# THE LINEAR SAMPLING METHOD REVISITED 

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Communicated by Charles Groetsch<br>This paper is dedicated to Professor Rainer Kress on the occasion of his 65th birthday.


#### Abstract

This paper is concerned with convergence results for the Linear Sampling method, a method in inverse scattering theory characterizing an unknown obstacle directly through an indicator function computed from the data. Three seperate but related results are shown. Firstly, sufficient conditions are formulated for the choice of the regularization parameter that guarantee that the method converges in the presence of noise for a sampling point inside the obstacle. Secondly, a new, very strong connection to the related Factorization method is proved. Thirdly, for the first time the behaviour of the indicator function for sampling points outside the obstacle is adequately explained.


1. Introduction. Inverse scattering problems for time-harmonic acoustic waves have been a popular research subject for a long time [7]. Among the methods employed for their solution are iterative Newtontype methods, where differentiability with respect to the scatterer is exploited, decomposition methods separating the reconstruction of the scattered fields from the reconstruction of an obstacle or inhomogeneity, and sampling methods. Such methods allow the computation of an indicator function characterizing the unknown obstacle directly from the data. It is the latter class of methods we are concerned with in this paper.

Theory on sampling methods started with the Linear Sampling method, first introduced in $[\mathbf{5}, \mathbf{6}]$. It requires the knowledge of the far field pattern $u^{\infty}(\hat{x}, d)$ of the scattered field for incident plane waves of all possible directions $d \in \mathbb{S}^{2}$ and all directions of observation $\hat{x} \in \mathbb{S}^{2}$. Here, $\mathbb{S}^{2}$ denotes the unit sphere in $\mathbb{R}^{3}$. From this data, the so-called

[^0]far field operator $F: L^{2}\left(\mathbb{S}^{2}\right) \rightarrow L^{2}(\mathbb{S})$ is defined by setting
$$
F g(\hat{x})=\int_{\mathbb{S}^{2}} u^{\infty}(\hat{x}, d) g(d) d s(d), \quad \hat{x} \in \mathbb{S}^{2}, \quad g \in L^{2}\left(\mathbb{S}^{2}\right)
$$

The idea is then to approximately solve an integral equation of the first kind, the so-called far field equation,

$$
F g_{z}=\Phi^{\infty}(\cdot, z)
$$

for every point $z \in \mathbb{R}^{3}$ using a regularization strategy. The right hand side denotes the far field pattern generated in free-field conditions by the point source $\Phi(\cdot, z)$. Explicitly,

$$
\Phi(x, z)=\frac{1}{4 \pi} \frac{\exp (i k|x-z|)}{|x-z|}, \quad x \in \mathbb{R}^{3}
$$

and

$$
\Phi^{\infty}(\hat{x}, z)=\frac{1}{4 \pi} \exp (-i k \hat{x} \cdot z), \quad \hat{x} \in \mathbb{S}^{2}
$$

By $k>0$ we denote the positive wave number.
The claim in the Linear Sampling method is that the norm of the approximate solution of the far field equation is an indicator for the obstacle in the scattering problem. Numerical experiments show that this is indeed the case. The method has been successfully applied to a large number of scattering problems. A recent overview of the literature available can be found in the monograph [4]. The attractions of the method are manifold: using the singular value decomposition of the operator $F$, it is very easy to implement, and, assuming that the necessary data is available, the reconstructions are obtained very quickly.

However, there are some gaps in the mathematical theory. Foremost, the right hand side of the far field equation is almost never in the range of the far field operator, and hence the equation has no solution. Thus, standard regularization theory will not guarantee that an approximate solution computed using a regularization strategy will have any meaning at all. To date, the only convergence results available for this method have been obtained in [3]. They are based on the related Factorization method first introduced by Kirsch in [10]. In the simplest
case, for example when considering scattering by a bounded sound soft obstacle, the Factorization method gives a rigorously justified characterization of the obstacle. To this end, a different equation is considered which is obtained from the far field equation by replacing $F$ with the operator $\left(F^{*} F\right)^{1 / 4}$. A more recent presentation of the Factorization method including the many modifications necessary for its application to broader classes of problems is contained in the monograph [11]. The convergence results presented in [3] are valid in principal whenever this latter method can be applied.

In the present paper, we only consider the case of a bounded sound soft obstacle. The results of [3] are extended in several ways. Firstly, the case of perturbed data is considered. Again, standard regularization theory for ill-posed operator equations fails in the situation of the Linear Sampling method in this case. In Section 3, the application of Tikhonov regularization to the far field equation is considered in the case of noisy data. A necessary condition for the choice of the regularization parameter is given that leads to a convergent method as the noise level tends to zero.

The main result of Section 4 is that for a sampling point inside the obstacle the indicator function proposed in [3] for the Linear Sampling method is equivalent to the indicator function computed by the Factorization method. This new result further clarifies the connection between these two sampling methods. Finally, the results of Section 4 are used in Section 5 to characterize the behaviour of the indicator function for sampling points outside the obstacle. Use is made of some results from perturbation theory applied to normal operators that were recently successfully applied to study the effect of noisy data on the Factorization method [12]. For completeness we collected some basics on perturbation theory in an appendix.
2. Preliminaries. The propagation of time harmonic acoustic waves of wave number $k>0$ in three-dimensional space is governed by the Helmholtz equation

$$
\begin{equation*}
\Delta u+k^{2} u=0 \quad \text { in } \mathbb{R}^{3} \tag{1}
\end{equation*}
$$

We consider here scattering of plane waves of incident direction $d$,

$$
u^{i}(x, d)=\exp (i k d \cdot x), \quad x \in \mathbb{R}^{3}, \quad d \in \mathbb{S}^{2}
$$

by a bounded obstacle $D \subset \mathbb{R}^{3}$. Throughout the paper, we will use the convention of noting the dependence of all fields on the direction of incidence as a second argument.

The total field $u$, which is the sum of the incident field $u^{i}$ and the scattered field $u^{s}$ is assumed to satisfy a homogeneous Dirichlet boundary condition on $\partial D$,

$$
\begin{equation*}
u^{i}+u^{s}=0 \quad \text { on } \partial D \tag{2}
\end{equation*}
$$

The scattered field is a solution of (1) in the domain $\mathbb{R}^{3} \backslash \bar{D}$.
The formulation of the scattering problem is completed by the requirement that the scattered field satisfy the Sommerfeld radiation condition,

$$
\begin{equation*}
\lim _{|x| \rightarrow \infty}|x|\left(\frac{\partial u^{s}}{\partial|x|}-i k u^{s}\right)=0 \tag{3}
\end{equation*}
$$

where the limit is obtained uniformly for all directions $\hat{x}=x /|x| \in \mathbb{S}^{2}$. As a consequence of this radiation condition, the scattered field has an asymptotic expansion for large $|x|$ of the form

$$
u^{s}(x, d)=\frac{\exp (i k|x|)}{|x|} u^{\infty}(\hat{x}, d)+\mathrm{O}\left(|x|^{-2}\right), \quad|x| \rightarrow \infty
$$

The function $u^{\infty}$ in this expansion is called the far field pattern of $u^{s}$. It can be used to define a linear integral operator $F: L^{2}\left(\mathbb{S}^{2}\right) \rightarrow L^{2}\left(\mathbb{S}^{2}\right)$, the far field operator, by setting

$$
\begin{equation*}
F g(\hat{x})=\int_{\mathbb{S}^{2}} u^{\infty}(\hat{x}, d) g(d) d s(d), \quad g \in L^{2}\left(\mathbb{S}^{2}\right), \quad \hat{x} \in \mathbb{S}^{2} \tag{4}
\end{equation*}
$$

It is this operator, a compact operator in $L^{2}\left(\mathbb{S}^{2}\right)$, that forms the basis of both the Linear Sampling and the Factorization method. The function $F g$ can be interpreted as the far field of the scattered field that is generated by the incident field $v_{g}$ given by

$$
\begin{equation*}
v_{g}(x)=\int_{\mathbb{S}^{2}} \exp (i k d \cdot x) g(d) d s(d), \quad g \in L^{2}\left(\mathbb{S}^{2}\right), \quad x \in \mathbb{R}^{3} \tag{5}
\end{equation*}
$$

The function $v_{g}$ is called the Herglotz wave function with density $g$.
The scattering problem $(1-3)$ can be viewed as a special case of the exterior boundary value problem

$$
\begin{align*}
\Delta v+k^{2} v=0 & \text { in } \quad \mathbb{R}^{3} \backslash \bar{D}  \tag{6}\\
v=\varphi & \text { on } \partial D \\
& v \text { satisfies }(3)
\end{align*}
$$

with given boundary values $\varphi \in H^{1 / 2}(\partial D)$. Here and in all subsequent arguments we will assume that $\partial D$ is Lipschitz. We denote by $G$ : $H^{1 / 2}(\partial D) \rightarrow L^{2}\left(\mathbb{S}^{2}\right)$ the operator mapping these boundary values to the far field pattern of the solution of (6). Further defining the operator $H: L^{2}\left(\mathbb{S}^{2}\right) \rightarrow H^{1 / 2}(\partial D)$ by $H g=\left.v_{g}\right|_{\partial D}, g \in L^{2}\left(\mathbb{S}^{2}\right)$, with $v_{g}$ given by (5), by the above comments we have the representation

$$
\begin{equation*}
F=-G H \tag{7}
\end{equation*}
$$

For the problem under consideration, the far field operator is normal, a fact central to the proof given in $[\mathbf{1 0}]$. As a consequence, there exist eigenvalues $\lambda_{n} \in \mathbb{C}$ of $F$ and corresponding eigenfunctions $g_{n} \in L^{2}\left(\mathbb{S}^{2}\right)$, $n \in \mathbb{N}$, such that the set $\left\{g_{n}\right\}$ forms a complete orthonormal system in $L^{2}\left(\mathbb{S}^{2}\right)$. The operator $F$ can hence be represented by its eigenexpansion,

$$
\begin{equation*}
F g=\sum_{n=1}^{\infty} \lambda_{n}\left(g, g_{n}\right) g_{n}, \quad g \in L^{2}\left(\mathbb{S}^{2}\right) \tag{8}
\end{equation*}
$$

We implicitly suppose in the sequel that the $\lambda_{n}$ are ordered, that is, $\left|\lambda_{n}\right| \geq\left|\lambda_{n+1}\right|, n \in \mathbb{N}$. Furthermore, we know from [10] that $\lambda_{n} \rightarrow 0$ as $n \rightarrow \infty$ with $\operatorname{Re}\left(\lambda_{n}\right)<0$ for all $n$ larger than some number $n_{0}$, and $\operatorname{Im}\left(\lambda_{n}\right)>0$ for all $n \in \mathbb{N}$. Lastly, it is shown in [10] that

$$
\begin{equation*}
\left|\lambda_{n}\right| \leq-2 \operatorname{Re}\left(\lambda_{n}\right), \quad n>n_{0} \tag{9}
\end{equation*}
$$

We note that Herglotz wave functions defined using the eigenfunctions of $F$ as a density can be expressed in the form

$$
\begin{align*}
v_{g_{n}}(x) & =\int_{\mathbb{S}^{2}} \exp (i k x \cdot d) g_{n}(d) d s(d)  \tag{10}\\
& =4 \pi \int_{\mathbb{S}^{2}} \overline{\Phi^{\infty}(d, x)} g_{n}(d) d s(d) \\
& =4 \pi \overline{\left(\Phi^{\infty}(\cdot, x), g_{n}\right)}, \quad x \in \mathbb{R}^{3} .
\end{align*}
$$

For the purpose of this paper, we will consider applying Tikhonov regularization to the far field equation, i.e. solving the equation

$$
\alpha g_{\alpha, z}+F^{*} F g_{\alpha, z}=F^{*} \Phi^{\infty}(\cdot, z)
$$

where $\alpha>0$ is the regularization parameter. Using the eigensystem of $F$, the unique solution to this equation can be written in the form

$$
\begin{equation*}
g_{\alpha, z}=\sum_{n=1}^{\infty} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n} \tag{11}
\end{equation*}
$$

The main result of $[\mathbf{3}]$ is that for $z \in D$,

$$
-H g_{\alpha, z} \rightarrow \Phi(\cdot, z) \quad \text { in } \quad H^{1 / 2}(\partial D) \quad(\alpha \rightarrow 0)
$$

and that $\left\|H g_{\alpha, z}\right\|_{H^{1 / 2}(\partial D)} \rightarrow \infty$ as $\alpha \rightarrow 0$ if $z \notin D$. Consequently, for $z \in D, v_{g_{\alpha, z}}(z)$ will converge to a limit as $\alpha \rightarrow 0$ and this limit becomes unbounded as $z \rightarrow \partial D$.
3. Convergence in the case of noisy data. In the case of noisy data, the far field operator $F$ has to be replaced by a perturbed version $F^{\delta}$ where we assume that

$$
\left\|F-F^{\delta}\right\| \leq \delta
$$

Note that we cannot assume that $F^{\delta}$ is normal. Hence, instead of using an eigensystem, we write the minimizer of the Tikhonov functional as the solution of the corresponding normal equation, i.e. as

$$
g_{\alpha, z}^{\delta}=\left[\alpha I+\left(F^{\delta}\right)^{*} F^{\delta}\right]^{-1}\left(F^{\delta}\right)^{*} \Phi^{\infty}(\cdot, z)
$$

Defining

$$
\varphi_{\alpha, z}^{\delta}=-H g_{\alpha, z}^{\delta}
$$

the goal in this section is to formulate conditions on the choice of the regularization parameter $\alpha(\delta)$ as a function of the noise level $\delta$ such that for $z \in D$,

$$
\varphi_{\alpha(\delta), z}^{\delta} \rightarrow \Phi(\cdot, z) \quad \text { in } \quad H^{1 / 2}(\partial D) \quad(\delta \rightarrow 0)
$$

We obtain the following result.

Theorem 3.1. Assume $z \in D$. Suppose further that $\alpha(\delta) \rightarrow 0$ and $\delta / \alpha(\delta)^{3 / 2} \rightarrow 0$ as $\delta \rightarrow 0$. Then

$$
\left\|\varphi_{\alpha(\delta), z}^{\delta}-\Phi(\cdot, z)\right\|_{H^{1 / 2}(\partial D)} \longrightarrow 0 \quad(\delta \rightarrow 0)
$$

Proof. We abbreviate $\varphi=\left.\Phi(\cdot, z)\right|_{\partial D}$ and $h=G \varphi=\Phi^{\infty}(\cdot, z)$. We write the difference

$$
\begin{align*}
\varphi_{\alpha(\delta), z}^{\delta}-\varphi= & -H\left[\alpha I+F^{*} F\right]^{-1} F^{*} h-\varphi  \tag{12}\\
& +H\left[\alpha I+F^{*} F\right]^{-1}\left(F^{*}-\left(F^{\delta}\right)^{*}\right) h \\
& +H\left\{\left[\alpha I+F^{*} F\right]^{-1}-\left[\alpha I+\left(F^{\delta}\right)^{*} F^{\delta}\right]^{-1}\right\}\left(F^{\delta}\right)^{*} h .
\end{align*}
$$

The first term was shown to converge to 0 as $\alpha \rightarrow 0$ in [3]. For the second term in (12), we have the estimate

$$
\begin{aligned}
\| H\left[\alpha I+F^{*} F\right]^{-1}\left(F^{*}-\left(F^{\delta}\right)^{*}\right) & h \|_{H^{1 / 2}(\partial D)} \\
& \leq\|H\|\left\|\left(\alpha I+F^{*} F\right)^{-1}\right\|\|h\|_{L^{2}\left(\mathbb{S}^{2}\right)} \delta
\end{aligned}
$$

As for any self-adjoint, positive operator $B$ in a Hilbert space, the estimate

$$
\left\|(\alpha I+B)^{-1}\right\| \leq \frac{1}{\alpha}
$$

holds, we obtain

$$
\left\|H\left[\alpha I+F^{*} F\right]^{-1}\left(F^{*}-\left(F^{\delta}\right)^{*}\right) h\right\|_{H^{1 / 2}(\partial D)} \leq\|H\|\|h\|_{L^{2}\left(\mathbb{S}^{2}\right)} \frac{\delta}{\alpha}
$$

Finally, for the third term in (12), we note (see [13]) the estimate

$$
\left\|\left[\alpha I+F^{*} F\right]^{-1}-\left[\alpha I+\left(F^{\delta}\right)^{*} F^{\delta}\right]^{-1}\right\| \leq \frac{2 \delta}{\alpha^{3 / 2}}
$$

Combining these estimates, it follows that

$$
\begin{gathered}
\left\|\varphi_{\alpha(\delta), z}^{\delta}-\varphi\right\|_{H^{1 / 2}(\partial D)} \leq\left\|H\left[\alpha I+F^{*} F\right]^{-1} F^{*} h+\varphi\right\|_{H^{1 / 2}(\partial D)} \\
+\|H\|\|h\|_{L^{2}\left(\mathbb{S}^{2}\right)}\left(\frac{\delta}{\alpha}+2\left\|\left(F^{\delta}\right)^{*}\right\| \frac{\delta}{\alpha^{3 / 2}}\right)
\end{gathered}
$$

From this estimate, the assertion follows immediately.

In standard regularization theory, when applying Tikhonov regularization or similar schemes, it is a well known result that a regularization strategy will be convergent if $\alpha(\delta) \rightarrow 0$ and $\delta / \sqrt{\alpha(\delta)} \rightarrow 0$ as $\delta \rightarrow 0$. These conditions are also met when using the discrepancy principle as a choice for the regularization parameter.

However, such results are based on estimates involving application of the perturbed operator to the correct solution of the ill-posed problem. The problem in the situation in Theorem 3.1 is that the method employed here must be viewed as a regularization strategy for solving the operator equation

$$
G \Phi(\cdot, z)=\Phi^{\infty}(\cdot, z)
$$

for $z \in D$. As $H$ is a compact operator, it is seen from (7) that information on a perturbation of $F$ cannot be used for estimates involving $G$.

Furthermore, the proof of Theorem 3.1 given here relies on estimates specific for the operators occurring in Tikhonov regularization. This is different from the results for noise free data in [3], where more general classes of regularization schemes were considered. It is an open question to generalize Theorem 3.1 to other regularizations.
4. A new characterization result. In the Factorization method, the equation

$$
\begin{equation*}
\left(F^{*} F\right)^{1 / 4} g_{z}=\Phi^{\infty}(\cdot, z) \tag{13}
\end{equation*}
$$

is studied. It is shown in $[\mathbf{1 0}]$ that

$$
\Phi^{\infty}(\cdot, z) \in \text { Range }\left(\left(F^{*} F\right)^{1 / 4}\right) \Longleftrightarrow z \in D
$$

Using the eigenexpansion (8) of $F$, the solution to (13) is given by

$$
g_{z}=\sum_{n=1}^{\infty} \frac{1}{\sqrt{\left|\lambda_{n}\right|}}\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n} \quad \text { for } \quad z \in D
$$

We now return to the Linear Sampling method. We will give a new proof for the behaviour of $v_{g_{\alpha, z}}(z)$ for $z \in D$, making even clearer the connection between Factorization and Linear Sampling method.

Assume $z \in D$. We simply compute the value $v_{g_{\alpha, z}}(z)$ using (10) and (11) as
(14) $v_{g_{\alpha, z}}(z)=\int_{\mathbb{S}^{2}} \exp (i k d \cdot z) g_{\alpha, z}(d) d s(d)$

$$
\begin{aligned}
& =\sum_{n=1}^{\infty} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left(\Phi^{\infty}(\cdot, z), g_{n}\right) \int_{\mathbb{S}^{2}} \exp (i k d \cdot z) g_{n}(d) d s(d) \\
& =4 \pi \sum_{n=1}^{\infty} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} .
\end{aligned}
$$

Now, denote by $g_{z}$ the solution of (13). Then

$$
\left(g_{z}, g_{n}\right)=\frac{1}{\sqrt{\left|\lambda_{n}\right|}}\left(\Phi^{\infty}(\cdot, z), g_{n}\right)
$$

and hence

$$
\begin{equation*}
v_{g_{\alpha, z}}(z)=4 \pi \sum_{n=1}^{\infty} \frac{\overline{\lambda_{n}}\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} . \tag{15}
\end{equation*}
$$

We directly obtain $\left|v_{g_{\alpha, z}}(z)\right| \leq 4 \pi\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}$ for $z \in D$.
In order to obtain a lower bound, we combine (14) and (15) and write

$$
\begin{aligned}
v_{g_{\alpha, z}}(z)= & 4 \pi \sum_{n=1}^{n_{0}} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} \\
& +4 \pi \sum_{n=n_{0}+1}^{\infty} \frac{\overline{\lambda_{n}}\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2},
\end{aligned}
$$

where $n_{0}$ is the number defined in Section 2 when discussing the eigenvalues of $F$. Recall from (9) that $n_{0}$ is independent of $\alpha$ and $z$.
Moreover, using (9), we can estimate

$$
\begin{aligned}
\left.\left.\left|\sum_{n=n_{0}+1}^{\infty} \frac{\overline{\lambda_{n}}\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\right|\left(g_{z}, g_{n}\right)\right|^{2} \right\rvert\, & \geq\left|\operatorname{Re}\left(\sum_{n=n_{0}+1}^{\infty} \frac{\overline{\lambda_{n}}\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2}\right)\right| \\
& =-\sum_{n=n_{0}+1}^{\infty} \frac{\operatorname{Re}\left(\lambda_{n}\right)\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} \\
& \geq \frac{1}{2} \sum_{n=n_{0}+1}^{\infty} \frac{\left|\lambda_{n}\right|^{2}}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} .
\end{aligned}
$$

Therefore, we conclude

$$
\begin{aligned}
\left|v_{g_{\alpha, z}}(z)\right| \geq & 2 \pi \sum_{n=1}^{\infty} \frac{\left|\lambda_{n}\right|^{2}}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} \\
& -4 \pi \sum_{n=1}^{n_{0}} \frac{\left|\lambda_{n}\right|}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} \\
\geq & 2 \pi \sum_{n=1}^{\infty} \frac{\left|\lambda_{n}\right|^{2}}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2}-4 \pi \sum_{n=1}^{n_{0}} \frac{1}{\left|\lambda_{n}\right|}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} \\
= & 2 \pi\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}-2 \pi \sum_{n=1}^{\infty} \frac{\alpha}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} \\
& -4 \pi \sum_{n=1}^{n_{0}} \frac{1}{\left|\lambda_{n}\right|}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} .
\end{aligned}
$$

Now, as $D$ is a bounded domain and the last term on the right hand side is a continuous function of $z \in \mathbb{R}^{3}$, it will attain a maximum on $\bar{D}$, say $M / 3$. Next choose $N \in \mathbb{N}$ such that

$$
\sum_{n=N+1}^{\infty} \frac{\alpha}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} \leq \sum_{n=N+1}^{\infty}\left|\left(g_{z}, g_{n}\right)\right|^{2} \leq \frac{M}{6 \pi}
$$

for all $\alpha>0$. Finally, we choose $\alpha_{0}$ such that

$$
\sum_{n=1}^{N} \frac{\alpha}{\alpha+\left|\lambda_{n}\right|^{2}}\left|\left(g_{z}, g_{n}\right)\right|^{2} \leq \frac{M}{6 \pi}
$$

for all $\alpha \leq \alpha_{0}$. Consequently, we have shown the estimate

$$
\left|v_{g_{\alpha, z}}(z)\right| \geq 2 \pi\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}-M
$$

for all $\alpha \leq \alpha_{0}$. We summarize these results in the following theorem.

Theorem 4.1. For $z \in D$, denote by $g_{z}$ the solution of (13) and let $g_{\alpha, z}$ be given by (11). There exists a constant $M>0$ such that for any $z \in D$ there is $\alpha_{0}(z)$ such that

$$
2 \pi\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}-M \leq\left|v_{g_{\alpha, z}}(z)\right| \leq 4 \pi\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}, \quad \alpha \leq \alpha_{0}(z)
$$

Consequently, $\lim _{\alpha \rightarrow 0} v_{g_{\alpha, z}}(z)$, known to exist by the results of $[\mathbf{3}]$, is bounded on compact subsets of $D$ and becomes unbounded for $z \rightarrow \partial D$.


Figure 1: Reconstructions of a kite-shaped obstacle with the Linear Sampling and the Factorization method. Plots of approximations to (a) $\left\|g_{\alpha, z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{-1}$, (b) $\left|v_{g_{\alpha, z}}\right|^{-1 / 2}(\mathrm{~b})$, and (c) $\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{-1}$ as functions of $z \in \mathbb{R}^{2}$.

The consequences of this theorem can be observed in numerical experiments. Figure 1 displays numerical results for the discussed methods in a two-dimensional situation. A discretized far field operator was obtained by replacing the integral in (4) with the composite rectangular rule with 32 quadrature points and evaluating this for the same 32 points for $\hat{x}$. This discretized operator was then used for the computation of $\left\|g_{\alpha, z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}$, of $\left|v_{g_{\alpha, z}}\right|$ and of $\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}$ with all series replaced by finite sums with 32 terms. The reciprocal value of each of the three quantities is displayed in figures (a), (b) and (c), respectively. The true obstacle is represented by a black line in all three cases.

Identical colours do not correspond to identical numerical values in these images. Only the qualitative behaviour is of interest here, hence no colour bar is presented. All three methods can be used to characterize the obstacle in the sense that there exists a contour line that approximates the obstacle well. However, both the plot of the Herglotz function and of $g_{z}$ form qualitatively far better approximations of the characteristic function of the obstacle. In addition, these two plots are very similar, completely in line with the statement of the theorem.

The estimates in Theorem 4.1 do not give any information regarding the rate of blow-up of the absolute value of the Herglotz wave function as $z$ approaches the boundary. Such an estimate is given in [3], however, the constants involved depend on the smoothness of the obstacle $D$. The estimates given here do not at all depend on the smoothness of $D$ and are hence valid for any bounded Lipschitz domain. Moreover,
using another result on the Factorization method, we are also able to give a blow up rate for $\left\|g_{z}\right\|$ in the next lemma.

Lemma 4.2. The function $\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}$ blows up as $\operatorname{dist}(z, \partial D)^{-1}$ when $z$ approaches the boundary $\partial D$ from the inside, that is, there is $C>0$ such that

$$
\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2} \geq \frac{C}{\operatorname{dist}(\mathrm{z}, \partial \mathrm{D})}, \quad z \in D
$$

Proof. The claimed blow up estimate relies on the operator $G: H^{1 / 2}(\partial D) \rightarrow L^{2}\left(\mathbb{S}^{2}\right)$ from Section 2. In [10, Theorem 3.6] it is proved that $\left(F^{*} F\right)^{-1 / 4} G$ is a norm isomorphism from $H^{1 / 2}(\partial D)$ to $L^{2}\left(\mathbb{S}^{2}\right)$. Therefore we find constants $0<C_{1}<C_{2}$ such that, for $z \in D$,

$$
\begin{aligned}
C_{1}\left\|G^{-1} \Phi^{\infty}(\cdot, z)\right\|_{H^{1 / 2}(\partial D)} & \leq\left\|\left(F^{*} F\right)^{-1 / 4} \Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}=\left\|g_{z}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& \leq C_{2}\left\|G^{-1} \Phi^{\infty}(\cdot, z)\right\|_{H^{1 / 2}(\partial D)}
\end{aligned}
$$

However, $\left\|G^{-1} \Phi^{\infty}(\cdot, z)\right\|_{H^{1 / 2}(\partial D)}=\|\Phi(\cdot, z)\|_{H^{1 / 2}(\partial D)}$ for $z \in D$. By the interpolation property of Sobolev spaces one can express the $H^{1 / 2}$ norm on $\partial D$ by simpler norms: there exist $0<C_{1}<C_{2}$ (possibly different from the above constants) such that
(16) $C_{1}\|\psi\|_{L^{2}(\partial D)}^{1 / 2}\|\psi\|_{H^{1}(\partial D)}^{1 / 2} \leq\|\psi\|_{H^{1 / 2}(\partial D)} \leq C_{2}\|\psi\|_{L^{2}(\partial D)}^{1 / 2}\|\psi\|_{H^{1}(\partial D)}^{1 / 2}$
for $\psi \in C^{\infty}(\partial D)$. Therefore it suffices to estimate $\|\Phi(\cdot, z)\|_{L^{2}(\partial D)}$ and $\|\Phi(\cdot, z)\|_{H^{1}(\partial D)}$ in the remainder of the proof.
Let us more generally investigate the $L^{2}$ norm of the function $\phi_{n}(x)=$ $|x-z|^{-n}$ for arbitrary $n \in \mathbb{N}$. We find

$$
\begin{aligned}
\int_{\partial D}|x-z|^{-2 n} d s(x) & \geq \int_{\partial D \cap B_{2} \operatorname{dist}(z, \partial D)}(z) \\
& x-\left.z\right|^{-2 n} d s(x) \\
& \geq \frac{\left|\partial D \cap B_{2 \operatorname{dist}(z, \partial D)}(z)\right|}{(2 \operatorname{dist}(z, \partial D))^{2 n}}
\end{aligned}
$$

where $B_{\rho}(z)$ denotes the open ball of radius $\rho$ centered at $z$. The quantity on the right hand side remains to be bounded from below.

As $D$ is assumed to be a Lipschitz domain, it can locally be represented by the graph of a Lipschitz continuous function. Such a function has a gradient almost everywhere which is essentially bounded. Therefore, a lower bound

$$
\left|\partial D \cap B_{2 \operatorname{dist}(z, \partial D)}(z)\right| \geq C^{\prime} \operatorname{dist}(z, \partial D)^{2}
$$

can be obtained, where the constant $C^{\prime}$ is essentially the bound on the gradient of the local representation of $\partial D$. Hence we arrive at

$$
\left\|\phi_{n}(\cdot, z)\right\|_{L^{2}(\partial D)} \geq C^{\prime \prime} \operatorname{dist}(z, \partial D)^{1-n}
$$

For estimating the $L^{2}$ norm of $\Phi(\cdot, z)$ we use $n=1$, for the $H^{1}$ norm, $n=2$ is necessary. Thus from (16), we obtain

$$
\|\Phi(\cdot, z)\|_{H^{1 / 2}(\partial D)} \geq C \operatorname{dist}(z, \partial D)^{-1 / 2}
$$

and the proof is complete.

If the boundary is smoother than Lipschitz, one can characterize the behaviour of $\left\|g_{z}\right\|$ near the boundary: Hähner [8] showed that for $C^{2, \alpha}$ boundaries one has, for some $0<C_{1}<C_{2}$,

$$
\begin{equation*}
C_{1} \operatorname{dist}(z, \partial D) \leq\left\|g_{z}\right\|^{-2} \leq C_{2} \operatorname{dist}(z, \partial D), \quad z \in D \tag{17}
\end{equation*}
$$

Precise blow-up characterization with less smoothness is technical. Note that Lemma 4.2 suggests that plotting the inverse of the norm of $g_{z}$, or equivalently, the inverse of $\sqrt{\left|v_{g_{\alpha, z}}(z)\right|}$, gives superior reconstructions than plotting its square: $1 /\left\|g_{z}\right\|^{2}$ decays linearly to 0 at the boundary of $\partial D$ whereas $1 /\left\|g_{z}\right\|$ decays as $\operatorname{dist}(z, \partial D)^{1 / 2}$, resulting in a steep downward slope and better contrast.
5. Points outside the obstacle. We now extend the result of Theorem 4.1 to points $z$ outside of $\bar{D}$. To this end we consider a family of open balls $B_{\delta}(z)$ of radius $\delta$ centred at $z$. Define

$$
D_{\delta}:=D \cup B_{\delta}(z)
$$

and denote by $F^{\delta}$ the far field operator of the scattering problem with $D$ replaced by $D_{\delta}$. We furthermore estimate the difference of $F$ and $F^{\delta}$ by

$$
\begin{equation*}
\left\|F-F^{\delta}\right\|=\mathrm{o}(\delta) \quad(\delta \rightarrow 0) \tag{18}
\end{equation*}
$$

Similar but much more precise results have been derived in $[\mathbf{1}, \mathbf{1 4}]$. For our purpose, however, the asymptotic behaviour in (18) is sufficient and we give an elementary proof of this in the following theorem.

Theorem 5.1. There exists a constant $C>0$ dependent on $z$ and $\delta_{0}>0$ such that

$$
\left\|F-F^{\delta}\right\| \leq C \delta^{2} \quad \text { for all } \quad 0<\delta \leq \delta_{0}
$$

Proof. We consider two scattering problems,

$$
\begin{align*}
\Delta u^{s}+k^{2} u^{s}=0 & \text { in } \quad \mathbb{R}^{3} \backslash \bar{D}  \tag{19}\\
u^{s}+u^{i}=0 & \text { on } \partial D \\
& u^{s} \text { satisfies }(3)
\end{align*}
$$

as well as the perturbed problem

$$
\begin{align*}
\Delta u_{\delta}^{s}+k^{2} u_{\delta}^{s}=0 & \text { in } \quad \mathbb{R}^{3} \backslash \overline{D_{\delta}}  \tag{20}\\
u_{\delta}^{s}+u^{i}=0 & \text { on } \quad \partial D_{\delta} \\
& u_{\delta}^{s} \text { satisfies (3). }
\end{align*}
$$

By $v_{\delta}$ we denote the difference between the solution to (20) and the solution to (19), $v_{\delta}=u_{\delta}^{s}-u^{s}$. Then, for sufficiently small $\delta, v_{\delta}$ is a solution to the following exterior boundary value problem,

$$
\begin{aligned}
\Delta v_{\delta}+k^{2} v_{\delta}=0 & \text { in } \quad \mathbb{R}^{3} \backslash \overline{D_{\delta}} \\
v_{\delta}=0 & \text { on } \quad \partial D \\
v_{\delta}+u^{s}+u^{i}=0 & \text { on } \partial B_{\delta}(z) \\
& v_{\delta} \text { satisfies }(3)
\end{aligned}
$$

For $\delta$ small enough, we can write $v_{\delta}$ as a double-layer potential,

$$
v_{\delta}(x)=\int_{\partial B_{\delta}(z)} \frac{\partial G(x, y)}{\partial \nu(y)} \psi(y) d s(y), \quad x \in \mathbb{R}^{3} \backslash \overline{D_{\delta}}
$$

where $G$ denotes the radiating Green's function to the Helmholtz equation in the exterior of $D$ satisfying homogeneous boundary conditions on $\partial D$ and $\psi \in C\left(\partial B_{\delta}(z)\right)$ satisfies the boundary integral equation
$\frac{1}{2} \psi(x)+\int_{\partial B_{\delta}(z)} \frac{\partial G(x, y)}{\partial \nu(y)} \psi(y) d s(y)=-\left(u^{s}(x)+u^{i}(x)\right), \quad x \in \partial B_{\delta}(z)$.
Transforming to an integral over the unit sphere, we instead obtain

$$
\begin{equation*}
v_{\delta}(x)=\delta^{2} \int_{\mathbb{S}^{2}} \hat{y} \cdot \nabla_{y} G(x, z+\delta \hat{y}) \varphi(\hat{y}) d s(\hat{y}), \quad x \in \mathbb{R}^{3} \backslash \overline{D_{\delta}}, \tag{21}
\end{equation*}
$$

with some density $\varphi \in C\left(\mathbb{S}^{2}\right)$ satisfying the integral equation

$$
\begin{align*}
& \frac{1}{2} \varphi(\hat{x})+\delta^{2} \int_{\mathbb{S}^{2}} \hat{y} \cdot \nabla_{y} G(z+\delta \hat{x}, z+\delta \hat{y}) \varphi(\hat{y}) d s(\hat{y})  \tag{22}\\
&=-\left(u^{s}(z+\delta \hat{x})+u^{i}(z+\delta \hat{x})\right), \quad \hat{x} \in \mathbb{S}^{2}
\end{align*}
$$

From (22), it follows that $\varphi$ is uniformly bounded for $0<\delta \leq \delta_{0}$. From (21) we then obtain a bound

$$
\left|v_{\delta}^{\infty}(\hat{x})\right| \leq C \delta^{2} .
$$

From this, the assertion follows directly.

In contrast to the situation of Section 3, here $F^{\delta}$ is not only a perturbation of $F$ but also a far field operator for a certain obstacle in its own right. Hence it is a normal operator. We now denote by $\lambda_{n}^{\delta}$ the eigenvalues of $F^{\delta}$ and by $g_{n}^{\delta}$ the corresponding eigenvectors.
Next, we limit ourselves to a finite approximation of these operators, i.e. for fixed $n_{1} \in \mathbb{N}, n_{1} \geq n_{0}$, we compute

$$
\begin{equation*}
g_{z}^{\delta}=\sum_{n=1}^{n_{1}} \frac{1}{\sqrt{\left|\lambda_{n}^{\delta}\right|}}\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}, \quad z \in \mathbb{R}^{3}, \tag{23}
\end{equation*}
$$

as an approximate solution to (13) and

$$
g_{\alpha, z}^{\delta}=\sum_{n=1}^{n_{1}} \frac{\overline{\lambda_{n}^{\delta}}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}, \quad z \in \mathbb{R}^{3}, \alpha>0 .
$$

By $g_{\alpha, z}$, we will from now on denote the function given by (11), but with the infinite series also replaced by a summation up to $n_{1}$.

The finite dimensional projections are introduced for technical reasons in the estimates below. Later on, we shall also state results concerning the limit behaviour as $n_{1} \rightarrow \infty$. Note, however, that finite dimensionality is always present in numerical computations. Therefore estimates for $g_{z}^{\delta}$ are of interest in their own right, even if the discretization in sampling methods is usually not done using spectral cut-off.

By similar calculations as above, we obtain

$$
\begin{align*}
\left|v_{g_{\alpha, z}^{\delta}}(z)\right| \geq 2 \pi \sum_{n=1}^{n_{1}} \frac{\left|\lambda_{n}^{\delta}\right|^{2}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}} & \left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}  \tag{24}\\
& -8 \pi \sum_{n=1}^{n_{0}} \frac{1}{\left|\lambda_{n}^{\delta}\right|}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right)\right|^{2}
\end{align*}
$$

Furthermore, we have

$$
\begin{equation*}
\left|v_{g_{\alpha, z}}(z)\right| \geq\left|v_{g_{\alpha, z}^{\delta}}(z)\right|-\left|v_{g_{\alpha, z}^{\delta}}(z)-v_{g_{\alpha, z}}(z)\right| . \tag{25}
\end{equation*}
$$

We first address the last term in (24).

Lemma 5.2. There exists a constant $M>0$ and $\delta_{0}>0$ such that

$$
8 \pi \sum_{n=1}^{n_{0}} \frac{1}{\left|\lambda_{n}^{\delta}\right|}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right)\right|^{2} \leq \frac{M}{3}, \quad \delta \leq \delta_{0}, \quad z \in \mathbb{R}^{3}
$$

Proof. As the functions $g_{n}^{\delta}$ form an orthonormal basis in $L^{2}\left(\mathbb{S}^{2}\right)$, it follows straight away that

$$
8 \pi \sum_{n=1}^{n_{0}} \frac{1}{\left|\lambda_{n}^{\delta}\right|}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right)\right|^{2} \leq \max _{n=1, \ldots, n_{0}} \frac{1}{\left|\lambda_{n}^{\delta}\right|}\left\|\Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{2}
$$

The far field pattern of point sources differs for varying $z$ only in a complex factor with absolute value 1 . Hence the bound on the right
hand side only depends on $\delta$. But from Lemma A. 1 in the appendix, it follows that $\lambda_{n}^{\delta} \rightarrow \lambda_{n}$ as $\delta \rightarrow 0$ for every $n \in \mathbb{N}$. Hence the first factor on the right hand side is bounded by $M / 3$ for some $M>0$ if $\delta \leq \delta_{0}$. ロ

Lemma 5.3. Given arbitrary $n_{1} \in \mathbb{N}, z \in \mathbb{R}^{3}$ and $c>0$, there is $\delta_{0}\left(n_{1}\right)>0$ such that

$$
\left|v_{g_{\alpha, z}^{\delta}}(z)-v_{g_{\alpha, z}}(z)\right| \leq c
$$

for all $0<\delta \leq \delta_{0}$ uniformly in $\alpha>0$ and $z \in \mathbb{R}^{3}$.

Proof. Interchanging absolute value and integration yields the estimate

$$
\left|v_{g_{\alpha, z}^{\delta}}(z)-v_{g_{\alpha, z}}(z)\right| \leq 2 \pi\left\|g_{\alpha, z}^{\delta}-g_{\alpha, z}\right\|_{L^{2}\left(S^{2}\right)} .
$$

We split up the difference of $g_{\alpha, z}^{\delta}$ and $g_{\alpha, z}$ as

$$
\begin{align*}
g_{\alpha, z}^{\delta}-g_{\alpha, z}= & \sum_{n=1}^{n_{1}}\left(\frac{\overline{\lambda_{n}^{\delta}}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}-\frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\right)\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}  \tag{26}\\
& +\sum_{n=1}^{n_{1}} \frac{\overline{\lambda_{n}}}{\left.d \lambda_{n}\right|^{2}}\left(\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}-\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n}\right)
\end{align*}
$$

and successively bound the two terms on the right hand side by choosing $\delta_{0}$ sufficiently small.

First, we use Lemma A. 1 and (18) to conclude that $\left|\lambda_{n}-\lambda_{n}^{\delta}\right| \leq$ $\left\|F-F^{\delta}\right\| \leq C \delta$ for some constant $C$ depending only on $D$. In consequence, we can choose $\delta_{0}=\delta_{0}\left(n_{1}\right)$ such that $\left|\lambda_{n}^{\delta}\right|^{2} \geq\left|\lambda_{n}\right|^{2} / 2$ for all $n=1, \ldots, n_{1}$ and $\left\|F^{\delta}\right\|=\left|\lambda_{1}^{\delta}\right| \leq 2\|F\|$. This allows to estimate

$$
\begin{aligned}
\left|\frac{\overline{\lambda_{n}^{\delta}}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}-\frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\right| & \leq \frac{\alpha\left|\lambda_{n}^{\delta}-\lambda_{n}\right|+2\|F\|^{2}\left|\lambda_{n}^{\delta}-\lambda_{n}\right|}{\alpha^{2}+\left|\lambda_{n_{1}}\right|^{4} / 2} \\
& \leq \delta \frac{\alpha+2\|F\|^{2}}{\alpha^{2}+\left|\lambda_{n_{1}}\right|^{4} / 2}
\end{aligned}
$$

Note that for fixed $n_{1}$ we can uniformly bound

$$
\frac{\alpha+2\|F\|^{2}}{\alpha^{2}+\left|\lambda_{n_{1}}\right|^{4} / 2} \leq C\left(\lambda_{n_{1}}\right) \quad \text { for all } \alpha>0
$$

which implies that the first term on the right hand side of $(26)$ is bounded by

$$
\begin{aligned}
& \| \sum_{n=1}^{n_{1}}\left(\frac{\overline{\lambda_{n}^{\delta}}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}\right.\left.-\frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\right)\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta} \|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& \leq \delta C\left(\lambda_{n_{1}}\right)\left\|\Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}
\end{aligned}
$$

Note that the norms $\left\|\Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}$ are uniformly bounded in $z \in \mathbb{R}^{3}$. Consequently, for $\delta_{0}=\delta_{0}\left(n_{1}\right)$ small enough, the left hand side is uniformly bounded in $\alpha$ by $c / 2$ for $0<\delta<\delta_{0}$ and fixed $n_{1}$.

Consider now the second term in (26). We introduce the two projections

$$
P_{m}=\sum_{\lambda_{n}=\lambda_{m}}\left(\cdot, g_{n}\right) g_{n} \quad \text { and } \quad P_{m}^{\delta}=\sum_{\lambda_{n}=\lambda_{m}}\left(\cdot, g_{n}^{\delta}\right) g_{n}^{\delta}, \quad m \in \mathbb{N}
$$

It is proved in Theorem A. 2 that $\left\|P_{m}-P_{m}^{\delta}\right\| \leq C \delta /(d-C \delta)$, where $C$ is the constant from Theorem 5.1 and $2 d$ is the distance of $\lambda_{m}$ to the rest of the spectrum of $F$. Denote by $\left(m_{j}\right)_{j \in \mathbb{N}}$ a sequence such that $\lambda_{m_{j}}$ is the ordered sequence of eigenvalues of $F$ counted without multiplicity and set $J\left(n_{1}\right)$ such that $\lambda_{m_{J}}=\lambda_{n_{1}}$. We estimate

$$
\begin{aligned}
& \left\|\sum_{n=1}^{n_{1}} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left(\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}-\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n}\right)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& =\left\|\sum_{j=1}^{J\left(n_{1}\right)} \frac{\overline{\lambda_{m_{j}}}}{\alpha+\left|\lambda_{m_{j}}\right|^{2}} \sum_{\lambda_{n}=\lambda_{m_{j}}}\left(\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}-\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n}\right)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& \leq \sum_{j=1}^{J\left(n_{1}\right)} \frac{1}{\left|\lambda_{m_{j}}\right|}\left\|\sum_{\lambda_{n}=\lambda_{m_{j}}}\left(\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) g_{n}^{\delta}-\left(\Phi^{\infty}(\cdot, z), g_{n}\right) g_{n}\right)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& =\sum_{j=1}^{J\left(n_{1}\right)} \frac{1}{\left|\lambda_{m_{j}}\right|}\left\|P_{m_{j}}^{\delta} \Phi^{\infty}(\cdot, z)-P_{m_{j}} \Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& \leq \sum_{j=1}^{J\left(n_{1}\right)} \frac{1}{\left|\lambda_{m_{j}}\right|} \frac{C \delta\left\|\Phi^{\infty}(\cdot, z)\right\|_{L^{2}\left(\mathbb{S}^{2}\right)}^{\operatorname{dist}\left(\lambda_{m_{j}}, \sigma(F) \backslash \lambda_{m_{j}}\right)-C \delta} .}{}
\end{aligned}
$$

If we suppose that $\delta_{0}$ is so small that $\operatorname{dist}\left(\lambda_{n}, \sigma(F) \backslash \lambda_{n}\right)-C \delta \geq$ $\operatorname{dist}\left(\lambda_{n}, \sigma(F) \backslash \lambda_{n}\right) / 2$ for $n \leq n_{1}$, we obtain

$$
\begin{aligned}
&\left\|\sum_{n=1}^{n_{1}} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}-g_{n}\right) g_{n}^{\delta}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \\
& \leq \frac{1}{\left|\lambda_{n_{1}}\right|} \frac{2 n_{1} \delta\left\|\Phi^{\infty}(\cdot, z)\right\|}{\inf _{n \leq n_{1}} \operatorname{dist}\left(\lambda_{n}, \sigma(F) \backslash \lambda_{n}\right)}
\end{aligned}
$$

Thus, choosing $\delta_{0}=\delta_{0}\left(n_{1}\right)$ small enough we conclude that

$$
\begin{aligned}
&\left\|\sum_{n=1}^{n_{1}} \frac{\overline{\lambda_{n}}}{\alpha+\left|\lambda_{n}\right|^{2}}\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}-g_{n}\right) g_{n}^{\delta}\right\|_{L^{2}\left(\mathbb{S}^{2}\right)} \leq \frac{c}{2} \\
& \text { for all } \delta_{0}>\delta>0, \alpha>0
\end{aligned}
$$

By combining the previous results, we arrive at the following theorem:

Theorem 5.4. There exists a constant $M$ such that for any compact set $K \subset \mathbb{R}^{3} \backslash \bar{D}$ and every $n_{1}>n_{0}$ there exists $\delta\left(n_{1}, K\right)>0$ and $\alpha_{0}\left(n_{1}, K\right)>0$ such that
$\left|v_{g_{\alpha, z}}(z)\right| \geq 2 \pi \sum_{n=1}^{n_{1}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}-M \quad$ for $z \in K$ and $\alpha \leq \alpha_{0}\left(n_{1}, K\right)$.
For $n_{1} \rightarrow \infty$, there also holds $\delta\left(n_{1}, K\right) \rightarrow 0$ and $\alpha_{0}\left(n_{1}, K\right) \rightarrow 0$.

Proof. Combining (24) and (25) with Lemmas 5.2 and 5.3, we obtain that there exists a constant $M$ such that for every $n_{1}>n_{0}$ there exists some $\delta_{0}>0$ such that

$$
\left|v_{g_{\alpha, z}^{\delta}}(z)\right| \geq 2 \pi \sum_{n=1}^{n_{1}} \frac{\left|\lambda_{n}^{\delta}\right|^{2}}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}-\frac{2 M}{3}
$$

for all $z \in \mathbb{R}^{3}, \alpha>0$ and $\delta \leq \delta_{0}$. We rewrite this estimate slightly to obtain

$$
\left|v_{g_{\alpha, z}^{\delta}}(z)\right| \geq 2 \pi \sum_{n=1}^{n_{1}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}-2 \pi \sum_{n=1}^{n_{1}} \frac{\alpha}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}-\frac{2 M}{3}
$$

Now, fix $\delta \leq \delta_{0}$. Then, for $z \in K,\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|, n=1, \ldots, n_{1}$, is uniformly bounded. Hence, also using Lemma A. 1 from the appendix, there exists some $\alpha_{0}$ such that

$$
2 \pi \sum_{n=1}^{n_{1}} \frac{\alpha}{\alpha+\left|\lambda_{n}^{\delta}\right|^{2}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2} \leq \frac{M}{3} \quad \text { for } \alpha \leq \alpha_{0}
$$

For $n_{1} \rightarrow \infty$, we observe from the proof of Lemmas 5.2 and 5.3 that $\delta_{0} \rightarrow 0$. Hence there also follows $\alpha_{0}\left(n_{1}\right) \rightarrow 0$.

Theorem 5.4 combined with Fatou's lemma implies that the absolute value of the Herglotz wave function $v_{g_{\alpha, z}}$ at $z$ diverges, when $z \notin D$ and more and more modes are taken into consideration, and when $\alpha$ is chosen permissibly small according to Theorem 5.4.

Lemma 5.5 Under the assumptions of Theorem 5.4 we have

$$
\begin{equation*}
\sum_{n=1}^{n_{1}}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2} \rightarrow \infty \quad\left(n_{1} \rightarrow \infty\right) \tag{27}
\end{equation*}
$$

where again $\delta\left(n_{1}\right)$ depends on $n_{1}>n_{0}$. Consequently, for $\alpha\left(n_{1}\right)$ being admissible in Theorem 5.4, we find that $\left|v_{g_{\alpha, z}}(z)\right| \rightarrow \infty$ as $n_{1} \rightarrow \infty$.

Proof. Since, for $m \in \mathbb{N}$,

$$
\begin{aligned}
& \sum_{\lambda_{n}^{\delta}=\lambda_{m}^{\delta}}\left(g_{z}^{\delta}, g_{n}^{\delta}\right)=\sum_{\lambda_{n}^{\delta}=\lambda_{m}^{\delta}} \frac{1}{\sqrt{\lambda_{n}^{\delta}}}\left(\Phi^{\infty}(\cdot, z), g_{n}^{\delta}\right) \\
& \rightarrow \sum_{\lambda_{n}=\lambda_{m}} \frac{1}{\sqrt{\lambda_{n}}}\left(\Phi^{\infty}(\cdot, z), g_{n}\right) \quad\left(n_{1} \rightarrow \infty\right)
\end{aligned}
$$

because $\delta\left(n_{1}\right) \rightarrow 0$, we obtain convergence of the terms $\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}$ in (27). Moreover, Fatou's lemma implies

$$
\sum_{n=1}^{\infty} \liminf _{n_{1} \rightarrow \infty}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2} \leq \liminf _{n_{1} \rightarrow \infty} \sum_{n=1}^{\infty}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}
$$

the numerical values on the left and right-hand side being possibly infinite. Note that the series in the latter inequality are for fixed $n_{1} \in \mathbb{N}$ finite due to the finite-dimensional projection $g_{z}^{\delta}$ in (23). However, the Fourier coefficients converge,

$$
\lim _{n_{1} \rightarrow \infty}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}=\frac{\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2}}{\left|\lambda_{n}\right|}
$$

Of course, the fundamental statement of the Factorization method is that for $z \notin \bar{D}$ the series $\left(\sum_{n=1}^{\infty}\left|\left(\Phi^{\infty}(\cdot, z), g_{n}\right)\right|^{2} /\left|\lambda_{n}\right|\right)$ diverges. Hence,

$$
\infty \leq \liminf _{n_{1} \rightarrow \infty} \sum_{n=1}^{\infty}\left|\left(g_{z}^{\delta}, g_{n}^{\delta}\right)\right|^{2}
$$

which finally gives the Lemma's claim.

Corollary 5.6. For any $z \in \mathbb{R}^{3} \backslash \bar{D}$, there is a sequence $\left(\alpha_{n}\right)$ with $\alpha_{n} \rightarrow 0(n \rightarrow \infty)$ such that

$$
\left|v g_{\alpha_{n}, z}(z)\right| \rightarrow \infty \quad(n \rightarrow \infty)
$$

A. Perturbation theory for normal operators. In this appendix, we will assume that $F$ denotes a bounded normal operator. For completeness of the paper we recall some important results. General references on this subject are, for instance, $[\mathbf{2}, \mathbf{9}]$.
From the eigenexpansion

$$
F=\sum_{n=1}^{\infty} \lambda_{n}\left(\cdot, g_{n}\right) g_{n}
$$

we see that the resolvent $R(\xi, F)=(\xi-F)^{-1}$ has the representation

$$
\begin{equation*}
R(\xi, F)=\sum_{n \in \mathbb{N}} \frac{1}{\xi-\lambda_{n}}\left(\cdot, g_{n}\right) g_{n}, \quad \xi \in \mathbb{C} \backslash \sigma(F) \tag{28}
\end{equation*}
$$

Here $\sigma(F)=\{0\} \cup\left\{\lambda_{n}: n \in \mathbb{N}\right\}$ denotes the spectrum of $F$. For $\xi \notin \sigma(F)$, the resolvent is a bounded operator on $L^{2}\left(S^{2}\right)$. Moreover, the representation (28) implies that

$$
\begin{equation*}
\|R(\xi, F)\|=\sup _{n \in \mathbb{N}}\left|\xi-\lambda_{n}\right|^{-1}, \quad\|F R(\xi, F)\|=\sup _{n \in \mathbb{N}}\left|\lambda_{n}\left(\xi-\lambda_{n}\right)^{-1}\right| \tag{29}
\end{equation*}
$$

## Lemma A.1. Let $F$ and $F^{\delta}$ be bounded normal operators. Then

$$
\operatorname{dist}\left(\sigma(F), \sigma\left(F^{\delta}\right)\right) \leq\left\|F-F^{\delta}\right\|
$$

Proof. By symmetry, it suffices to prove that $\sup _{\xi \in \sigma(F)} \operatorname{dist}\left(\xi, \sigma\left(F^{\delta}\right)\right) \leq$ $\left\|F-F^{\delta}\right\|$. Therefore we show that any $\xi$ with $\operatorname{dist}(\xi, \sigma(F))>\left\|F-F^{\delta}\right\|$ belongs to the resolvent set $\rho\left(F^{\delta}\right)$. Using (29) we infer that $\|R(\xi, F)\| \leq$ $\left\|F-F^{\delta}\right\|^{-1}$, thus, $I+\left(F-F^{\delta}\right) R(\xi, F)$ is invertible. We compute

$$
\begin{aligned}
R\left(\xi, F^{\delta}\right) & =R(\xi, F)\left[I+\left(F-F^{\delta}\right) R(\xi, F)\right]^{-1} \\
& =R(\xi, F) \sum_{n \in \mathbb{N}}\left(-\left(F-F^{\delta}\right) R(\xi, F)\right)^{n}
\end{aligned}
$$

and the latter Neumann series converges.

The spectral projection on the eigenspaces of the $m$ th eigenvector of $F$ and $F^{\delta}$ is given by

$$
P_{m}=\sum_{\lambda_{n}=\lambda_{m}}\left(\cdot, g_{n}\right) g_{n} \quad \text { and } \quad P_{m}^{\delta}=\sum_{\lambda_{n}^{\delta}=\lambda_{m}^{\delta}}\left(\cdot, g_{n}^{\delta}\right) g_{n}^{\delta}
$$

respectively. Cauchy's theorem states that

$$
P_{m}=\frac{1}{2 \pi i} \int_{\gamma} R(\xi, F) \mathrm{d} \xi
$$

for any contour $\gamma$ around $\lambda_{m}$ such that the rest of $\sigma(F)$ is outside of $\gamma$. Let us assume that the distance of $\lambda_{m}$ to the rest of $\sigma(F)$ is $2 d$ and choose the contour $\left\{\xi \in \mathbb{C},\left|\xi-\lambda_{m}\right|=d\right\}$. If $\left\|F-F^{\delta}\right\| \leq \delta<d$, we find that $P_{m}^{\delta}=(2 \pi i)^{-1} \int_{\gamma} R\left(\xi, F^{\delta}\right) \mathrm{d} \xi$ and estimate

$$
\begin{aligned}
\left\|P_{m}-P_{m}^{\delta}\right\| & =\frac{1}{2 \pi}\left\|\int_{\gamma}\left(R(\xi, F)-R\left(\xi, f^{\delta}\right)\right) \mathrm{d} \xi\right\| \\
& \leq d \sup _{\xi \in \gamma}\left\|R(\xi, F)\left(F-F^{\delta}\right) R\left(\xi, F^{\delta}\right)\right\| \\
& \leq d \delta \sup _{\xi \in \gamma} \sup _{\zeta \in \sigma(F)}|\xi-\zeta|^{-1} \sup _{\zeta \in \sigma\left(F^{\delta}\right)}|\xi-\zeta|^{-1} \\
& \leq d \delta \sup _{\xi \in \gamma}\left|\xi-\lambda_{m}\right|^{-1}\left(\left|\xi-\lambda_{m}\right|-\delta\right)^{-1}=\frac{\delta}{d-\delta}
\end{aligned}
$$

We formulate this estimate in a lemma.

Lemma A.2. Assume that $\operatorname{dist}\left(\lambda_{m}, \sigma(F) \backslash\left\{\lambda_{m}\right\}\right)=2 d$ and $\left\|F-F^{\delta}\right\| \leq \delta<d$. Then

$$
\left\|P_{m}-P_{m}^{\delta}\right\| \leq \frac{\delta}{d-\delta}
$$

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