AN INVERSE PROBLEM FOR POINT INHOMOGENEITIES

FRITZ GESZTESY AND ALEXANDER G. RAMM

ABSTRACT. We study quantum scattering theory off n point inhomogeneities ($n \in \mathbb{N}$) in three dimensions. The inhomogeneities (or generalized point interactions) positioned at $\{\xi_1, \dots, \xi_n\} \subset \mathbb{R}^3$ are modeled in terms of the n^2 (real) parameter family of self-adjoint extensions of $-\Delta|_{C_0^\infty(\mathbb{R}^3 \backslash \{\xi_1,\dots,\xi_n\})}$ in $L^2(\mathbb{R}^3)$. The Green's function, the scattering solutions and the scattering amplitude for this model are explicitly computed in terms of elementary functions. Moreover, using the connection between fixed energy quantum scattering and acoustical scattering, the following inverse spectral result in acoustics is proved: The knowledge of the scattered field on a plane outside these point-like inhomogeneities, with all inhomogeneities located on one side of the plane, uniquely determines the positions and boundary conditions associated with them.

1. INTRODUCTION

To describe the inverse problem solved in this paper in some detail we need a few preparations. Let $\mathbb{R}^3_\pm = \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_3 \gtrless 0\}$, $P = \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_3 = 0\}$, $D \subset \mathbb{R}^3_-$ a domain with smooth boundary and finitely many connected components, and $v \in L^2(D)$, $\operatorname{supp}(v) \subseteq D$, v real-valued . Consider the fixed energy scattering problem

$$\begin{cases} [- \nabla_x^2 - k_0^2 - k_0^2 v(x)] u(x,y) = \delta(x-y), \quad x, y \in \mathbb{R}^3,\ x \neq y, \\ \lim_{|x|\to\infty} |x| \big[\frac{\partial}{\partial |x|} u(x,y) - ik_0 u(x,y)\big] = 0 \quad \text{uniformly in directions } \omega = |x|^{-1}x \\ \qquad\qquad \text{and uniformly in } y \text{ for } y \text{ varying in compact sets,} \end{cases} \tag{1.1}$$

with $k_0 > 0$ (the wave number) a fixed positive constant. Here $c(x) = [v(x)+1]^{-1/2}$ has the physical meaning of the wave velocity profile in the medium, $v(x)$ is the inhomogeneity in the velocity profile, and $u(x,y)$ represents the acoustic pressure generated by a point source at the point $y \in \mathbb{R}^3$.

The inverse problem (IP) associated with (1.1), more precisely, the inversion of the surface data $u(x,y)$ for the velocity profile $c(x)$, then can be formulated as follows:

IP 1.1. Given the data $\{u(x,y)\}_{\substack{x,y\in P \\ x\neq y}}$ at fixed $k_0 > 0$, determine $v(x)$, $x \in D$.

A solution of this inverse problem (i.e., uniqueness of $v(x)$ and recovery of $v(x)$ from the prescribed data) is described in [11, Sects. III.6, IV.2]. Numerical methods in connection with IP 1.1 are discussed in [11, Sect. V.3].

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Since $u(x,y)$ in (1.1) can be identified with the Green's function at fixed energy $k_0^2>0$,

$$G(k_0^2,x,y)=(-\Delta-k_0^2v-k_0^2)^{-1}(x,y),\quad x,y\in\mathbb{R}^3,\, x\neq y, \tag{1.2}$$

associated with the self-adjoint (Schrödinger-type) operator

$$H=-\Delta-k_0^2v,\quad \operatorname{dom}(H)=H^{2,2}(\mathbb{R}^3) \tag{1.3}$$

in $L^2(\mathbb{R}^3)$, we can reformulate the inverse problem IP 1.1 in the following equivalent form:

IP 1.1'. Given the data $\{G(k_0^2,x,y)\}_{\substack{x,y\in P\\ x\neq y}}$ at a fixed energy $k_0^2>0$, determine $v(x)$, $x\in D$.

For practical applications in connection with ultrasound mammography tests (as opposed to x-ray mammography) and in the area of material science in connection with the detection of cracks and cavities, it is of relevance to consider inhomogeneities $v(x)$ of the special form

$$v(x)=\sum_{j=1}^n v_j(x-\xi_j),\quad \{\xi_1,\dots,\xi_n\}\subset\mathbb{R}^3_-, \tag{1.4}$$

where $v_j\in L^2(D_j)$, $\operatorname{supp}(v_j(\cdot-\xi_j))\subseteq D_j$, and $D_j\subset\mathbb{R}^3_-$ are connected domains with smooth boundaries and sufficiently small diameters d_j with respect to the wave length (i.e., $(\max_{1\le j\le n} d_j)k_0\ll 1$). A numerical procedure recovering the ξ_j (and hence the approximate position of the small inhomogeneities) and the intensities of the inhomogeneities, defined by $V_j=\int_{D_j}dx\, v_j(x-\xi_j)$, $1\le j\le n$, has recently been discussed in [12].

At this point we are in a position to describe the inverse problem considered in this paper. In view of the physical applications mentioned in connection with (1.4), we will now consider the idealized situation of inhomogeneities $v_j(x-\xi_j)$ of *point-like* support at ξ_j, $1\le j\le n$. Intuitively, we want to solve the inverse problem

$$\begin{cases}[-\nabla_x^2-k_0^2-k_0^2\sum_{j=1}^n v_j(x-\xi_j)]u(x,y)=\delta(x-y), \quad x,y\in\mathbb{R}^3,\, x\neq y,\\ \lim_{|x|\to\infty}|x|\big[\frac{\partial}{\partial|x|}u(x,y)-ik_0u(x,y)\big]=0 \quad \text{uniformly in directions } \omega=|x|^{-1}x\\ \qquad\qquad \text{and uniformly in } y \text{ for } y \text{ varying in compact sets,}\end{cases} \tag{1.5}$$

where formally

$$v_j(x-\xi_j)=a_j\delta(x-\xi_j),\quad 1\le j\le n, \tag{1.6}$$

for some "coupling" constants $a_j\in\mathbb{R}$, $1\le j\le n$. However, as is well-known, point-like inhomogeneities of the type (1.6) as potential coefficients in a Schrödinger-type operator in dimensions $d\ge 2$ do not lead to an operator or quadratic form perturbation of the Laplacian $-\Delta$, $\operatorname{dom}(-\Delta)=H^{2,2}(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$, where d denotes the corresponding space dimension. One possible way around this difficulty for $d=2$ and $d=3$ is the introduction of an appropriate coupling constant renormalization procedure. This point of view is presented in detail in [3, Ch. II.1]. Alternatively to this renormalization procedure for $d=2,3$, one can apply the theory of self-adjoint extensions of closed symmetric densely defined linear operators in a Hilbert space to the operator

$$\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}, \quad \Xi = \{\xi_1, \dots, \xi_n\} \subset \mathbb{R}^3_- \tag{1.7}$$

in $L^2(\mathbb{R}^3)$. (Here the $\overline{T}$ denotes the operator closure of T and we refer to Remark 3.5 for a brief discussion of the situation in different dimensions $d \in \mathbb{N}$.) In this paper we follow the latter approach and model the Laplacian $-\Delta$ perturbed by point-like perturbations of the type $-k_0^2 \sum_{j=1}^n a_j \delta(x - \xi_j)$ by self-adjoint extensions of $\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}$, denoted by $-\Delta_{\theta,\Xi}$, parametrized by the n^2 (real) parameter family of self-adjoint matrices θ in $\mathbb{C}^n$.

Taking advantage of the equivalence of the inverse problems IP 1.1 and IP 1.1', we can now formulate the inverse problem associated with point-like inhomogeneities, as studied in this paper, in a precise manner as follows:

IP 1.2. Prove that the data $\{G_{\theta,\Xi}(k_0^2, x, y)\}_{\substack{x,y \in P\\ x\neq y}}$ at fixed energy $k_0^2 > 0$, uniquely determine $\Xi = \{\xi_1, \dots, \xi_n\} \subset \mathbb{R}^3_-$ and the self-adjoint $n \times n$ matrix θ in $\mathbb{C}^n$.

Here $G_{\theta,\Xi}(k_0^2, x, y)$ denotes the Green's function associated with $-\Delta_{\theta,\Xi}$, that is,

$$G_{\theta,\Xi}(z, x, y) = (-\Delta_{\theta,\Xi} - z)^{-1}(x, y), \quad \det(P_{\theta,\Xi}(z)) \neq 0, \ x, y \in \mathbb{R}^3\backslash\Xi, \, x \neq y. \tag{1.8}$$

While IP 1.1 (resp., (IP 1.1') is concerned with uniqueness and reconstruction of $v(x)$, $x \in \overline{D}$, IP 1.2, as studied in this paper, focuses on the unique determination of Ξ and θ by the data measured on the plane P.

In Section 2 we present a detailed account of Krein's formula of self-adjoint extensions of closed symmetric operators in a Hilbert space, our principal tool in describing the n^2 (real) parameter family of self-adjoint extensions $-\Delta_{\theta,\Xi}$ of (1.7) in Section 3. In particular, we explicitly describe the Green's function, the scattering solutions, and the scattering amplitude associated with $-\Delta_{\theta,\Xi}$ in Section 3. The inverse problem IP 1.2 is solved in our final Section 4.

2. Krein's Formula for Self-adjoint Extensions

In this section we recall Krein's formula, which describes the resolvent difference of two self-adjoint extensions A_1 and A_2 of a densely defined closed symmetric linear operator A with deficiency indices (n, n), $n \in \mathbb{N}$. (Reference [7] treats this topic in the general case where $n \in \mathbb{N} \cup \{\infty\}$. Here we restrict ourselves to the case $n < \infty$.) We start with the basic setup following [2].

Let $\mathcal{H}$ be a separable complex Hilbert space, $\dot{A} : \mathrm{dom}(\dot{A}) \to \mathcal{H}$, $\overline{\mathrm{dom}(\dot{A})} = \mathcal{H}$ a densely defined closed symmetric linear operator in $\mathcal{H}$ with finite and equal deficiency indices $\mathrm{def}(\dot{A}) = (r, r)$, $r \in \mathbb{N}$. Let A_ℓ, $\ell = 1, 2$, be two distinct self-adjoint extensions of $\dot{A}$ and denote by A the maximal common part of A_1 and A_2, that is, A is the largest closed extension of $\dot{A}$ with $\mathrm{dom}(A) = \mathrm{dom}(A_1) \cap \mathrm{dom}(A_2)$. In this case one calls A_1 and A_2 *relatively prime* with respect to A. Let $0 \leq p \leq r-1$ be the maximal number of elements in $\mathrm{dom}(A) = \mathrm{dom}(A_1) \cap \mathrm{dom}(A_2)$ which are linearly independent modulo $\mathrm{dom}(\dot{A})$. Then A has deficiency indices $\mathrm{def}(A) = (n, n)$, $n = r - p$. Next, denote by $\ker(A^* - z)$, $z \in \mathbb{C}\backslash\mathbb{R}$ the deficiency subspaces of A and define

$$W_{1,z,z_0} = I + (z - z_0)(A_1 - z)^{-1} = (A_1 - z_0)(A_1 - z)^{-1}, \ z, z_0 \in \rho(A_1), \tag{2.1}$$

where I denotes the identity operator in $\mathcal{H}$ and $\rho(T)$ abbreviates the resolvent set of T. One verifies

$$W_{1,z_0,z_1} W_{1,z_1,z_2} = W_{1,z_0,z_2}, \ z_0, z_1, z_2 \in \rho(A_1) \tag{2.2}$$

and

$$W_{1,z,z_0} \ker(A^* - z_0) = \ker(A^* - z). \tag{2.3}$$

Let $\{u_j(i)\}_{1\leq j\leq n}$ be an orthonormal basis for $\ker(A^* - i)$ and define

$$u_j(z) = W_{1,z,i} u_j(i) = (A_1 - i)(A_1 - z)^{-1} u_j(i), \quad 1 \leq j \leq n, \ z \in \rho(A_1). \tag{2.4}$$

Then $\{u_j(z)\}_{1\leq j\leq n}$ is a basis for $\ker(A^* - z)$, $z \in \rho(A_1)$ and since $W_{1,-i,i} = (A_1 - i)(A_1 + i)^{-1}$ is the unitary Cayley transform of A_1, $\{u_j(-i)\}_{1\leq j\leq n}$ is in fact an orthonormal basis for $\ker(A^* + i)$.

The basic result on Krein's formula, as presented by Akhiezer and Glazman [2], Sect. 84, then reads as follows.

Theorem 2.1. (Krein's formula, [2, Sect. 84].)
There exists a $P_{1,2}(z) = \big(P_{1,2}(z)_{j,j'}\big)_{1\leq j,j'\leq n} \in M_n(\mathbb{C})$, $z \in \rho(A_2) \cap \rho(A_1)$, *such that*

$$\det(P_{1,2}(z)) \neq 0, \ z \in \rho(A_2) \cap \rho(A_1), \tag{2.5}$$

$$P_{1,2}(z)^{-1} = P_{1,2}(z_0)^{-1} - (z - z_0)\big((u_j(\bar{z}), u_{j'}(z_0))\big)_{1\leq j,j'\leq n}, \ z, z_0 \in \rho(A_1), \tag{2.6}$$

$$\mathrm{Im}\,(P_{1,2}(i)^{-1}) = -I_n, \tag{2.7}$$

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,j'=1}^{n} P_{1,2}(z)_{j,j'} (u_{j'}(\bar{z}), \cdot\,) u_j(z), \quad z \in \rho(A_2) \cap \rho(A_1). \tag{2.8}$$

Here $\mathrm{Im}(T) = (T - T^*)/(2i)$ and $\mathrm{Re}(T) = (T + T^*)/2$ denote the imaginary and real parts of the matrix T, respectively.

We note that $P_{1,2}(z)^{-1}$ extends by continuity from $z \in \rho(A_2) \cap \rho(A_1)$ to all of $\rho(A_1)$ since the right-hand side of (2.6) is continuous for $z \in \rho(A_1)$. The normalization condition (2.7) is not mentioned in [2] but it trivially follows from (2.6) and the fact

$$(u_j(i), u_{j'}(i)) = \delta_{j,j'}, \quad 1 \leq j, j' \leq n \tag{2.9}$$

(where $\delta_{j,j'}$ denotes Kronecker's symbol) and from

$$P_{1,2}^*(z) = P_{1,2}(\bar{z}), \quad z \in \rho(A_1) \cap \rho(A_2). \tag{2.10}$$

Taking $z = \overline{z_0}$ in (2.6) shows that $-P_{1,2}(z)^{-1}$ and hence $P_{1,2}(z)$ is a matrix-valued Herglotz function, that is,

$$\mathrm{Im}\,(P_{1,2}(z)) > 0, \ z \in \mathbb{C}_+. \tag{2.11}$$

Strict positive definiteness in (2.11) follows from the fact that $\{u_j(z)\}_{1\leq j\leq n}$ are linearly independent for $z \in \mathbb{C}_+$ and hence $((u_j(z), u_{j'}(z))_{1\leq j,j'\leq n} > 0$.

Next we turn to the connection between $P_{1,2}(z)$ and von Neumann's parametrization of self-adjoint extensions of A as discussed in detail in [7]. Due to (2.6),

$P_{1,2}(z)^{-1}$ is determined for all $z \in \rho(A_1)$ in terms of $P_{1,2}(i)^{-1}$, $(A_1 - z)^{-1}$ and $\{u_j(i)\}_{1\le j\le n}$,

$$P_{1,2}(z)^{-1} = P_{1,2}(i)^{-1} - (z-i)I_n - (1+z^2)\big((u_j(i),(A_1-z)^{-1}u_{j'}(i))\big)_{1\le j,j'\le n}, \quad z \in \rho(A_1). \tag{2.12}$$

Hence it suffices to focus on

$$P_{1,2}(i)^{-1} = \operatorname{Re}(P_{1,2}(i)^{-1}) - iI_n. \tag{2.13}$$

Let

$$\mathcal{U}_\ell : \ker(A^*-i) \to \ker(A^*+i), \quad \ell = 1,2, \tag{2.14}$$

be the linear isometric isomorphisms that parameterize A_ℓ according to von Neumann's formula

$$\begin{aligned} &A_\ell(f + (I+\mathcal{U}_\ell)u_+) = Af + i(I-\mathcal{U}_\ell)u_+, \\ &\operatorname{dom}(A_\ell) = \{(g + (I+\mathcal{U}_\ell)u_+) \in \operatorname{dom}(A^*) \,|\, g \in \operatorname{dom}(A),\, u_+ \in \ker(A^*-i)\}, \\ &\qquad \ell = 1,2. \end{aligned} \tag{2.15}$$

Next, denote by $U_\ell = (U_{\ell,j,j'})_{1\le j,j'\le n} \in M_n(\mathbb{C})$, $\ell = 1,2$ the unitary matrix representation of $\mathcal{U}_\ell$ with respect to the bases $\{u_j(i)\}_{1\le j\le n}$ and $\{u_{1,j}(-i)\}_{1\le j\le n}$ of $\ker(A^*-i)$ and $\ker(A^*+i)$ respectively, that is,

$$\mathcal{U}_\ell u_j(i) = \sum_{j'=1}^n U_{\ell,j',j}u_{1,j'}(-i),\ 1\le j\le n,\ \ell = 1,2. \tag{2.16}$$

Lemma 2.2. ([7].)
(i) $U_1 = -I_n$.
(ii) $-1 \notin \operatorname{spec}(U_2)$.
(iii) U_ℓ, $\ell = 1,2$ and $P_{1,2}(i)$ are connected by

$$P_{1,2}(i) = \frac{i}{2}(I_n + U_2^{-1}) = \frac{i}{2}(U_2^{-1} - U_1^{-1}). \tag{2.17}$$

Here $\operatorname{spec}(T)$ denotes the spectrum of T.

Next, writing

$$U_2 = \exp(i\theta_2), \quad \theta_2^* = \theta_2 \tag{2.18}$$

for the matrix representation of $\mathcal{U}_2$ with respect to the bases $\{u_j(i)\}_{1\le j\le n}$ and $\{u_{1,j}(-i)\}_{1\le j\le n}$ of $\ker(A^*-i)$ and $\ker(A^*+i)$, one verifies

$$\operatorname{Re}(P_{1,2}(i)^{-1}) = \tan(\theta_2/2). \tag{2.19}$$

Introducing the matrix-valued Herglotz function $M_1(z)$ associated with A_1 (cf. [6], [7]) by

$$M_1(z) = zI_n + (1+z^2)\big((u_j(i),(A_1-z)^{-1}u_{j'}(i))_{1\le j,j'\le n}\big), \quad z \in \rho(A_1), \tag{2.20}$$

$P_{1,2}(z)$ in Krein's formula (2.8) then can be rewritten as

$$\begin{aligned} P_{1,2}(z) &= (\tan(\theta_2/2) - M_1(z))^{-1} \\ &= \big(\tan(\theta_2/2) - zI_n - (1+z^2)\big((u_j(i),(A_1-z)^{-1}u_{j'}(i))_{1\le j,j'\le n}\big)\big)^{-1}, \\ &\qquad z \in \rho(A_1). \end{aligned} \tag{2.21}$$

We emphasize that

$$\{((1/2)+m)\pi\}_{m\in\mathbb{Z}} \notin \operatorname{spec}(\theta_2) \tag{2.22}$$

according to Lemma 2.2 (ii), due to our hypothesis that A_1 and A_2 are relatively prime with respect to A.

For subsequent purposes it is useful to introduce the self-adjoint operator $\vartheta_2 \in \mathcal{B}(\ker(A^* - i))$ defined through its matrix representation θ_2 with respect to the basis $\{u_j(i)\}_{1\leq j\leq n}$, that is,

$$\theta_{2,j,j'} = (u_j(i), \vartheta_2 u_{j'}(i)), \quad 1 \leq j, j' \leq n. \tag{2.23}$$

The discussion of Krein's formula thus far dealt exclusively with the orthonormal bases $\{u_j(i)\}_{1\leq j\leq n}$ and $\{u_{1,j}(-i)\}_{1\leq j\leq n}$ of $\ker(A^* - i)$ and $\ker(A^* + i)$ following our discussion in [7] and [8, Appendix B]. In the remainder of this paper, however, it will be be more convenient to discuss matrix representations of $M_1(z)$ and $\mathcal{U}_2$ with respect to a natural (cf. the comment following (3.6)), but not necessarily orthogonal basis. Hence we briefly discuss the effect of a change of basis in connection with Krein's formula (2.8). Let $\{\tilde u_j(i)\}_{1\leq j\leq n}$ be another (not necessarily orthogonal basis) of $\ker(A^* - i)$ and define

$$\tilde u_j(z) = (A_1 - i)(A_1 - z)^{-1}\tilde u_j(i), \quad 1 \leq j \leq n,\ z \in \rho(A_1), \tag{2.24}$$

$$\mathcal{U}_\ell \tilde u_j(i) = \sum_{j'=1}^n \widetilde U_{\ell,j',j}\tilde u_{j'}(-i), \quad 1 \leq j \leq n,\ \ell = 1,2, \tag{2.25}$$

$$\widetilde U_2 = \exp(i\tilde\theta_2), \quad \tilde\theta_2^* = \tilde\theta_2. \tag{2.26}$$

In addition, one verifies

$$\widetilde U_1 = -I_n \tag{2.27}$$

as in Lemma 2.2 (i). Krein's formula (2.8) then can be rewritten in the form

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,j'=1}^n \widetilde P_{1,2}(z)_{j,j'}(\tilde u_{j'}(\bar z), \cdot)\tilde u_j(z), \quad z \in \rho(A_2)\cap\rho(A_1), \tag{2.28}$$

where

$$\begin{aligned}\widetilde P_{1,2}(z) &= (\tan(\tilde\theta_2/2) - \widetilde M_1(z))^{-1}\\ &= \big(\tan(\tilde\theta_2/2) - zI_n - (1+z^2)\big((\tilde u_j(i), (A_1 - z)^{-1}\tilde u_{j'}(i))_{1\leq j,j'\leq n}\big)\big)^{-1},\\ &\hspace{20em} z \in \rho(A_1),\end{aligned} \tag{2.29}$$

and (cf. (2.23))

$$\tilde\theta_{2,j,j'} = (\tilde u_j(i), \vartheta_2 \tilde u_{j'}(i)), \quad 1 \leq j, j' \leq n. \tag{2.30}$$

The proof of (2.28)–(2.30) is based on the following elementary result.

Lemma 2.3. *Let $\mathcal{H}_n$, $n \in \mathbb{N}$ be an n-dimensional complex Hilbert space, $T \in \mathcal{B}(\mathcal{H})$ a bounded linear operator in $\mathcal{H}$ with $T^{-1} \in \mathcal{B}(\mathcal{H})$. Assume that $\{\psi_j\}_{1\leq j\leq n}$ and $\{\tilde\psi_j\}_{1\leq j\leq n}$ are (not necessarily orthogonal) bases in $\mathcal{H}$. Then*

$$\begin{aligned}&\sum_{j,j'=1}^n \big(\big((\psi_\ell, T\psi_m)_{1\leq \ell,m\leq n}\big)^{-1}\big)_{j,j'}(\psi_{j'}, \cdot)\psi_j\\ &= \sum_{j,j'=1}^n \big(\big((\tilde\psi_\ell, T\tilde\psi_m)_{1\leq \ell,m\leq n}\big)^{-1}\big)_{j,j'}(\tilde\psi_{j'}, \cdot)\tilde\psi_j.\end{aligned} \tag{2.31}$$

3. The Direct Scattering Problem for Generalized Point Interactions

In the principal part of this section we apply the abstract framework surrounding Krein's formula (2.28) to the concrete situation of n generalized point interactions in $\mathbb{R}^3$. At the end we derive the corresponding quantum mechanical scattering formalism, including explicit expressions for the scattering wave functions and the scattering amplitude.

In order to apply the results of Section 2, we now make a series of identifications:

$$\mathcal{H} = L^2(\mathbb{R}^3), \tag{3.1}$$

$$A = \overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\{\xi_1,\dots,\xi_n\})}}, \quad \{\xi_1,\dots,\xi_n\} \subset \mathbb{R}^3,\ \xi_j \neq \xi_{j'} \text{ for } j \neq j', \tag{3.2}$$

$$\ker(A^* - i) = \operatorname{span}\{\tilde u_j(i,x) = G_0(i, x-\xi_j)\}_{1\le j\le n}, \tag{3.3}$$

$$G_0(z, x-y) = (-\Delta - z)^{-1}(x,y) = \frac{\exp(iz^{1/2}|x-y|)}{4\pi|x-y|}, \tag{3.4}$$

$$z \in \mathbb{C}\backslash\mathbb{R},\ \operatorname{Im}(z^{1/2}) > 0,\ x,y \in \mathbb{R}^3,\ x \neq y,$$

$$A_1 = -\Delta, \quad \operatorname{dom}(-\Delta) = H^{2,2}(\mathbb{R}^3), \tag{3.5}$$

$$\tilde u_j(z) = (-\Delta - i)(-\Delta - z)^{-1}\tilde u_j(i) = G_0(z, \cdot - \xi_j), \tag{3.6}$$

$$z \in \mathbb{C}\backslash\mathbb{R},\ \operatorname{Im}(z^{1/2}) > 0,\ 1 \le j \le n.$$

In particular, a comparison of (3.3) and

$$\ker(A^* - z) = \operatorname{span}\{\tilde u_j(z,x) = G_0(z, x-\xi_j)\}_{1\le j\le n}, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.7}$$

shows that $\{\tilde u_j(z)\}_{1\le j\le n}$ is a natural (though, not orthogonal) basis of $\ker(A^* - z)$.

We note that the fact (3.3) can be found, for instance, in [3, Sect. II.1.1] and [14].

Straightforward computations using

$$(\pm i)^{1/2} = 2^{-1/2}(\pm 1 + i), \quad \overline{i(i)^{1/2}} = i(-i)^{1/2} \tag{3.8}$$

and the first resolvent equation

$$(-\Delta - z_1)^{-1}(-\Delta - z_2)^{-1} = (z_1 - z_2)^{-1}[(-\Delta - z_1)^{-1} - (-\Delta - z_2)^{-1}], \quad z_1, z_2 \in \rho(-\Delta) \tag{3.9}$$

repeatedly, then yield the following results.

Lemma 3.1. *Let $z \in \rho(-\Delta)$ and $j, j' \in \{1,\dots,n\}$. Then*

$$(\tilde u_j(i), \tilde u_{j'}(i)) = \begin{cases} \|u_j(i)\|^2 = (4\pi 2^{1/2})^{-1}, & j = j', \\ \operatorname{Im}(G_0(i, \xi_j - \xi_{j'})), & j \neq j', \end{cases} \tag{3.10}$$

$$(\tilde u_j(i), (-\Delta - z)^{-1}\tilde u_j(i)) = (4\pi)^{-1}(z^2+1)^{-1}[iz^{1/2} - i(-i)^{1/2} - 2^{-1/2}(z+i)], \tag{3.11}$$

$$\begin{aligned}(\tilde u_j(i), (-\Delta - z)^{-1}\tilde u_{j'}(i)) = {} & (z^2+1)^{-1}[G_0(z, \xi_j - \xi_{j'}) - G_0(-i, \xi_j - \xi_{j'})] \\ & - (z-i)^{-1}\operatorname{Im}(G_0(i, \xi_j - \xi_{j'})), \quad j \neq j',\end{aligned} \tag{3.12}$$

$$\operatorname{Im}(z)((\tilde u_j(i), \tilde u_{j'}(i)) = \begin{cases} (4\pi)^{-1}\operatorname{Re}(z^{1/2}), & j = j', \\ \operatorname{Im}(G_0(z, \xi_j - \xi_{j'})), & j \neq j', \end{cases} \tag{3.13}$$

where

$$\operatorname{Im}(G_0(z,\xi_j-\xi_{j'}))=[G_0(z,\xi-\xi_{j'})-G_0(\overline{z},\xi_j-\xi_{j'})]/(2i). \tag{3.14}$$

Given these preliminaries, one can now describe the n^2 (real) parameter family of all self-adjoint extensions of A, relatively prime to $A_1=-\Delta$ with respect to A, by appealing to Krein's formula (2.28), (2.29) as follows. (In passing we note that $A_1=-\Delta$, as defined in (3.5), is the Friedrichs extension of A.) One defines

$$\Xi=\{\xi_1,\dots,\xi_n\}\subset\mathbb{R}^3 \tag{3.15}$$

and denotes by

$$\theta=\big(\theta_{j,j'}\big)_{1\le j,j'\le n}=\theta^* \tag{3.16}$$

a self-adjoint $n\times n$ matrix in $\mathbb{C}^n$. Combining Krein's formula (2.28), (2.29) with (3.11) and (3.12) then yields the principal result of this section.

Theorem 3.2. *Let $z\in\mathbb{C}\backslash\mathbb{R}$. Then the n^2 (real) parameter family of all self-adjoint extensions $-\Delta_{\theta,\Xi}$ of $\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}$, relatively prime to $-\Delta$ with respect to $\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}$, can be parametrized by all self-adjoint $n\times n$ matrices θ in $\mathbb{C}^n$ with*

$$\{((1/2)+m)\pi\}_{m\in\mathbb{Z}}\notin\operatorname{spec}(\theta). \tag{3.17}$$

An explicit representation for $-\Delta_{\theta,\Xi}$ is provided by

$$(-\Delta_{\theta,\Xi}-z)^{-1}=(-\Delta-z)^{-1}+\sum_{j,j'=1}^{n}P_{\theta,\Xi}(z)_{j,j'}(G_0(\overline{z},\cdot-\xi_{j'}),\cdot)G_0(z,\cdot-\xi_j), \tag{3.18}$$

where

$$\begin{aligned}&\big(P_{\theta,\Xi}(z)^{-1}\big)_{j,j'} \qquad\qquad (3.19)\\ &=\begin{cases}-(4\pi)^{-1}iz^{1/2}-(4\pi)^{-1}2^{-1/2}+(\tan(\theta/2)_{j,j}, & j=j',\\ -G_0(z,\xi_j-\xi_{j'})+\operatorname{Re}(G_0(i,\xi_j-\xi_{j'}))+(\tan(\theta/2))_{j,j'}, & j\ne j',\end{cases}\end{aligned}$$

and

$$\operatorname{Re}(G_0(z,\xi_j-\xi_{j'}))=[G_0(z,\xi_j-\xi_{j'})+G_0(\overline{z},\xi_j-\xi_{j'})]/2. \tag{3.20}$$

Remark 3.3. (i) Whenever θ in (3.18) has an eigenvalue $((1/2)+m_0)\pi$ for some $m_0\in\mathbb{Z}$, $\widetilde{P}_{\theta,\Xi}(z)$ becomes a singular matrix, $\det(\widetilde{P}_{\theta,\Xi}(z))=0$, $z\in\mathbb{C}\backslash\mathbb{R}$. In this case at least one point ξ_{j_0} is removed from Ξ and one effectively considers self-adjoint extensions of $A=\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\{\Xi\backslash\{\xi_{j_0}\}\})}}$, parametrized in terms of $(n-1)\times(n-1)$ (or less) dimensional self-adjoint matrices θ. In particular, the Friedrichs extension of $A=\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}$, given by $A_1=-\Delta$, formally corresponds to the extreme case $\theta=\pi I_n$ in (3.18), (3.19).
(ii) It seems appropriate to call the n^2-parameter family $-\Delta_{\theta,\Xi}$ defined by (3.18), (3.19) the *generalized* point interaction Hamiltonian, distinguishing it from the usually considered n-parameter family of (local) point interactions. In fact, introducing $\underline{\alpha}=(\alpha_1,\dots,\alpha_n)\in\mathbb{R}^n$, the standard n-parameter family of self-adjoint extensions $-\Delta_{\underline{\alpha},\Xi}$ of $\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^3\backslash\Xi)}}$ emerges as a special case of (3.18), (3.19) by choosing

$$\tan(\theta/2)=\big((\alpha_j+(4\pi)^{-1}2^{-1/2})\delta_{j,j'}-\operatorname{Re}(\widetilde{G}_0(i,\xi_j-\xi_{j'}))\big)_{1\le j,j'\le n}, \tag{3.21}$$

where

$$\widetilde{G}_0(z,x) = \begin{cases} G_0(z,x) & \text{if } x \neq 0, \\ 0 & \text{if } x = 0 \text{ (or if } n = 1), \end{cases} \tag{3.22}$$

and $\mathrm{Re}(\widetilde{G}_0(z,\xi_j - \xi_{j'})) = [\widetilde{G}_0(z,\xi - \xi_{j'}) + \widetilde{G}_0(\overline{z},\xi_j - \xi_{j'})]/2$. Insertion of (3.21) into (3.18), (3.19) then yields

$$(-\Delta_{\underline{\alpha},\Xi} - z)^{-1} = (-\Delta - z)^{-1} + \sum_{j,j'=1}^{n} \big(\Gamma_{\underline{\alpha},\Xi}(z)^{-1}\big)_{j,j'} (G_0(\overline{z},\cdot - \xi_{j'}),\cdot) G_0(z,\cdot - \xi_j), \tag{3.23}$$

where

$$\Gamma_{\underline{\alpha},\Xi}(z) = \big((-(4\pi)^{-1} i z^{1/2} + \alpha_j)\delta_{j,j'} - \widetilde{G}_0(z,\xi_j - \xi_{j'})\big)_{1\leq j,j'\leq n}, \tag{3.24}$$

in accordance with [3, p. 113]. While most efforts in connection with finitely many point interactions focus on the n-parameter family $-\Delta_{\underline{\alpha},\Xi}$ (cf. the detailed discussion in [3, Ch. II.1] and the references therein), the general n^2-parameter family of generalized point interactions has been discussed by Dabrowski and Grosse [5] in 1985. The treatment in [5] also combines Krein's resolvent formula with von Neumann's parametrization of self-adjoint extensions, but is somewhat less detailed than our present approach. (In particular, their matrix $S(\overline{z},z_0)$, and hence their $M(z)$, are not explicitly computed in section II of [5], although these quantities can be inferred from the scaling limit approach in section IV via their formula (4.18).)

Finally, we briefly discuss stationary quantum scattering theory following the lines of [3, Sect. II.1.5] and [10]. Given the resolvent kernel of $-\Delta_{\theta,\Xi}$ in (3.18), one computes

$$\begin{aligned} &\lim_{\varepsilon\downarrow 0} \lim_{\substack{|y|\to\infty \\ -|y|^{-1}y=\omega}} 4\pi |y| e^{-i(k+i\varepsilon)|y|} (-\Delta_{\theta,\Xi} - (k+i\varepsilon)^2)^{-1}(x,y) \\ &= e^{ik\omega\cdot x} + \sum_{j,j'=1}^{n} P_{\theta,\Xi}(k^2)_{j,j'} e^{ik\omega\cdot\xi_{j'}} G_0(k^2, x - \xi_j) \\ &= \Psi_{\theta,\Xi}(x,k,\omega), \quad k\in\mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0,\ \omega\in S^2,\ x\in\mathbb{R}^3\backslash\Xi\,. \end{aligned} \tag{3.25}$$

Moreover, since

$$(-\Delta\Psi)(x,k,\omega) = k^2\Psi(x,k,\omega), \quad x\in\mathbb{R}^3\backslash\Xi \tag{3.26}$$

in the distributional sense as well as pointwise, $\Psi_{\theta,\Xi}(k\omega,x)$, $k\in\mathbb{R}$, $\det(P_{\theta,\Xi}(k^2)) \neq 0$, $\omega\in S^2$, $x\in\mathbb{R}^3\backslash\Xi$, represent the generalized eigenfunctions, that is, the quantum scattering wave functions associated with $-\Delta_{\theta,\Xi}$.

The corresponding quantum scattering amplitude $A_{\theta,\Xi}(\omega',\omega,k)$ is then computed as follows,

$$\begin{aligned} A_{\theta,\Xi}(\omega',\omega,k) &= \lim_{\substack{|x|\to\infty \\ |x|^{-1}x=\omega'}} |x| e^{-ik|x|} \big[\Psi_{\theta,\Xi}(x,k,\omega) - e^{ik\omega\cdot x}\big] \\ &= (4\pi)^{-1} \sum_{j,j'=1}^{n} P_{\theta,\Xi}(k^2)_{j,j'} e^{ik(\omega\cdot\xi_{j'} - \omega'\cdot\xi_j)}, \\ &\qquad k\in\mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0,\ \omega,\omega'\in S^2. \end{aligned} \tag{3.27}$$

The corresponding scattering matrix $S_{\theta,\Xi}(k)$ in $L^2(S^2)$ is then given by

$$S_{\theta,\Xi}(k) = I + \frac{ik}{8\pi^2} \sum_{j,j'=1}^{n} P_{\theta,\Xi}(k^2)_{j,j'} \left(e^{-ik\xi_{j'}\cdot(\cdot)}, \cdot\right) e^{-ik\xi_j\cdot(\cdot)}, \quad k \in \mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0. \tag{3.28}$$

Remark 3.4. Since $S_{\theta,\Xi}(k)$ is unitary in $L^2(S^2)$ (this either follows from abstract methods since $-\Delta$ and $-\Delta_{\theta,\Xi}$ are self-adjoint and the second term on the right-hand side of (3.18) is of rank n and hence a trace class operator, or directly from (3.19) and (3.28)), the scattering amplitude $A_{\theta,\Xi}(\omega', \omega, k)$ (the integral kernel of $S_{\theta,\Xi}(k) - I$) automatically satisfies the (generalized) *optical theorem*, that is,

$$\mathrm{Im}(A_{\theta,\Xi}(\omega', \omega, k)) = (4\pi)^{-1} k \int_{S^2} d\omega''\, A_{\theta,\Xi}(\omega'', \omega, k) \overline{A_{\theta,\Xi}(\omega'', \omega', k)}, \quad k \in \mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0,\ \omega, \omega' \in S^2. \tag{3.29}$$

On the other hand, *reciprocity* of the scattering amplitude $A_{\theta,\Xi}(\omega', \omega, k)$, defined by

$$A_{\theta,\Xi}(\omega', \omega, k) = A_{\theta,\Xi}(-\omega, -\omega', k), \quad k \in \mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0,\ \omega, \omega' \in S^2 \tag{3.30}$$

is satisfied if and only if

$$\theta^t = \theta, \tag{3.31}$$

where T^t denotes the transpose of the matrix T. Together with the requirement of self-adjointness of θ, $\theta^* = \theta$, this yields an $n(n+1)/2$ (real) parameter family of operators $-\Delta_{\theta,\Xi}$ satisfying $\theta = \theta^* = \theta^t$. (The number of real elements above and on the diagonal of θ equals $\sum_{j=1}^n j = n(n+1)/2$.)

Similarly, the *reality* constraint on $A_{\theta,\Xi}(\omega', \omega, k)$, that is, the requirement

$$\overline{A_{\theta,\Xi}(\omega', \omega, k)} = A_{\theta,\Xi}(\omega', \omega, -k), \quad k \in \mathbb{R},\ \det(P_{\theta,\Xi}(k^2)) \neq 0,\ \omega, \omega' \in S^2 \tag{3.32}$$

is satisfied if and only if θ is a real matrix,

$$\theta_{j,j'} = \overline{\theta_{j,j'}}, \quad 1 \leq j, j' \leq n. \tag{3.33}$$

Together with self-adjointness of θ this again results in $\theta = \theta^* = \theta^t$ and hence is equivalent to the reciprocity requirement. (For background material on properties of the scattering amplitude, such as the optical theorem, reciprocity, and reality, we refer to [10, Sect. I.4] for obstacle scattering and [13, Sect. 3.6] in the context of potential scattering.)

It is interesting to observe that these natural requirements on the scattering amplitude, such as the optical theorem, reciprocity, and reality, are satisfied for an $n(n+1)/2$-parameter family of generalized point interactions (though, not for the full n^2-parameter family) and hence for a larger family than the usually considered n-parameter family of (local) point interactions $-\Delta_{\underline{\alpha},\Xi}$.

We conclude this section with the following remark on space dimensions other than three (the interested reader can find many more details in [3]).

Remark 3.5. All results of this section immediately extend to the case of two space dimensions replacing the Green's function (3.4) of the three-dimensional Laplacian by the corresponding two-dimensional Green's function

$$G_0(z, x-y) = (-\Delta - z)^{-1}(x, y) = (i/4) H_0^{(1)}(z^{1/2}|x-y|), \tag{3.34}$$

$$\mathrm{Im}(z^{1/2}) > 0,\ x, y \in \mathbb{R}^2,\ x \neq y.$$

Here $H_0^{(1)}(\cdot)$ denotes the Hankel function of order zero and first kind (cf. [1, Sect. 9.1]). There are only minor changes required in (3.10), (3.11), and (3.12) due to the $\ln(z)$-behavior of (3.34) as $z \to 0$. Analogous results apply to the one-dimensional case using

$$G_0(z, x-y) = (-\Delta - z)^{-1}(x, y) = (i/2) z^{-1/2} e^{iz^{1/2}|x-y|}, \qquad \mathrm{Im}(z^{1/2}) > 0,\ x, y \in \mathbb{R}. \tag{3.35}$$

The one-dimensional case, however, differs from the two and three-dimensional cases since $B = \overline{-\frac{d^2}{dx^2}\big|_{C_0^\infty(\mathbb{R}\setminus\{\xi_1,\dots,\xi_n\})}}$ now has deficiency indices $(2n, 2n)$ (as opposed to (n, n) in two and three dimensions, cf. (3.3)). Consequently, B admits a $4n^2$ (real) parameter family of self-adjoint extensions and hence additional types of (generalized) point interactions in dimension one. The proper definition of A with

$$\ker(A^* - z) = \mathrm{span}\{G_0(z, \cdot - \xi_j)\}_{1\leq j\leq n} \tag{3.36}$$

in one dimension is given by

$$A = -\frac{d^2}{dx^2}, \quad \mathrm{dom}(A) = \{g \in H^{2,2}(\mathbb{R}) \,|\, g(\xi_j) = 0,\ 1 \leq j \leq n\}. \tag{3.37}$$

Finally, since

$$\overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^d\setminus\{\xi_1,\dots,\xi_n\})}} = -\Delta\big|_{H^{2,2}(\mathbb{R}^d)} \text{ for } d \geq 4 \tag{3.38}$$

(i.e., $-\Delta\big|_{C_0^\infty(\mathbb{R}^d\setminus\{\xi_1,\dots,\xi_n\})}$ is essentially self-adjoint for $d \geq 4$), there are no (generalized) point interactions in four dimensions or higher.

4. A Uniqueness Result

Given the preparations in Section 3, the principal purpose of our final Section 4 is to provide a solution of the inverse problem IP 1.2 formulated in Section 1. More precisely, we will prove the following uniqueness result (we freely use the notation established in Sections 1–3 throughout this section).

Theorem 4.1. *Let $k_0 > 0$ and assume that $\det(P_{\theta,\Xi}(k_0^2)) \neq 0$. Then the data $\{G_{\theta,\Xi}(k_0^2, x, y)\}_{\substack{x,y\in P\\ x\neq y}}$ uniquely determine $\Xi = \{\xi_1, \dots, \xi_n\} \subset \mathbb{R}^3_-$ and the self-adjoint $n \times n$ matrix θ in $\mathbb{C}^n$.*

Proof. Given the data $G_{\theta,\Xi}(k_0^2, x, y)$ for all $x, y \in P$, $x \neq y$, $\det(P_{\theta,\Xi}(k_0^2)) \neq 0$, the Poisson-type formula,

$$\begin{aligned} w(s, y) = \int_P d^2\sigma\, G_{\theta,\Xi}(k_0^2, (\sigma, 0), y) \frac{\partial}{\partial \sigma_3} \big[&G_0(k_0^2, (\sigma, \sigma_3) - s) \\ &- G_0(k_0^2, (\sigma, -\sigma_3) - s)\big]\big|_{\sigma_3 = 0}, \\ &s \in \mathbb{R}^3_+,\ y \in P \end{aligned} \tag{4.1}$$

(here $\sigma = (\sigma_1, \sigma_2) \in \mathbb{R}^2$) yields the solution of the problem

$$\begin{cases} (-\nabla_x^2 - k_0^2) w(x,y) = 0, \quad x \in \mathbb{R}^3_+, \\ \lim_{|x|\to\infty} |x| \big[\frac{\partial}{\partial |x|} w(x,y) - ik_0 w(x,y)\big] = 0 \text{ uniformly in directions } \omega = |x|^{-1}x \\ \qquad\qquad\qquad \text{and uniformly in } y \text{ for } y \text{ varying in compact sets,} \\ w(x,y)\big|_{x_3=0} = G_{\theta,\Xi}(k_0^2, x, y) \end{cases} \tag{4.2}$$

for each fixed $y \in P$. In particular, $w(x,y)$ in (4.1) represents

$$G_{\theta,\Xi}(k_0^2, x, y) \text{ for all } x \in \mathbb{R}^3_+ \cup P,\ y \in P,\ x \neq y. \tag{4.3}$$

By symmetry of the Green's function $G_{\theta,\Xi}(k_0^2, x, y)$ with respect to x and y,

$$G_{\theta,\Xi}(k_0^2, x, y) = G_{\theta,\Xi}(k_0^2, y, x), \quad x, y \in \mathbb{R}^3,\ x \neq y, \tag{4.4}$$

we also determined

$$G_{\theta,\Xi}(k_0^2, x, y) \text{ for all } x \in P,\ y \in \mathbb{R}^3_+ \cup P,\ x \neq y. \tag{4.5}$$

Moreover, using $G_{\theta,\Xi}(k_0^2, (\sigma, 0), y)$ with $y \in \mathbb{R}^3_+ \cup P$ (instead of $y \in P$) in (4.1) then determines

$$G_{\theta,\Xi}(k_0^2, x, y) \text{ for all } x, y \in \mathbb{R}^3_+ \cup P,\ x \neq y. \tag{4.6}$$

In other words, we managed to lift the data from P to $\mathbb{R}^3_+ \cup P$.

Next, the explicit formula (3.18) for $(-\Delta_{\theta,\Xi} - z)^{-1}$ yields

$$G_{\theta,\Xi}(z, x, y) = G_0(z, x, y) + \sum_{j,j'=1}^{n} P_{\theta,\Xi}(z)_{j,j'} G_0(z, x - \xi_j) G_)(z, y - \xi_{j'}), \tag{4.7}$$
$$\det(P_{\theta,\Xi}(z)) \neq 0,\ x, y \in \mathbb{R}^3 \backslash \Xi,\ x \neq y,$$

with $P_{\theta,\Xi}(z)$ defined in (3.19). Hence one concludes

$$(-\nabla_x^2 - z) G_{\theta,\Xi}(z, x, y) = 0, \quad x, y \in \mathbb{R}^3 \backslash \Xi,\ x \neq y. \tag{4.8}$$

Thus, the data $\{G_{\theta,\Xi}(k_0^2, x, y)\}_{\substack{x,y \in P \\ x \neq y}}$, $\det(P_{\theta,\Xi}(k_0^2)) \neq 0$ uniquely determine

$$G_{\theta,\Xi}(k_0^2, x, y) \text{ for all } x, y \in \mathbb{R}^3 \backslash \Xi,\ x \neq y \tag{4.9}$$

by the unique continuation property [9, Sect. 17.2] applied to (4.8). The singularity structure of (4.7) then determines $\xi_1, \dots, \xi_n$ and hence Ξ. Similarly, taking $x \to \xi_j$ and $y \to \xi_{j'}$ independently, determines $P_{\theta,\Xi}(k_0^2)_{j,j'}$, $1 \leq j, j' \leq n$, and hence θ. Thus, Theorem 4.1 is proved. ☐

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Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: fritz@math.missouri.edu
URL: http://www.math.missouri.edu/people/fgesztesy.html

Department of Mathematics, Kansas State University, Manhattan, KS 66506-2602, USA
E-mail address: ramm@math.ksu.edu