , so

$$|(Kv)(t)| \leq rac{C}{t(t-2i)} \int_0^t (t-t_1) t_1^{lpha-1} \, \mathrm{d}t_1 = rac{C}{t|t-2i|} (2lpha+1) t^{1+lpha} o 0$$

as  $t \to 0$ . This shows  $\psi_+ \in C([0,\infty))$  and (27a).

Assume now that  $\psi_+ \in C^k([0,\infty))$ ,  $k \geq 0$ . Then there exists a function  $R_k$  such that  $\psi(t) = \sum_{j=0}^k \frac{\psi^{(j)}(0)}{j!} t^j + R_k(t)$  and  $R_k(t) = o(t^k)$  as  $t \to 0$ . We have

$$|(KR_k)(t)| \leq rac{1}{t|t-2i|} \int_0^t |P(t-t_1)| \, \mathrm{d}t_1 \sup_{0 < t_1 < t} |R_k(t_1)| = \mathrm{o}\Big(t^{k+1}\Big)$$

since  $P(t) = \mathcal{O}(t)$  as  $t \to 0$ . Therefore,  $KR_k \in C^{k+1}([0,\infty))$  and  $(KR_k)^{(k+1)}(0) = 0$ . Now it follows from (75), (76) and the analyticity of  $t \mapsto \frac{-P(t)}{t(t-2i)}$  that  $\psi \in C^{k+1}([0,\infty))$  and that  $\psi^{(k+1)}(0)$  satisfies (27b).  $\square$ 

Proof of Lemma 19. We may assume w.r.o.g. that  $\Delta_2(\rho+i\sigma)\neq 0$  for all  $\rho\in[a,A]$  and  $\sigma\in\mathbb{R}$ . Otherwise, if  $\Delta_2(\rho_0+i\sigma_0)=0$ , then  $\Delta_2(\rho_0+i\sigma;\nu)=0$  for all  $\sigma\in\mathbb{R}$  due to the uniqueness of initial value problems for (48), and then (50) is trivially satisfied for  $\rho=\rho_0$ . Our proof is based on the observation that the function  $\sigma\mapsto |\Delta_2(\rho+i\sigma;\nu)|$  is decreasing at the point  $\sigma$  if and only if  $\partial_\sigma(|\Delta_2(\rho+i\sigma;\nu)|^2)\leq 0$ , if and only if  $\mathrm{Re}(\dot{\Delta}_2/\Delta_2)(\rho+i\sigma;\nu)\leq 0$  (divide by  $|\Delta_2(\rho+i\sigma;\nu)|^2$ ). Due to (48),  $\sigma\mapsto |\Delta_2(\rho+i\sigma;\nu)|$  is decreasing at  $\sigma$  if and only if  $\Delta_2(\rho+i\sigma;\nu)\in G(\rho+i\sigma;\nu)$  where

$$G(z;
u) := \left\{\delta \in \mathbb{C} : \operatorname{Re}[-\delta + 2\gamma_2(z;
u) + rac{\dot{\gamma}_2(z;
u) - \dot{\gamma}_1(z;
u)}{\delta}] \leq 0 
ight\}.$$

Introducing the variable x for the expression in brackets and solving a quadratic equation for  $\delta$  shows that  $G = G^+ \cup G^-$  with

$$G^{\pm} := \left\{ \left( \gamma_2 - \frac{x}{2} \right) \left( 1 \pm \sqrt{1 + \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{(\gamma_2 - x/2)^2}} \right) : \operatorname{Re} x \le 0 \right\}.$$

For the following arguments we introduce the strips  $S_{\lambda} := \{\rho + i\sigma : a \leq \rho \leq A, \sigma \geq \lambda\}$   $(\lambda \geq 0)$  in the complex plane. Note that there exist constants C, N > 0 such that

$$\frac{1}{|z\gamma_1|} = \frac{1}{\nu|\sqrt{\nu^{-2}z^2(1+p)-1}|} = \begin{cases} \frac{C}{\nu}, & \sigma \le \nu, \\ \frac{C}{\sigma}, & \sigma > \nu, \end{cases}$$
(77)

for all  $z \in S_0$  and all  $\nu \geq N$  and that

$$\dot{\gamma}_1 = i \frac{\nu^2}{z^3 \gamma_1} \left( 1 + \frac{z^3 \dot{p}}{2\nu^2} \right). \tag{78}$$

Therefore,

$$\gamma_2^2 - 1 = \gamma_1^2 - 1 - \dot{\gamma}_1 = -\frac{\nu^2}{z^2} \left( 1 + \mathcal{O}\left(\frac{1}{\nu}\right) \right), \qquad \nu \to \infty, \quad (79)$$

uniformly for  $z \in S_0$ . Using (79) and  $\gamma_2 = \frac{i\nu}{z} \sqrt{1 - \nu^{-2} z^2 + \mathcal{O}(\nu^{-1})}$ , it can be shown that there exist constants C, N > 0 such that

$$|z|\operatorname{Re}\gamma_{2}(z) \geq \begin{cases} C\nu\sigma, & 0 \leq \sigma < 1, \\ C\nu, & 1 \leq \sigma < \nu, \\ C\sigma, & \nu \leq \sigma \end{cases}$$
(80)

for all  $\nu \geq N$  and all  $z \in S_0$ . As  $\gamma_2 = \gamma_1 \sqrt{1 + \frac{\dot{\gamma}_1}{\gamma_1^2}}$ , we have

$$\dot{\gamma}_2 - \dot{\gamma}_1 = \dot{\gamma}_1 \left( \sqrt{1 + \frac{\dot{\gamma}_1}{\gamma_1^2}} - 1 \right) + \left( 1 + \frac{\dot{\gamma}_1}{\gamma_1^2} \right)^{-1/2} \left( \frac{\ddot{\gamma}_1}{\gamma_1} - 2 \frac{\dot{\gamma}_1^2}{\gamma_1^2} \right).$$

Since  $\frac{\dot{\gamma}_1}{\gamma_1^2} = \mathcal{O}(\frac{1}{\nu})$  uniformly for  $z \in S_0$  due to (77) and (78), we have

$$\dot{\gamma}_1\left(\sqrt{1+\frac{\dot{\gamma}_1}{\gamma_1^2}}-1\right)=\frac{1}{2}\left(\frac{\dot{\gamma}_1}{\gamma_1}\right)^2+\mathcal{O}\!\left(\frac{\dot{\gamma}_1^3}{\gamma_1^4}\right)=\mathcal{O}\!\left(|z|^{-2}\right).$$

Moreover,

$$\frac{\ddot{\gamma}_{1}}{\gamma_{1}} = \frac{3\nu^{2}}{z^{2}(z\gamma_{1})^{2}} \left(1 + \frac{z^{4}\ddot{p}}{\nu^{2}}\right) - \frac{2i}{z^{2}} \left(\frac{\nu\dot{\gamma}_{1}}{\gamma_{1}^{2}}\right) \left(\frac{\nu}{z\gamma_{1}}\right) \left(1 + \frac{z^{3}\dot{p}}{2i\nu^{2}}\right) = \frac{\mathcal{O}(1)}{z^{2}}$$

uniformly for  $z \in S_0$ , so

$$|\dot{\gamma}_2 - \dot{\gamma}_1| = \mathcal{O}(|z|^{-2}) \tag{81}$$

uniformly for  $z \in S_0$ . Hence,

$$\left| \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{(\gamma_2 - x/2)^2} \right| = \mathcal{O}\left(\frac{1}{|z|^2 (\operatorname{Re} \gamma_2)^2}\right) = \begin{cases} \mathcal{O}\left((\nu\sigma)^{-2}\right), & 0 \le \sigma < 1, \\ \mathcal{O}\left(\nu^{-2}\right), & 1 \le \sigma < \nu, \\ \mathcal{O}\left(\sigma^{-2}\right), & \nu \le \sigma \end{cases}$$

uniformly for  $z \in S_0$  and Re  $x \le 0$  (cf. (80)). Now the Taylor formula  $\sqrt{1+\epsilon} = 1+\epsilon/2 + \mathcal{O}(\epsilon^2)$  ( $\epsilon \to 0$ ) implies that there exist constants  $\Gamma, N > 0$  such that

$$\left| \left( \gamma_2 - \frac{x}{2} \right) \left( 1 - \sqrt{1 + \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{(\gamma_2 - x/2)^2}} \right) \right|$$

$$= \left| \left( \gamma_2 - \frac{x}{2} \right) \left( 1 - 1 - \frac{1}{2} \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{(\gamma_2 - x/2)^2} + \mathcal{O}\left( \left| \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{(\gamma_2 - x/2)^2} \right|^2 \right) \right) \right|$$

$$\leq \frac{1}{2} \left| \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{\operatorname{Re} \gamma_2} \right| + \mathcal{O}\left( \frac{|\dot{\gamma}_2 - \dot{\gamma}_1|}{|\operatorname{Re} \gamma_2|^3} \right) \leq \begin{cases} \Gamma(\sigma \nu)^{-1}, & \Gamma/\nu \leq \sigma < \nu, \\ \Gamma/\sigma^{-2}, & \nu \leq \sigma \end{cases}$$

for all  $\nu \geq N$ ,  $z \in S_{\Gamma/\nu}$  and  $\operatorname{Re} x \geq 0$ . Performing an analogous computation for  $G^+(z;\nu)$ , we obtain that for  $\nu \geq N$ 

$$G^{-}(z;\nu) \subset \begin{cases} \{\zeta : |\zeta| \le \Gamma/(\sigma\nu)\}, & \Gamma/\nu \le \sigma < \nu, \\ \{\zeta : |\zeta| \le \Gamma/\sigma^{-2}\}, & \nu \le \sigma, \end{cases}$$
(82a)

$$G^+(z;\nu) \subset \{\zeta : \operatorname{Re} \zeta \ge 1\}, \qquad \Gamma/\nu \le \sigma.$$
 (82b)

Now we are going to show that (82) and (45) imply (50) for  $z \in S_{\Gamma/\nu}$ . Let  $\rho_0 \in [a,A]$ . By virtue of (45) and the fact that  $\lim_{\sigma \to \infty} (1-\gamma_2(\rho_0+i\sigma;\nu)) = 0$  for all  $\nu$ , there exists a sequence  $\Gamma/\nu = \sigma_0 < \sigma_1 < \ldots$  such that  $\lim_{l\to\infty} \sigma_l = \infty$  and  $|\Delta_2(\rho_0+i\sigma_l;\nu)| < 1/(l+1)$  for  $l \geq 1$ . We may also arrange that  $\partial_{\sigma}|\Delta_2(\rho_0+i\sigma_l;\nu)| < 0$ . Then the maximum of the function  $\sigma \mapsto |\Delta_2(\rho_0+i\sigma;\nu)|$  on the interval  $[\sigma_l,\sigma_{l+1}]$  is attained at the point  $\sigma_l^* \in [\sigma_l,\sigma_{l+1})$ , and  $\partial_{\sigma}|\Delta_2(\rho_0+i\sigma_l^*;\nu)| \leq 0$ , i.e.  $\Delta(\rho_0+i\sigma_l^*;\nu) \in G(\rho_0+i\sigma_l^*;\nu)$ . If  $\Delta(\rho_0+i\sigma_0;\nu) \in G^+(\rho_0+i\sigma_0;\nu)$  then, due to (82b) and the choice of the  $\sigma_l$ 's, there exists a largest  $\tilde{\sigma} \in (\sigma_l^*,\sigma_{l+1})$  such that  $|\Delta_2(\rho_0+i\tilde{\sigma};\nu)| = \frac{1}{2}$ , and  $\Delta_2(\rho_0+i\tilde{\sigma};\nu) \in G(\rho_0+i\sigma_*;\nu)$  since  $\partial_{\sigma}|\Delta(\rho_0+i\tilde{\sigma};\nu)| \leq 0$ . This contradicts (82). Hence,  $\Delta(\rho_0+i\sigma_l^*;\nu) \in G^-(\rho_0+i\sigma_l^*;\nu)$ , and (50) follows from (82a).

It remains to show (50) for  $0 \le \sigma \le \Gamma/\nu$ . In this case, there exists constants C, N > 0 such

$$\operatorname{Re} \frac{\dot{\Delta}_2}{\Delta_2} = -\operatorname{Re} \Delta_2 + 2\operatorname{Re} \gamma_2 + \operatorname{Re} \frac{\dot{\gamma}_2 - \dot{\gamma}_1}{\Delta_2} \ge -C$$

if  $\Delta_2(z;\nu)$  is in the annulus  $1 \leq |\Delta_2(z;\nu)| \leq 2$  and  $\nu \geq N$  (cf. (80) and (81)). Since

$$|\Delta_2(
ho+i\sigma;
u)| = \left|\Delta_2(
ho+irac{\Gamma}{
u};
u)
ight| \exp\left(\int_{\Gamma/
u}^\sigma {
m Re}\,rac{\dot{\Delta}_2(
ho+i\sigma_1;
u)}{\Delta_2(
ho+i\sigma_1;
u)}\,{
m d}\sigma_1
ight)$$

and since  $|\Delta_2(\rho + i\Gamma/\nu; \nu)| \leq 1$ , it follows that  $|\Delta_2(\rho + i\sigma; \nu)| \leq \exp(C(\Gamma/\nu - \sigma)) \leq 2$  for  $0 \leq \sigma \leq \Gamma/\nu$  and  $\nu \geq \max(N, C\Gamma/\ln 2)$ .

#### References

- D. Colton and R. Kreß. Inverse Acoustic and Electromagnetic Scattering. Springer Verlag, Berlin Heidelberg New York, second edition, 1997.
- P. Deuflhard and F. Bornemann. Numerische Mathematik II. Walter de Gruyter, Berlin, New York, 1994.
- G. Doetsch. Handbuch der Laplace-Transformation, volume 2. Birkhäuser Verlag, Basel, Stuttgart, 1955.
- 4. H. W. Engl. Integralgleichungen. Springer, Vienna, 1997.
- E. Heinz. Beiträge zur Störungstheorie der Spektralzerlegung. Math. Ann., 123:425–438, 1951.
- T. Hohage, F. Schmidt, and L. Zschiedrich. Solving time-harmonic scattering problems based on the pole condition: Convergence of the PML method. in preparation.
- T. Hohage, F. Schmidt, and L. Zschiedrich. Solving time-harmonic scattering problems based on the pole condition: Numerical algorithms. in preparation.
- F. Ihlenburg. Finite Element Analysis of Acoustic Scattering. Springer Verlag, 1998
- R. Kreß. Linear Integral Equations. Springer Verlag, Berlin Heidelberg New York, 1989.
- 10. M. Renardy and R. C. Rogers. An Introduction to Partial Differential Equations. Springer-Verlag, 1992.
- 11. F. Schmidt. An alternative derivation of the exact DtN-map on a circle. Technical Report SC 98-32, Konrad-Zuse-Zentrum, Berlin, December 1998.
- F. Schmidt. Construction of discrete transparent boundary conditions for Schrödinger-type equations. Surv. Math. Ind., 9:87-100, 1999.
- F. Schmidt and P. Deuflhard. Discrete transparent boundary conditions for the numerical solution of Fresnel's equation. Computers Math. Appl., 29:53– 76, 1995.
- F. Schmidt, T. Friese, and D. Yevick. Transparent boundary conditions for split-step Padé approximations of the one-way Helmholtz equation. Preprint SC 99-46, ZIB, 1999. to appear in J. Comp. Phys.
- 15. A. Sommerfeld. Die Greensche Function der Schwingungsgleichung. In Jahresber. Deutsch. Math.-Verein. -, 1912.
- A. Sommerfeld. Lectures on Theoretical Physics, volume 6. Academic Press, 1964.
- M. Taylor. Partial Differential Equations, volume 1-3. Springer Verlag, New York, 1996.
- 18. G. N. Watson. *Theory of Bessel Functions*. Cambridge University Press, London, 1922.