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s-POINTS IN THREE-DIMENSIONAL ACOUSTICAL SCATTERING*

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Abstract. The notion of s-points was introduced by the authors in [*SIAM J. Math. Anal.*, 39 (2008), pp. 1821–1850] in connection with the control problem for the dynamical system governed by the three-dimensional acoustical equation $u_{tt}-\Delta u+qu=0$ with a real potential $q\in C_0^\infty(\mathbb{R}^3)$ and controlled by incoming spherical waves. In the generic case, this system is controllable in the relevant sense, whereas $a\in\mathbb{R}^3$ is called an *s-point* (we write $a\in\Upsilon_q$) if the system with the shifted potential $q_a=q(\,\cdot-a)$ *is not controllable*. Such a lack of controllability is related to the subtle physical effect: in the system with the potential q_a, there exist the finite energy waves vanishing in the past and future cones simultaneously. The subject of this paper is the set Υ_q: we reveal its relation to the factorization of the S-matrix, connections with the discrete spectrum of the Schrödinger operator $-\Delta+q$, and the jet degeneration of the polynomially growing solutions to the equation $(-\Delta+q)p=0$.

Key words. three-dimensional acoustical equation, time domain scattering problem, reversing waves, stop-points, R. Newton's factorization, discrete spectrum

AMS subject classifications. 35Bxx, 35Lxx, 35P25, 47Axx

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0. Introduction.

0.1. Dynamical system. An acoustical scattering problem is the system of the form

$$u_{tt}-\Delta u+qu=0, \qquad (x,t)\in\mathbb{R}^3\times(-\infty,\infty), \tag{0.1}$$

$$u\,|_{|x|<-t}=0, \qquad t<0, \tag{0.2}$$

$$\lim_{s\to\infty} su((s+\tau)\omega,-s)=f(\tau,\omega), \qquad (\tau,\omega)\in[0,\infty)\times S^2\,, \tag{0.3}$$

where $u=u^f(x,t)$ is a solution (*wave*), $q=q(x)$ is a real valued smooth[1] compactly supported function (*potential*), and $f\in\mathcal{F}:=L_2\left([0,\infty);L_2\left(S^2\right)\right)$ is a *control*. With the system one associates the *control operators* $W:\mathcal{F}\to\mathcal{H}:=L_2(\mathbb{R}^3)$, $Wf:=u^f(\,\cdot\,,0)$ and the subspaces $\mathcal{U}:=\operatorname{Ran}W$ (*reachable set*), $\mathcal{D}:=\mathcal{H}\ominus\mathcal{U}$ (*defect subspace*), $\mathcal{N}:=\operatorname{Ker}W\subset\mathcal{F}$ (*null control subspace*). The relations $0\le\dim\mathcal{D}=\dim\mathcal{N}<\infty$ hold [2]. If $\mathcal{D}=\{0\}$, then the system (0.1)–(0.3) is said to be controllable;[2] the case of $\mathcal{D}\ne\{0\}$ is referred to as a lack of controllability.

0.2. *s*-points. As is shown in [2], the case $\dim\mathcal{D}\ne0$ is realizable and corresponds to the curious effect that for $f\in\mathcal{N}$, the function $w^f(x,t):=\int_0^t u^f(x,s)\,ds$ is a finite energy solution of (0.1), which satisfies $w^f(\,\cdot\,,-t)=w^f(\,\cdot\,,t)$ and

$$w^f\,|_{|x|<|t|}=\,0\,, \tag{0.4}$$

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[1]Throughout the paper, "smooth" means C^∞-smooth.
[2]Note that the unperturbed system (with $q=0$) is controllable.

i.e., it describes the wave vanishing in the past and future cones simultaneously. This wave comes from infinity, stops at the moment $t = 0$,[3] and then returns to infinity along the same trajectory. Such a behavior motivates us to call it a *reversing wave* and to regard the coordinate system origin $x = 0$ as a point that is able to stop incoming waves ("stop point"). Looking for such points in the space, we change the coordinates $x \mapsto x - a$ and deal with the system (0.1)–(0.3) with the shifted potential $q_a := q(x-a)$, the objects corresponding to q_a being labelled with the subscript a. An $a \in \mathbb{R}^3$ is said to be an *s-point of the potential* q if $\mathcal{D}_a \neq \{0\}$ holds. By Υ_q we denote the set of such points.

To the best of our knowledge, s-points are something new in acoustical scattering, and the set Υ_q is worth studying for its own sake. The goal of our paper is to originate such a study: we reveal certain relations between Υ_q and the known objects of the scattering theory.

0.3. Results. Evolution of the system (0.1)–(0.3) is governed by the Schrödinger operator $H := -\Delta + q$ in $\mathcal{H}$, $\operatorname{Dom} H = H^2(\mathbb{R}^3)$. This operator may have a finite discrete spectrum $\sigma_{\rm disc}(H) \subset (-\infty, 0]$ (see, e.g., [8]) and in this paper, for the sake of simplicity, we accept the following assumption.

Assumption 1. *The potential q is such that the equation*

$$(-\Delta + q)\,\varphi = 0 \qquad \text{in } \mathbb{R}^3 \tag{0.5}$$

has no nonzero solutions, which satisfy $\varphi(x) \to 0$ as $|x| \to 0$.

In physical terms, this means that the Hamiltonian H has neither a bound nor a semibound state at the zero energy level (see, e.g., [7]). If it exists, such a level can be removed by an arbitrarily small perturbation of the potential q, so that the assumption is not restrictive and we deal with a generic case.

Our results are the following.

- Let $S_a(k)$, $k \in \mathbb{R}$, be the Schrödinger S-matrix of the potential q_a. In the series of papers cited in his book [7], R. Newton introduced the Riemann–Hilbert factorization of the form

  $$S_a(k) = \Pi_a^-(k)\left[S_a^-(k) S_a^+(k)\right]\Pi_a^+(k)\,, \quad k \in \mathbb{R}\,, \tag{0.6}$$

  where $\Pi_a^\pm$ are the Blaschke-type rational operator-valued functions and $S_a^\pm$ are the operator-valued functions that are holomorphic and boundedly invertible in the half-planes $\{k \in \mathbb{C} \mid \pm\Im k > 0\}$, respectively. This representation is used for solving the inverse problem that determines the potential q from the scattering data: it is shown that knowledge of the family $\{S_a^\pm\}_{a\in\mathbb{R}^3}$ enables one to recover q. In the meantime, in the aforementioned papers it is assumed that such a factorization is realizable for any $a \in \mathbb{R}^3$. *We show that for $a \in \Upsilon_q$, the representation* (0.6) *fails; i.e., the factorization is impossible.*[4]
- In [2] we suggested that the presence of s-points is connected with the discrete spectrum of the operator H: the conjecture was that $\Upsilon_q \neq \emptyset$ is equivalent to $\sigma_{\rm disc}(H) \neq \emptyset$. Here this conjecture is partially justified as follows.

  Let a point $a \in \mathbb{R}^3$, an integer $m \geq 1$, and a function $h \in \mathcal{H}$ be such that

  $$(-\Delta + q)^m\, h = 0 \qquad \text{in } \mathbb{R}^3 \setminus \{a\} \tag{0.7}$$

[3] We mean $w_t^f(\,\cdot\,, 0) = 0$.

[4] However, we do not claim that this fact cancels the determination of the potential by R. Newton's procedure.

holds, whereas $(-\Delta + q)^{m-1}h$ does not vanish identically. As is shown in [2] (see the proof of Theorem 1, the relation (3.1)), such an a is necessarily an s-point; by $\Upsilon_q^m \subset \Upsilon_q$ we denote the set of these points and specify m as the order of a. *We prove that* $\Upsilon_q^1 \neq \emptyset$ *is equivalent to* $\sigma_{\rm disc}(H) \neq \emptyset$.

- We show that the points $a \in \Upsilon_q^{\rm fin} := \cup_{m\geq 1}\Upsilon_q^m$[5] can be specified as the *jet degeneration points of polynomially growing solutions* to the equations $(-\Delta + q)\, p = 0$ in $\mathbb{R}^3$. By this, typically, the set $\Upsilon_q^{\rm fin}$ consists of s-surfaces. If the potential is radially symmetric, i.e., $q = q(|x|)$, the s-surfaces are spheres, and their position in the space can be studied in more detail.

1. s-points and R. Newton's factorization.

1.1. Scattering matrix. We begin with a few words on history. In L. Faddeev's approach to the three-dimensional inverse quantum scattering problem, there is a certain difficulty related to the so-called *exceptional points* on the spectral parameter complex plane connected with the discrete spectrum of the Schrödinger operator. The presence of these points complicates the procedure of solving the inverse problem.[6] These complications were one of the reasons that motivated R. Newton to elaborate on another approach that makes use of the Riemann–Hilbert factorization of the S-matrix (for the arbitrary choice of the coordinate system origin). However, R. Newton's scheme is based on the assumption that the S-matrix can be factorized for *any choice of origin.*

In this paper we show that this assumption is not valid: if the discrete spectrum does occur, then there is a set of space points in which the factorization by R. Newton is impossible. Moreover, it is shown that this set coincides with the set of s-points introduced in [2] in the framework of the acoustical scattering problem. The physical meaning of s-points is quite transparent: they are connected with a lack of controllability of the hyperbolic dynamical system governed by the acoustical equation.

We regard our work as a step toward solving the three-dimensional acoustical scattering inverse problem by the BC-method. The method is based upon the controllability properties of the acoustical system, and the study of such properties (and in particular, the effects related to s-points) is helpful and unavoidable.

We now recall the basic definitions and facts (see, e.g., [7]).

The Schrödinger *scattering operator* of the pair $H_0 = -\Delta$, $H = -\Delta + q$ is $S : \mathcal{H} \to \mathcal{H}$, $S := W_+^* W_-$, where $W_\pm := \lim_{t\to\pm\infty} e^{-itH}e^{itH_0}$ are the *wave operators.* Let $(Fy)\,(p) = (2\pi)^{-\frac{3}{2}} \int_{\mathbb{R}^3} e^{ipx}y(x)\,dx$ be the Fourier transform. The operator $\tilde{S} := FSF^{-1}$ is of the form

$$\left(\widetilde{S}v\right)(p) = \left(S(k)\,[v(k,\,\cdot\,)]\right)(\theta)\,,$$

where $v(k,\omega) := v(k\omega)$, $k := |p|$, $\theta := \frac{p}{|p|}$, $\omega, \theta \in S^2 := \{p \in \mathbb{R}^3 \mid |p| = 1\}$, whereas $S(k)$ is an operator acting in $L_2(S^2)$ on the angle variable by the rule

$$\left(S(k)\,g\right)(\theta) := \int_{S^2} s(\theta,\omega;k) g(\omega)\,d\omega\,,$$

dependent on k as a parameter and called the *S-matrix* of the potential q. So, we regard the S-matrix as an operator-valued function of $k > 0$, with the values taken

[5]Presumably, $\Upsilon_q^{\rm fin}$ exhausts Υ_q but it is still a conjecture.

[6]To the best of our knowledge, the physical meaning of the exceptional points is so far not clear.

in the bounded operator algebra $\mathcal{B}\left(L_2(S^2)\right)$. The kernel $s(\theta,\omega;k)$ is a distribution of the form $\delta(\theta-\omega)+\widetilde{s}(\theta,\omega;k)$ with a smooth $\widetilde{s}$, so that each $S(k)$ is of the form "identity + compact operator." Moreover, each $S(k)$ is a unitary operator. Also, the well-known high energy asymptotic $S(k)\to\mathbb{I}$ as $k\to\infty$ holds.

In what follows, we assume $S(k)$ extended to $k<0$ by $S(k):=S^*(-k)$. The index of the S-matrix is defined by

$$\operatorname{ind}S := \frac{1}{4\pi i}\left[\ln\det S(k)\right]\Big|_{k=-\infty}^{k=+\infty};$$

by the Levinson theorem it is equal to the total multiplicity of the discrete spectrum $\sigma_{\rm disc}(H)$. The representation

$$S(k)=\Pi^-(k)\,S^{\rm red}(k)\,\Pi^+(k)\,,\qquad k\in\mathbb{R}, \tag{1.1}$$

is valid, where $S^{\rm red}$ is the so-called *reduced S-matrix*, which satisfies $\operatorname{ind}S^{\rm red}=0$, and Π is a $\mathcal{B}\left(L_2(S^2)\right)$-valued function of the form

$$\Pi^{\pm}(k)=\prod_{n=1}^{l}\left(\mathbb{I}+\frac{2ik}{k-ik_n}\,B_n^{\pm}\right),\qquad k\in\mathbb{R},$$

with the certain projections $B_n^{\pm}=(\,\cdot\,,\psi_n^{\pm})_{L_2(S^2)}\,\psi_n^{\pm}$, where $\psi^+(\omega)=\psi^-(-\omega)$, and $k_n>0$ such that $-k_n^2\in\sigma_{\rm disc}(H)$ (see [7]).

1.2. Factorization by R. Newton. In solving the scattering inverse problem by R. Newton, the following Riemann–Hilbert-type representation of the reduced S-matrix plays a key role:

$$S^{\rm red}(k)=S^-(k)S^+(k)\,,\qquad k\in\mathbb{R}\,, \tag{1.2}$$

where $S^{\pm}$ are the $\mathcal{B}\left(L_2(S^2)\right)$-valued operator functions, which are holomorphic, bounded, and boundedly invertible, respectively, in the complex half-planes $\mathbb{C}^{\pm}=\{k\in\mathbb{C}\mid\pm\Im k>0\}$. More specifically, to recover the potential q via its S-matrix, one needs

- to find, for a fixed $a\in\mathbb{R}^3$, the S-matrix S_a of the shifted potential q_a that can be done in a simple and explicit way;
- to determine ${S^{\rm red}}_a$ from (1.1) and represent ${S^{\rm red}}_a=S_a^-S_a^+$ by (1.2);
- to collect the families $\{S_a^{\pm}\}_{a\in\mathbb{R}^3}$ by varying a; each family determines the potential q.

However, in [6], [7], the author assumes that the second step can be fulfilled *for all* $a\in\mathbb{R}^3$. The following result shows that such an assumption may be invalid.

THEOREM 1. *If $a\in\Upsilon_q$, then representation* (1.2) *for ${S^{\rm red}}_a$ does not hold; i.e., the factorization ${S^{\rm red}}_a=S_a^-S_a^+$ is impossible.*

We postpone the proof until section 1.4 and begin with preliminaries concerning the well-known facts of the Lax–Phillips theory.

1.3. On the Lax–Phillips scheme. The Cauchy problem for the acoustical equation is the system

$$v_{tt}-\Delta v+qv=0,\qquad (x,t)\in\mathbb{R}^3\times(-\infty,\infty), \tag{1.3}$$

$$v\mid_{t=0}=\varphi,\quad v_t\mid_{t=0}=\psi\qquad \text{in }\mathbb{R}^3 \tag{1.4}$$

with the finite energy data $d := \{\varphi, \psi\} \in D := H^1(\mathbb{R}^3) \times L_2(\mathbb{R}^3)$; the solution is denoted by $v = v^d(x,t)$. A peculiarity of the acoustical scattering is that the *energy form*

$$E[d, d'] := \int_{\mathbb{R}^3} \psi\psi' + \nabla\varphi \cdot \nabla\varphi' + q\varphi\varphi' \,,$$

with which the set of data is equipped, is indefinite. However, the form turns out to be positive definite on the *absolutely continuous subspace* $D_{\rm ac} := D \ominus_E D_{\rm disc}$, where $D_{\rm disc}$ is the finite dimensional subspace spanned on the data $\{\varphi_k, \pm k\varphi_k\}$ such that $-k^2 \in \sigma_{\rm disc}(H)$ and $H\varphi_k = -k^2\varphi_k$. By $P_{\rm ac}$ we denote the projection on the first summand of the decomposition $D = D_{\rm ac} \oplus_E D_{\rm disc}$.

In the framework of the Lax–Phillips theory [5], there is a certain freedom in the choice of the pair of the *incoming* and *outgoing subspaces* $D^{\pm}$. Once such a choice is made, for each $d \in D$, the corresponding *incoming* and *outgoing spectral representatives* $\widetilde{d}_{\mp}$, which are the S^2-valued functions of $k \in \mathbb{R}$ of the class $L_2\left(\mathbb{R}; L_2(S^2)\right)$, do appear. In the spectral representation, the scattering process is described by the *Lax–Phillips scattering operator* $\widetilde{S} : \widetilde{d}_- \mapsto \widetilde{d}_+$, which acts in $L_2\left(\mathbb{R}; L_2(S^2)\right)$ by

$$\left(\widetilde{S}g\right)(k) \;=\; \widetilde{S}(k)g(k)\,, \qquad k \in \mathbb{R}\,,$$

where $\widetilde{S}(\,\cdot\,)$ is a $\mathcal{B}\left(L_2(S^2)\right)$-valued operator function (*the Lax–Phillips S-matrix*). Two possible variants of the choice are the following.

1. Assign a $d \in D$ to the subspace $D_0^- \subset D$ if $v^d\mid_{|x|<-t} = 0$ for $t < 0$, and the subspace $D_0^+ \subset D$ if $v^d\mid_{|x|<t} = 0$ for $t > 0$. The subspaces
$$D^{\mp} \;:=\; P_{\rm ac} D_0^{\mp}$$
constitute an incoming/outgoing pair [5]. By $\widetilde{S}$ and $\widetilde{S}(\,\cdot\,)$, we denote the corresponding scattering operator and its S-matrix.
2. One can reduce the incoming/outgoing subspaces to the smaller ones
$$D^{\mp}_{\rm red} \;:=\; D_0^{\mp} \cap D_{\rm ac} \subset D^{\mp}.$$
By $\widetilde{S}^{\rm red}$ and $\widetilde{S}^{\rm red}(\,\cdot\,)$, we denote the corresponding operator and S-matrix.

The important fact, which relates the quantum scattering and acoustical scattering objects and follows from the above accepted definitions, is that the equalities

$$\widetilde{S}(k) \;=\; S(k)\,, \quad \widetilde{S}^{\rm red}(k) = S^{\rm red}(k)\,, \qquad k \in \mathbb{R}, \tag{1.5}$$

hold (see [5, Chapter VI, Part 2, relation (3.4)]). Note in addition that (1.5) and (1.1) imply

$$\widetilde{S}(k) = \Pi^-(k)\,\widetilde{S}^{\rm red}(k)\,\Pi^+(k)\,, \qquad k \in \mathbb{R}\,,$$

whereas the factors $\Pi^{\mp}(\,\cdot\,)$ can also be interpreted in terms of the Lax–Phillips theory as S-matrices corresponding to the certain choice of the incoming/outgoing subspaces.

Let

$$L_2\left(\mathbb{R}; L_2(S^2)\right) \;=\; \mathcal{H}^- \oplus \mathcal{H}^+ \tag{1.6}$$

be the decomposition on the Hardy subspaces $\mathcal{H}^{\mp}$ which consist of functions holomorphic in $\{k \in \mathbb{C} \mid \mp\Im k > 0\}$, respectively; by $P^{\mp}$ we denote the projections on $\mathcal{H}^{\mp}$.

As is known, if d belongs to the incoming (outgoing) subspace, then its spectral representative lies in $\mathcal{H}^-$ ($\mathcal{H}^+$). Representing the scattering operator in the matrix form in accordance with (1.6), one has

$$\widetilde{S}^{\rm red} = \begin{pmatrix} P^-\widetilde{S}^{\rm red}P^- & P^-\widetilde{S}^{\rm red}P^+ \\ \mathcal{P}^+\widetilde{S}^{\rm red}P^- & P^+\widetilde{S}^{\rm red}P^+ \end{pmatrix} . \tag{1.7}$$

1.4. Proof of Theorem 1. Assume that $a \in \mathbb{R}^3$ is an s-point of the potential q. As is evident, by shifting the coordinate system, one can provide $a = 0$. So, let $0 \in \Upsilon_q$.

Let w^f be a reversing wave (see section 0.2) and $d_0 := \{w^f(\,\cdot\,, 0), 0\}$ its Cauchy data. By (0.4), one has $d_0 \in D^- \cap D^+$; moreover, the results [2] on the stability of trajectories easily imply $d_0 \in D^-_{\rm red} \cap D^+_{\rm red}$. The latter leads to $\widetilde{d}_0^- \in \mathcal{H}^-$ and $\widetilde{d}_0^+ \in \mathcal{H}^+$. Therefore,

$$\widetilde{S}^{\rm red}\widetilde{d}_0^- = \widetilde{d}_0^+ \in \mathcal{H}^+$$

and, applying the projection P^-, one gets $P^-\widetilde{S}^{\rm red}\widetilde{d}_0^- = P^-\widetilde{S}^{\rm red}P^-\widetilde{d}_0^- = 0$. Thus, we see that $\operatorname{Ker} P^-\widetilde{S}^{\rm red}P^- \neq \{0\}$; i.e., the block $P^-\widetilde{S}^{\rm red}P^-$ in (1.7) is not invertible.

By (1.5), the block $P^-S^{\rm red}P^-$ is also not invertible. However, as is well known, such an invertibility is the necessary condition that provides the Riemann–Hilbert factorization (1.2) (see, e.g., [7]). Hence, in the case of $a \in \Upsilon_q$, to represent ${S^{\rm red}}_a$ in the form (1.2) is impossible. $\square$

In addition, note the following. Although representation (1.2) fails for $a \in \Upsilon_q$, by very general results of the Riemann–Hilbert theory one can factorize the reduced S-matrix as

$${S^{\rm red}}_a(k) = \check{\Pi}_a^-(k)\left[\check{S}_a^-(k)\check{S}_a^+(k)\right]\check{\Pi}_a^+(k)\,, \qquad k \in \mathbb{R}, \tag{1.8}$$

with the Blaschke-type operator functions $\check{\Pi}_a, \check{\Pi}_a^*$, which have the certain complex poles, and $\check{S}_a^\pm$ are holomorphic and boundedly invertible in $\{k \in \mathbb{C} \mid \pm\Im k > 0\}$ [3]. Moreover, it is the presence of the Blaschke factors that renders representation (1.2) impossible. In this connection, intriguing questions arise: What is the physical meaning of the factorization (1.8) and the corresponding Blaschke poles? Can one characterize them in terms of the Lax–Phillips theory? These questions remain open.

2. s-points and the discrete spectrum.

2.1. Theorem 2. Assume that for a point $a \in \mathbb{R}^3$ there exist a function $h \in \mathcal{H}$ and an integer $k \geq 1$ such that

$$(-\Delta + q)^k\, h = 0 \qquad \text{in } \mathbb{R}^3 \setminus \{a\},$$

and let m be the minimal of such k's. As is shown in [2], this a is necessarily an s-point, whereas m is specified as the order of a. By $\Upsilon_q^m \subset \Upsilon_q$, we denote the set of s-points of the order m.

Remark. In light of these definitions, Assumption 1 is motivated as follows. If $0 \in \sigma_{\rm disc}(H)$ and $\varphi_0 \in \mathcal{H}$ is a zero energy level eigenfunction, then $(-\Delta + q)\,\varphi_0 = 0$ *everywhere* in $\mathbb{R}^3$, and we are forced to accept $\Upsilon_q^1 = \Upsilon_q = \mathbb{R}^3$. The assumption excludes such a degeneration.

The following result partially explains why s-points do appear; one of the reasons is the presence of the discrete spectrum of the operator H.

THEOREM 2. *$\Upsilon_q^1 \neq \emptyset$ holds if and only if $\sigma_{\rm disc}(H) \neq \emptyset$.*

The rest of section 2 provides the proof of the theorem.

2.2. Green function. We define the *Green function* of the operator H as an $L_2^{\rm loc}(\mathbb{R}^3)$-solution of the integral equation

$$G(x,y) = \frac{1}{4\pi|x-y|} - \int_{\mathbb{R}^3} \frac{q(s)}{4\pi|x-s|}\, G(s,y)\, ds\,, \qquad x \in \mathbb{R}^3\,, \tag{2.1}$$

where $y \in \mathbb{R}^3$ is a parameter. This definition is correct since this equation is uniquely solvable. Indeed, otherwise, there is a nonzero solution φ of the homogeneous equation

$$\varphi(x) = -\int_{\mathbb{R}^3} \frac{\varphi(s)}{4\pi|x-s|}\, q(s)\, ds\,, \qquad x \in \mathbb{R}^3\,.$$

As is easy to see, such a solution satisfies (0.5) and vanishes at infinity, which is forbidden by Assumption 1. To establish the solvability, one can reduce the equation to a large enough ball $B \supset \operatorname{supp} q$, prove the solvability there, and then extend the solution to $\mathbb{R}^3 \backslash B$ as a right-hand side (r.h.s.) of (2.1).

Also, the integral equation implies the symmetry property $G(x,y) = G(y,x)$, $x \neq y$. From (2.1) one derives that in the sense of distributions on $C_0^\infty(\mathbb{R}^3)$ the function G satisfies

$$(-\Delta + q)\, G(\,\cdot\,, y) = \delta_y\,, \tag{2.2}$$

where δ_y is the Dirac measure supported in y.

LEMMA 1. *The asymptotic*

$$G(x,y) \underset{|x|\to\infty}{=} \frac{\Phi(y)}{4\pi|x|} + O\left(\frac{1}{|x|^2}\right), \qquad y \in \mathbb{R}^3, \tag{2.3}$$

holds, where Φ is a smooth function obeying

$$(-\Delta + q)\, \Phi = 0 \qquad \text{in } \mathbb{R}^3, \tag{2.4}$$

$$\Phi(x) \to 1 \quad \text{as } |x| \to \infty \tag{2.5}$$

with the asymptotics (2.3) *and* (2.5) *uniform w.r.t.* $\frac{x}{|x|} \in S^2$.

Proof. Fix x in (2.1) and let $|y| \to \infty$. Using the symmetry property and looking for the solution in the form (2.3), we have

$$\frac{\Phi(x)}{4\pi|y|} + O\left(\frac{1}{|y|^2}\right) = \frac{1}{4\pi|y|} + O\left(\frac{1}{|y|^2}\right) - \int_{\mathbb{R}^3} \frac{q(s)}{4\pi|x-s|} \left[\frac{\Phi(s)}{4\pi|y|} + O\left(\frac{1}{|y|^2}\right)\right] ds,$$

which easily leads to the integral equation

$$\Phi(x) = 1 - \int_{\mathbb{R}^3} \frac{q(s)}{4\pi|x-s|}\, \Phi(s)\, ds\,, \qquad x \in \mathbb{R}^3\,. \tag{2.6}$$

The latter equation implies (2.4) and (2.5), and justifies (2.3). ◻

Now we are ready to prove Theorem 2.

2.3. Necessity. Let $\sigma_{\rm disc}(H) \neq \emptyset$ and $H\chi = -k_0^2\chi$ for $-k_0^2 = \inf \sigma_{\rm disc}(H)$, so that χ is a ground state of the operator H. As is well known, $-k_0^2$ is an ordinary eigenvalue of H, whereas the eigenfunction χ behaves as $\chi(x) \sim_{|x|\to\infty} e^{-k_0|x|}$ and can be chosen positive: $\chi > 0$ *everywhere* in $\mathbb{R}^3$. Integrating by parts, we have

$$0 = (\text{see } (2.4)) = \int_{\mathbb{R}^3} \chi(x)\,[(-\Delta + q)\,\Phi]\,(x)\,dx = -k_0^2 \int_{\mathbb{R}^3} \chi(x)\Phi(x)\,dx\,.$$

Hence, Φ has to change sign, and there is an $a \in \mathbb{R}^3$ such that $\Phi(a) = 0$. As a result, we conclude that $G(\,\cdot\,, a) \in \mathcal{H}$ (see (2.3)), whereas $(-\Delta + q)\,G(\,\cdot\,, a) = 0$ in $\mathbb{R}^3 \setminus \{a\}$ (see (2.2)). Thus $a \in \Upsilon_q^1$ and hence $\Upsilon_q^1 \neq \emptyset$.

2.4. Sufficiency. The sufficiency will be proved by contradiction. Assume that $\sigma_{\rm disc}(H) = \emptyset$ but $\Upsilon_q^1 \neq \emptyset$; hence there is a point $a \in \mathbb{R}^3$ and a function $h \in \mathcal{H}$ such that $(-\Delta + q)\,h = 0$ holds in $\mathbb{R}^3 \setminus \{a\}$.

Show that $\Phi(a) = 0$. Indeed, considering $(-\Delta+q)\,h$ as a distribution on $C_0^\infty\left(\mathbb{R}^3\right)$, we see that it is supported at $x = a$. Such a distribution has to be a linear combination of the Dirac measure derivatives:

$$(-\Delta + q)\,h = \sum_{|j|=0}^{N} \alpha_j D_x^j \delta_a = \sum_{|j|=0}^{N} \alpha_j (-1)^{|j|} D_a^j \delta_a\,,$$

where $j = \{j_1, j_2, j_3\}$ is a multi-index, $|j| = j_1 + j_2 + j_3$, $D_x^j = \partial_{x^1}^{j_1}\partial_{x^2}^{j_2}\partial_{x^3}^{j_3}$ is a differentiation, and α_j are constants (see, e.g., [9]). Therefore, by (2.2), the function h has to be of the form

$$h(x) = \sum_{|j|=0}^{N} \alpha_j (-1)^{|j|} D_a^j G(x, a) + \widetilde{h}(x)\,, \tag{2.7}$$

with an $\widetilde{h}$ satisfying $-(\Delta + q)\widetilde{h} = 0$ as a distribution. Hence, $\widetilde{h}$ is a smooth function, and

$$-(\Delta + q)\widetilde{h} = 0 \qquad \text{in } \mathbb{R}^3 \tag{2.8}$$

holds in the classical sense. As can be shown from (2.1), for $|j| \geq 1$ the derivatives $D_a^j G(\,\cdot\,, a)$ are not square-summable near $x = a$. Therefore, the only option for the sum in (2.7) (and, hence, for h) to belong to $\mathcal{H}$ (to be square-summable near $x = a$) is $\alpha_j = 0$ for $|j| \geq 1$, and we get

$$h(x) = \alpha_0 G(x, a) + \widetilde{h}(x) \qquad \text{in } \mathbb{R}^3\backslash\{0\}.$$

For large enough $|x| > \operatorname{diam}\operatorname{supp} q$, we have $\Delta h = 0$, and we know that $h \in \mathcal{H}$. Such a function vanishes as $|x| \to \infty$. Hence, by (2.3), the function $\widetilde{h}$ also tends to zero as $|x| \to \infty$ and, at the same time, satisfies (2.8). By Assumption 1, one has $\widetilde{h} = 0$. Thus, h is proportional to the Green function $G(\,\cdot\,, a)$, whereas $G(\,\cdot\,, a) \in \mathcal{H}$ implies $\Phi(a) = 0$ by (2.3).

Now we apply the perturbation theory arguments. Consider an operator family $\{-\Delta + \varepsilon q\}_{\varepsilon\in[0,1]}$; let Φ^ε be the corresponding analogue of the function $\Phi \equiv \Phi^1$ that appears in the asymptotic (2.3). Note that for $\varepsilon = 0$ one has $\Phi^0 = 1$. As is easy to see from the integral equation (2.1), for small ε the inequality $\Phi^\varepsilon(\,\cdot\,) > 0$ holds everywhere in $\mathbb{R}^3$, whereas

$$\Phi^\varepsilon(x) \to 1 \quad \text{as } |x| \to \infty \tag{2.9}$$

uniformly w.r.t. ε.

Since Φ^ε depends on ε continuously,[7] there is the minimal $\varepsilon_0 \in (0, 1]$ such that the function Φ^{ε_0} satisfies $\Phi^{\varepsilon_0} \geq 0$ and, in the meantime, is not strictly positive (i.e., it has zeros). Shifting (if necessary) the origin of coordinates, assume that $\Phi^{\varepsilon_0}(0) = 0$ and recall that Φ^{ε_0} satisfies $(-\Delta + \varepsilon_0 q)\,\Phi^{\varepsilon_0} = 0$ in $\mathbb{R}^3$.

Fix a positive r; let $B_r := \{x \in \mathbb{R}^3 \mid |x| < r\}$ and $S_r := \partial B_r$. Integration by parts implies

$$\begin{aligned}\varepsilon_0 \int_{B_r} q(\xi)\Phi^{\varepsilon_0}(\xi)\left(\frac{1}{|\xi|} - \frac{1}{r}\right) d\xi \;&=\; \int_{B_r} \Delta\Phi^{\varepsilon_0}(\xi)\left(\frac{1}{|\xi|} - \frac{1}{r}\right) d\xi \\ = -4\pi\Phi^{\varepsilon_0}(0) + \frac{1}{r^2}\int_{S_r} \Phi^{\varepsilon_0}(\omega)\, d\omega &= \int_{S_1} \Phi^{\varepsilon_0}(r\theta)\, d\theta \;=: U(r)\,.\end{aligned}$$

On the other hand, we have

$$\begin{aligned}&\left|\int_{B_r} q(\xi)\Phi^{\varepsilon_0}(\xi)\left(\frac{1}{|\xi|} - \frac{1}{r}\right) d\xi\right| \;\leq\; \max_{B_r}|q| \int_0^r d\tau\, \tau^2 \left(\frac{1}{\tau} - \frac{1}{r}\right)\int_{S_1} \Phi^{\varepsilon_0}(\tau\theta)\, d\theta \\ &\leq\; \max_{B_r}|q|\, r \int_0^r U(\tau)\, d\tau \leq \left[\max_{B_r}|q|\right]\, r^2\, \left[\max_{[0,r]} U\right],\end{aligned}$$

and we arrive at the estimate

$$U(r) \;\leq\; cr^2 \max_{[0,r]} U(\,\cdot\,)\,.$$

Choosing r small enough such that $U(r) = \max_{[0,r]} U(\,\cdot\,)$, we see that this estimate is possible only if $U(r_1)$ vanishes identically for $r_1 < r$. Since $\Phi^{\varepsilon_0} \geq 0$, this means that $\Phi^{\varepsilon_0} \equiv 0$ in a small ball B_r.

So, Φ^{ε_0} is a solution of an elliptic equation vanishing in a ball. By the Landis uniqueness theorem [4], such a solution vanishes everywhere and we have $\Phi^{\varepsilon_0} = 0$ in $\mathbb{R}^3$, which contradicts (2.9). ∎

3. s-points and degeneration of jets.

3.1. Jets and polynomials. Recall what a *jet* is. For a fixed $a \in \mathbb{R}^3$ and an integer $k \geq 0$, we say that the smooth functions u and v are equivalent (and write $u \sim v$) if $u(x) - v(x) = o\left(|x - a|^k\right)$ as $x \to a$. With respect to the relation $\sim$, the set $C^\infty(\mathbb{R}^3)$ decomposes into the equivalence classes $j_a^k[u] := \{v \mid v \sim u\}$, called the jets of u (at the point a, of the order k). Setting up $\alpha j_a^k[u] + \beta j_a^k[u] := j_a^k[\alpha u + \beta v]$ for $\alpha, \beta \in \mathbb{R}$, one makes the set of jets into a linear space $\mathcal{J}_a^k\left[C^\infty(\mathbb{R}^3)\right]$.

As is easy to recognize, the jet $j_a^k[u]$ can be identified with the collection of the derivatives $\{D_x^j u(a)\}_{|j|=0}^k$, and $\dim \mathcal{J}_a^k\left[C^\infty(\mathbb{R}^3)\right]$ is equal to the number d^k of such derivatives: $d^0 = 1$, $d^1 = 1{+}3 = 4$, $d^2 = 1{+}3{+}6 = 10, \ldots, d^k = \frac{1}{6}(k{+}1)(k{+}2)(k{+}3)$.

Let $\mathcal{L} \subset C^\infty(\mathbb{R}^3)$ be a linear set; introduce a subspace

$$\mathcal{J}_a^k\left[\mathcal{L}\right] := \left\{j_a^k[u] \mid u \in \mathcal{L}\right\} \subset \mathcal{J}_a^k\left[C^\infty(\mathbb{R}^3)\right],$$

and denote by $d_a^k[\mathcal{L}]$ its dimension.

[7] In fact, analytically.

Fix an integer $l \geq 0$; the functions belonging to a linear set

$$\mathcal{P}_q^l := \left\{ p \in C^\infty(\mathbb{R}^3) \mid (-\Delta + q)\, p = 0 \text{ in } \mathbb{R}^3,\ |p(x)| \leq \text{const}\,(1+|x|)^l \right\}$$

are said to be *q-harmonic polynomials* of the order $\leq l$. The existence of such functions is established in a standard way: one puts $p = p_l + w$, where p_l is a harmonic polynomial (see, e.g., [9]), derives the relevant integral equation for w of the form analogous to (2.1), and proves its solvability and uniqueness of the solution by the same arguments as for (2.1), i.e., referring to Assumption 1. For instance, the function Φ determined by (2.4), (2.5) is an element of $\mathcal{P}_q^0$. Also, as is easy to verify, $\mathcal{P}_q^l \subset \mathcal{P}_q^{l'}$ for $l < l'$, and the relations

$$\dim \mathcal{P}_q^l = \dim \mathcal{P}_0^l = (l+1)^2, \qquad d_a^k[\mathcal{P}_q^k] \leq d_a^k[\mathcal{P}_0^k] = (k+1)^2 \tag{3.1}$$

hold.

The main result of this section is the following theorem.

THEOREM 3. *For $m = 2, 3, \dots$, the inclusion $a \in \Upsilon_q^m$ is equivalent to the relation*

$$d_a^{2m-2}[\mathcal{P}_q^{2m-2}] < (2m-1)^2\,. \tag{3.2}$$

Since in the generic case one has $d_a^{2m-2}[\mathcal{P}_q^{2m-2}] = (2m-1)^2$ (see (3.1) for $k = 2m-2$), it is reasonable to refer to (3.2) as a jet degeneration of $\mathcal{P}_q^{2m-2}$ at the point $x = a$. Also, Theorem 2 can be interpreted in the same terms: $\Phi(a) = 0$ means that $\dim \mathcal{J}_a^0\left[\mathcal{P}_q^0\right] = 0 < 1$.

The proof is postponed until section 3.3. For the sake of simplicity, it will be demonstrated for the case $m = 2$; the way to handle the general case will be clear.

3.2. Green function. Here we deal with the q-biharmonic equation $(-\Delta + q)^2\, u = h$. For $x, y \in \mathbb{R}^3$, $\langle x, y\rangle := x_1y_1 + x_2y_2 + x_3y_3$ is the inner product.

Unperturbed case. For $q = 0$, we set

$$B_0(x,y) \;:=\; -\frac{|x-y|}{8\pi}$$

and, in view of the well-known relation

$$(-\Delta)^2\, B_0(\,\cdot\,, y) = \delta_y\,, \tag{3.3}$$

we refer to B_0 as the *unperturbed Green function.* The following is a standard way to derive the asymptotic of B_0 as $|x| \to \infty$:

$$\begin{aligned}
|x-y| &= \left(|x|^2 - 2\langle x,y\rangle + |y|^2\right)^{\frac12}\\
&= |x|\left(1 + \frac{|y|^2}{|x|^2} - \frac{2}{|x|}\left\langle \frac{x}{|x|}, y\right\rangle\right)^{\frac12}\\
&= |x|\left(1 + \frac12\left(\frac{|y|^2}{|x|^2} - \frac{2}{|x|}\left\langle \frac{x}{|x|}, y\right\rangle\right) - \frac18\left(\frac{|y|^2}{|x|^2} - \frac{2}{|x|}\left\langle \frac{x}{|x|}, y\right\rangle\right)^2 + O(|x|^{-3})\right)\\
&= |x|\left(1 + \frac{|y|^2}{2|x|^2} - \frac{1}{|x|}\left\langle \frac{x}{|x|}, y\right\rangle - \frac{1}{2|x|^2}\left\langle \frac{x}{|x|}, y\right\rangle^2 + O(|x|^{-3})\right)\\
&= |x| + \frac{|y|^2}{2|x|} - \left\langle \frac{x}{|x|}, y\right\rangle - \frac{1}{2|x|}\left\langle \frac{x}{|x|}, y\right\rangle^2 + O(|x|^{-2})\\
&= |x| + \frac{|y|^2}{2|x|} - \frac{1}{|x|}\sum_i x_iy_i - \frac{1}{|x|^3}\sum_{i\neq j} x_ix_j\, y_iy_j - \frac{1}{2|x|^3}\sum_i x_i^2\, y_i^2 + O\left(\frac{1}{|x|^2}\right),
\end{aligned}$$

where i and j run over $1, 2, 3$. To clarify the structure of this expression, one can use the identity

$$\sum_i x_i^2\, y_i^2 = \frac{1}{2}(x_1^2 - x_2^2)\,(y_1^2 - y_2^2) + \frac{1}{6}(x_1^2 + x_2^2 - 2x_3^2)\,(y_1^2 + y_2^2 - 2y_3^2) + \frac{1}{3}|x|^2\,|y|^2$$

and write the result in the form

$$\begin{aligned}|x-y| = &\left\{|x| + \frac{|y|^2}{3|x|}\right\} - \left\{\sum_i \left[\frac{x_i}{|x|}\right] y_i\right\} - \frac{1}{|x|}\left\{\sum_{i\neq j}\left[\frac{x_i x_j}{|x|^2}\right] y_i y_j\right. \\ &\left. - \frac{1}{4}\left[\frac{x_1^2 - x_2^2}{|x|^2}\right](y_1^2 - y_2^2) - \frac{1}{12}\left[\frac{x_1^2 + x_2^2 - 2x_3^2}{|x|^2}\right](y_1^2 + y_2^2 - 2y_3^2)\right\} \\ &+ O\left(\frac{1}{|x|^2}\right). \qquad (3.4)\end{aligned}$$

As is seen now, this is an expansion over the spherical harmonics: the terms in the first curly braces do not depend on angle variables, and those in the second and third braces are proportional to $Y_1^m(\frac{x}{|x|})$ and $Y_2^m(\frac{x}{|x|})$, respectively.[8] One more peculiarity of such a representation is that, among the y-dependent coefficients

$$\begin{aligned}&\Phi_1^0 = 1\,, \quad \Psi^0 = |y|^2\,, \\ &\Phi_2^0 = y_1\,, \quad \Phi_3^0 = y_2\,, \quad \Phi_4^0 = y_3\,, \\ &\Phi_5^0 = y_1 y_2\,, \quad \Phi_6^0 = y_2 y_3\,, \quad \Phi_7^0 = y_1 y_3\,, \quad \Phi_8^0 = y_1^2 - y_2^2\,, \quad \Phi_9^0 = y_1^2 + y_2^2 - 2y_3^2, \qquad (3.5)\end{aligned}$$

there are nine *harmonic* functions $\Phi_1^0, \ldots, \Phi_9^0$ and one *biharmonic* Ψ^0.

REMARK 1. *So, the leading part of the unperturbed Green function asymptotic* (3.4) *is of the following structure:*

- *the term harmonic w.r.t. x has the coefficient Ψ^0 biharmonic w.r.t. y;*
- *the other terms are biharmonic w.r.t. x and have the coefficients Φ_i^0 harmonic w.r.t. y.*

A quite analogous picture will be observed in the perturbed case.

Perturbed case. For $q \neq 0$, we *define* the (perturbed) Green function as an $L_\infty^{\rm loc}(\mathbb{R}^3)$ -solution of the equation

$$B(x,y) = -\frac{|x-y|}{8\pi} + \int_{\mathbb{R}^3} \frac{|x-t|}{8\pi}\, LB(t,y)\, dt\,, \qquad x \in \mathbb{R}^3, \qquad (3.6)$$

where $y \in \mathbb{R}^3$ is a parameter and $L := (-\Delta + q)^2 - (-\Delta)^2$ is a second-order differential operator[9] such that $\operatorname{supp} Lu \subset \operatorname{supp} q \cap \operatorname{supp} u$. The following result shows that this definition is correct.

LEMMA 2. *Equation* (3.6) *is uniquely solvable.*

Proof. Let the homogeneous equation

$$\psi(x) = \int_{\mathbb{R}^3} \frac{|x-t|}{8\pi}\, L\psi(t)\, dt$$

have a nonzero solution ψ. Such a solution satisfies

$$(-\Delta + q)^2\, \psi = 0 \quad \text{in } \mathbb{R}^3\,;$$

[8] The harmonics are selected by the square brackets.

[9] In the integral, L acts on the variable t.

by (3.4), for large $|x|$ it behaves as

$$\psi(x) \underset{|x|\to\infty}{=} \alpha|x| + \sum_{i=1}^{3} \beta_i \frac{x_i}{|x|} + \widetilde{\psi}(x)\,,$$

where $\widetilde{\psi} = O(\frac{1}{|x|}) \to 0$.

Assume that ψ is q-harmonic: $(-\Delta + q)\psi = 0$ in $\mathbb{R}^3$. If so, we have $\Delta\psi = 0$ for large $|x|$, which implies $\alpha = \beta_i = 0$ and $\psi = \widetilde{\psi}$. Hence, ψ is a q-harmonic function vanishing as $|x| \to \infty$, which is forbidden by Assumption 1.

Thus, $\varphi := (-\Delta + q)\,\psi$ is a nonzero function, which satisfies $(-\Delta + q)\,\varphi = 0$ in $\mathbb{R}^3$, and

$$\varphi(x) \underset{|x|\to\infty}{=} -\alpha\Delta|x| - \sum_{i=1}^{3} \beta_i \Delta \frac{x_i}{|x|} + \Delta\widetilde{\psi}(x) \;=\; O\left(\frac{1}{|x|}\right) \to 0,$$

which is impossible in view of Assumption 1. So, assuming $\psi \neq 0$ we arrive at a contradiction. □

As easily follows from (3.6), the relation

$$(-\Delta + q)^2\, B(\,\cdot\,, y) = \delta_y, \tag{3.7}$$

analogous to (3.3), is valid. Also, the symmetry property $B(x,y) = B(y,x)$ holds.

The way to derive the asymptotic of B analogous to (3.4) is also quite standard. Namely, we represent

$$B(x,y) = -\frac{1}{8\pi}\, A(x,y) + O(|x|^{-2}) \tag{3.8}$$

with an ansatz of the form[10]

$$\begin{aligned} A(x,y) = &\left\{ |x|\Phi_1(y) + \frac{\Psi(y)}{3|x|} \right\} \\ &- \left\{ \left[\frac{x_1}{|x|}\right] \Phi_2(y) + \left[\frac{x_2}{|x|}\right] \Phi_3(y) + \left[\frac{x_3}{|x|}\right] \Phi_4(y) \right\} \\ &- \frac{1}{|x|}\left\{ \left[\frac{x_1x_2}{|x|^2}\right] \Phi_5(y) \;+\; \left[\frac{x_2x_3}{|x|^2}\right] \Phi_6(y) \;+\; \left[\frac{x_1x_3}{|x|^2}\right] \Phi_7(y) \right. \\ &\left. + \frac{1}{4}\left[\frac{x_1^2 - x_2^2}{|x|^2}\right] \Phi_8(y) \;-\; \frac{1}{12}\left[\frac{x_1^2 + x_2^2 - 2x_3^2}{|x|^2}\right] \Phi_9(y) \right\}. \end{aligned} \tag{3.9}$$

Let $|y| \to \infty$ in (3.6). Using the symmetry property, substitute this representation into (3.6), and by equaling the coefficients at the proper spherical harmonics, we eventually get the "transport equations" of the form

$$\Phi_i(x) = \Phi_i^0(x) \;+\; \int_{\mathbb{R}^3} \frac{|x-t|}{8\pi}\, L\Phi_i(t)\, dt\,, \qquad i = 1, \dots, 9, \tag{3.10}$$

$$\Psi(x) = \Psi^0(x) \;+\; \int_{\mathbb{R}^3} \frac{|x-t|}{8\pi}\, L\Psi(t)\, dt\,. \tag{3.11}$$

[10]Compare with (3.4)!

By the same arguments, which provide the unique solvability of (3.6), these equations are also solvable uniquely.

As is easy to see from (3.10) and (3.11), the solutions Ψ and Φ_i are q-biharmonic. Moreover, we have the following lemma.

LEMMA 3. *The functions $\Phi_1, \dots, \Phi_9$ are q-harmonic polynomials of the order ≤ 2 and constitute a basis in $\mathcal{P}_q^2$.*

Proof.

Step 1: *q-harmonicity.* Take an $f \in C_0^\infty(\mathbb{R}^3)$, denote $\hat{H} := (-\Delta + q)$,[11] and set

$$F(x) := \int_{\mathbb{R}^3} B(x,y)\, \hat{H} f(y)\, dy\,, \qquad x \in \mathbb{R}^3. \tag{3.12}$$

Applying $\hat{H}^2$ and taking into account (3.7), we get $\hat{H}^2 F = \hat{H} f$ and, hence,

$$\hat{H}\left(\hat{H}F - f\right) = 0 \qquad \text{in } \mathbb{R}^3.$$

As is easily seen from (3.12) and (3.8), (3.9), the function $\hat{H}F$ vanishes as $|x| \to \infty$. Hence, the same is valid for $\hat{H}F - f$. In the meantime, the latter difference is annulated by $\hat{H}$ and, whence, it has to vanish identically by Assumption 1. Thus, we arrive at $\hat{H}F - f = 0$, i.e.,

$$(-\Delta + q(x)) \int_{\mathbb{R}^3} B(x,y)\, \hat{H} f(y)\, dy \;=\; f(x)\,, \qquad x \in \mathbb{R}^3. \tag{3.13}$$

Now, tending $|x| \to \infty$ and taking into account the structure of the asymptotic (3.8), (3.9), it is easy to see that the asymptotic of the l.h.s. contains certain linearly independent harmonic (w.r.t. x) terms[12] with coefficients of the form $\int_{\mathbb{R}^3} \Phi_i(y)\, \hat{H} f(y)\, dy$. In the meantime, the r.h.s. in the equality (3.13) is compactly supported and, hence, the equality forces all harmonic terms to vanish identically. This follows to

$$0 = \int_{\mathbb{R}^3} \Phi_i(y)\, \hat{H} f(y)\, dy = \int_{\mathbb{R}^3} \hat{H}\Phi_i(y)\, f(y)\, dy,$$

which is equivalent to $\hat{H}\Phi_i = 0$ in $\mathbb{R}^3$ by the arbitrariness of f. So, Φ_i are q-harmonic.

Step 2: *Integral equations.* The functions Φ_i satisfy the integral equations, which are different from and more informative than (3.10). These equations can be derived as follows.

By (2.2), for any $f \in C_0^\infty(\mathbb{R}^3)$, one has the relation

$$(-\Delta + q(x)) \int_{\mathbb{R}^3} G(x,y)\, f(y)\, dy \;=\; f(x)\,, \qquad x \in \mathbb{R}^3\,.$$

Comparing it with (3.13) we get

$$\int_{\mathbb{R}^3} G(x,y)\, f(y)\, dy \;=\; \int_{\mathbb{R}^3} B(x,y)\, \hat{H} f(y)\, dy\,,$$

whereas integration by parts easily implies

$$(-\Delta + q(y))\, B(x,y) \;=\; G(x,y)\,, \qquad x,y \in \mathbb{R}^3,\;\; x \ne y. \tag{3.14}$$

[11] So, $\hat{H}$ is understood as a differential expression that can be applied to any smooth enough function not necessarily belonging to $\mathcal{H}$.

[12] For large enough $|x|$, "harmonic" and "q-harmonic" are the same.

In the unperturbed case, for the Green functions B_0 and G_0, we have just

$$-\Delta\left[-\frac{|x-y|}{8\pi}\right] = \frac{1}{4\pi|x-y|}\,, \qquad x,y\in\mathbb{R}^3,\ x\neq y. \tag{3.15}$$

These relations enable us to get the asymptotics for G and G_0 through (3.8) and (3.4), respectively, *the coefficients of the asymptotics being expressed through* Φ_i, Ψ *and* Φ_i^0, Ψ^0. Surely, the asymptotic of G obtained in this way is just a more detailed version of (2.3), which takes into account the structure of the lower order terms. Also, the comparison of the coefficients at $\frac{1}{|x|}$ in the detailed asymptotic and (2.3) easily implies the important relation

$$\Phi(y) = -\frac{1}{6}\left(\Delta+q(y)\right)\Psi(y)\,, \tag{3.16}$$

which will be required later on.

Thereafter, the trick, which was used for the derivation of (2.6), is repeated: substituting the detailed asymptotics of G and G_0 into (2.1) and comparing the terms on the l.h.s. and r.h.s., we can arrive at the equations

$$\Phi_i(x) = \Phi_i^0(x) - \int_{\mathbb{R}^3}\frac{q(s)}{4\pi|x-s|}\,\Phi_i(s)\,ds\,, \quad x\in\mathbb{R}^3\,, \quad i=1,\ldots,9\,, \tag{3.17}$$

the first one being identical to (2.6).

Step 3: *Completing the proof.* The estimates $|\Phi_i(x)|\leq c\,(1+|x|)^2$ easily follow from the integral equations (3.17) and the evident estimates of the same form for Φ_i^0. Thus, we have $\Phi_i\in\mathcal{P}_q^2$.

As is well known, the polynomials $\Phi_1^0,\ldots,\Phi_9^0$ form a basis in (unperturbed) $\mathcal{P}_0^2$. Using (3.17), it is not difficult to conclude that the same is valid for $\Phi_1,\ldots,\Phi_9$ in the perturbed $\mathcal{P}_q^2$. ∎

3.3. Proving Theorem 3. Recall that we are dealing with the case $m=2$.

Necessity. Assume that $a\in\Upsilon_q^2$ holds. This means that there is a function $h\in\mathcal{H}$ such that $(-\Delta+q)^2h=0$ in $\mathbb{R}^3\backslash\{a\}$ and, at the same time, $(-\Delta+q)h$ does not vanish identically.

Considering $(-\Delta+q)^2\,h$ as a distribution on $C_0^\infty\left(\mathbb{R}^3\right)$, we see that it is supported at $x=a$. Such a distribution has to be a linear combination of the Dirac measure derivatives:

$$(-\Delta+q)^2\,h = \sum_{|j|=0}^{N}\alpha_j D_x^j\delta_a = \sum_{|j|=0}^{N}\alpha_j(-1)^{|j|}D_a^j\delta_a \;=:\; P_N(\nabla_a)\,\delta_a\,,$$

where $P_N(\nabla_a)$ is a differential polynomial of the order N with constant coefficients, which acts on the variable a. Therefore, in accordance with (3.7), the function h has to be of the form

$$h(x) = P_N(\nabla_a)\,B(x,a)+\widetilde{h}(x)\,, \qquad x\in\mathbb{R}^3\backslash\{a\},$$

with a smooth q-biharmonic in $\mathbb{R}^3$ function $\widetilde{h}$.

Since

$$B(x,a) = c|x-a| + \text{smoother terms}$$

near $x = a$ (see (3.6)), the only option for h to belong to $\mathcal{H}$ (to be square-summable near $x = a$) is $\alpha_j = 0$ for $|j| \geq 3$; hence, we have $N \leq 2$, i.e.,

$$h(x) = P_2(\nabla_a)\, B(x,a) + \widetilde{h}(x)\,, \qquad x \in \mathbb{R}^3\backslash\{a\}.$$

Let us show that $\widetilde{h} = 0$. At first h is of the class $L_2(\mathbb{R}^3)$ and is biharmonic outside of a (large enough) ball. Therefore, as is well known, such a function satisfies $h(x) \leq \frac{c}{|x|^2}$, whereas all its derivatives decrease even faster. In the meantime, by (3.8), (3.9) (with $y = a$), a function $\widetilde{h} = h - P_N(\nabla_a)\, B(x,a)$ has to be of the same asymptotic behavior as $P_N(\nabla_a)\, A(x,a)$. Applying $-\Delta + q$ to $\widetilde{h}$ we conclude that $\psi := (-\Delta + q)\widetilde{h}$ is a *decreasing* solution to the equation $(-\Delta + q)\psi = 0$. Assumption 1 implies $\psi = 0$, i.e., $\widetilde{h}$ satisfies $(-\Delta + q)\widetilde{h} = 0$. On the other hand, if $\widetilde{h}$ contains nondecreasing terms entering the r.h.s. of (), then $\Delta\widetilde{h}$ cannot vanish at infinity. Hence $\psi = (-\Delta + q)\widetilde{h} \neq 0$, in contradiction to that which was proved above. Therefore, we have to conclude that $\widetilde{h} \to 0$, whereas Assumption 1 implies $\widetilde{h} = 0$.

Thus, we get

$$h(x) = P_2(\nabla_a)\, B(x,a)\,, \qquad x \in \mathbb{R}^3\backslash\{a\}. \tag{3.18}$$

Recall that $h \in \mathcal{H}$ and let $|x| \to \infty$. Turning to the structure of the asymptotic of B (see (3.8), (3.9) with $y = a$) and taking into account the linear independence of the spherical harmonics (the square brackets in (3.9)), we easily conclude that the r.h.s. of (3.18) can be square-summable if and only if the coefficients of the terms that behave as $|x|$ and $\frac{1}{|x|}$ vanish, i.e.,

$$P_2(\nabla_a)\, \Phi_i(a) \,=\, 0, \quad i = 1, \ldots, 9, \qquad P_2(\nabla_a)\, \Psi(a) \,=\, 0\,. \tag{3.19}$$

The obtained relations for *q-harmonic* Φ_i are nontrivial only if $P_2(\nabla_a) \neq -\Delta + q(a)$. Otherwise we have

$$\Phi(a) = \langle \text{see (3.16)} \rangle = -\frac{1}{6}\, P_2(\nabla)\Psi(a) = \langle \text{see (3.19)} \rangle \,= 0\,.$$

By (2.3), we conclude that $G(\,\cdot\,, a) \in \mathcal{H}$; i.e., a is an s-point of the *first* order, i.e., $a \in \Upsilon_q^1$, which contradicts the assumption.

Since $\Phi_1, \ldots, \Phi_9$ constitute a basis in $\mathcal{P}_q^2$, any q-harmonic polynomial $p \in \mathcal{P}_q^2$ satisfies $P_2(\nabla)p(a) = 0$. Hence, $d_a^2\left[\mathcal{P}_q^2\right] < 9$; i.e., the jet degeneration at the point a does occur.

Sufficiency. Assume that at a point $a \in \mathbb{R}^3$ the jet degeneration occurs, i.e., $d_a^2\left[\mathcal{P}_q^2\right] < 9$. Let $\mathcal{L}$ be the 10-dimensional subspace spanned on $\Phi_1, \ldots, \Phi_9, \Psi$; the degeneration evidently implies $d_a^2[\mathcal{L}] < 10$. By the latter, there exists a second-order differential polynomial $P_2(\nabla)$ such that (3.19) is valid. In the meantime, the same arguments as in the item below (3.19) imply $P_2(\nabla) \neq -\Delta + q(a)$.

Defining a function h by the r.h.s. of (3.18) and taking into account the form of the asymptotic (3.8) and the relations (3.19), it is easy to see that $h \in \mathcal{H}$ and $(-\Delta + q)^2 h = 0$ in $\mathbb{R}^3\backslash\{a\}$. Hence, $a \in \Upsilon_q^2$ holds. ∎

REMARK 2. *Choose a basis $F = F_1, F_2 \cdots F_9$ in the space $\mathcal{P}_q^2$; compose a column $F := \mathrm{col}\{F_1, F_2 \cdots F_9\}$ and a 9×10 matrix $(F, F_x, F_y \cdots F_{xx}, F_{yy}, F_{zz})$ of the 2-jets. Reduce it to a 9×9 matrix by removing the column $F_{zz} = -F_{xx} - F_{yy} + qF$. Let δ_q^2 be the determinant of the latter matrix. By Theorem 3, the condition $a \in \Upsilon_q^2$ is equivalent to $\delta_q^2(a) = 0$. As is easy to show, $\lim_{|x|\to\infty} \delta_q^2(x) = c \neq 0$, whereas a* *function* $\frac{1}{c}\,\delta_q^2$ *is determined by the potential* q *(does not depend on the choice of the basis* F*).*

In the case of $a \in \Upsilon_q^m$ for $m > 2$, the proof is just more complicated in notation. However, it exploits the same idea: a linear combination of the relevant q-m-harmonic Green function and its derivatives can belong to the space $\mathcal{H}$ if and only if the proper analogue of the relations (3.19) does hold and that is equivalent to a certain jet degeneration at $x = a$. Also, as a generalization of δ_q^2, an invariant δ_q^{2m-2} can be introduced as a determinant of the relevant square matrix of the order $(2m-2)^2$.

3.4. Radially symmetric potential. If the potential is of the form $q = q(|x|)$, much more can be said about the structure of the s-point set Υ_q. As is evident, Υ_q consists of spheres in $\mathbb{R}^3$ centered at $x = 0$. Here we briefly announce some results on this case.

1. For a fixed $l \geq 0$, the set Υ_q^l can be characterized as follows. Let φ_l be a *regular* solution of the radial Schrödinger equation

$$-\varphi_l'' + \frac{l(l+1)}{r^2}\,\varphi_l + q(r)\varphi_l \,=\, 0\,, \qquad r > 0, \tag{3.20}$$

that behaves as $\varphi_l(r) \sim r^{l+1}$ near $r = 0$. Note that, in this case, the functions

$$\frac{\varphi_l(|x|)}{|x|}\;Y_l^m\left(\frac{x}{|x|}\right) \qquad (|m| \leq l+1)$$

are q-harmonic and belong to $\mathcal{P}_q^l$. Introduce the Kram determinants[13]

$$\Delta_l^m\,(r) := \begin{vmatrix} \varphi_m(r) & \varphi_m'(r) & \cdots & \varphi_m^{(l-m)}(r) \\ \varphi_{m+1}(r) & \varphi_{m+1}'(r) & \cdots & \varphi_{m+1}^{(l-m)}(r) \\ \cdots & \cdots & \cdots & \cdots \\ \varphi_l(r) & \varphi_l'(r) & \cdots & \varphi_l^{(l-m)}(r) \end{vmatrix}, \qquad m = 0, 1, \ldots, l.$$

Let N_j be the number of the eigenvalues of the partial Schrödinger operator $-d_r^2 + \frac{j(j+1)}{r^2} + q(r)$ in $L_2(0,\infty)$ and let $z(\Delta_l^m)$ be the number of zeros of the Kram determinant. The relation

$$z(\Delta_l^m) \,=\, \sum_{k=0}^{l-m} (-1)^k N_{m+k} \tag{3.21}$$

is valid.

2. As we saw in section 2, $\sigma_{\mathrm{disc}}(H) \neq \emptyset$ implies $\Upsilon_q \neq \emptyset$. Our hypothesis is that the converse is also valid, so that the equivalence

$$\{\sigma_{\mathrm{disc}}(H) = \emptyset\} \Leftrightarrow \{\Upsilon_q \neq \emptyset\} \tag{3.22}$$

holds. It can be shown that *for radial symmetric potentials, if* $\sigma_{\mathrm{disc}}(H) = \emptyset$, *then* $\Upsilon_q^k = \emptyset$ *holds for all* $k \geq 1$. This fact is established in the following way. The determinant δ_q^l can be calculated explicitly and takes the form

$$\delta_q^l(r) = \Delta_l^0\left(\Delta_l^1(r)\right)^2 \ldots \left(\Delta_l^l(r)\right)^2,$$

which enables one to find the zeros of δ_q^l using (3.21) and, hence, to verify the presence/absence of the jet degeneration points.

[13] It is worth noting that these determinants appear in Darboux' transform theory.

3. The picture of s-spheres is rather curious. For instance, in the case of $H_\alpha = -\Delta + \alpha q$ with an interaction constant $\alpha \geq 0$, the following scenario is possible as α grows:

   (a) For small enough $\alpha \in [0, \alpha_1]$, one has $\sigma_{\rm disc}(H_\alpha) = \emptyset$ and $\Upsilon_q^k = \emptyset$ for all $k \geq 1$.

   (b) For $\alpha \in [\alpha_1, \alpha_2)$, $\sigma_{\rm disc}(H_\alpha)$ consists of a single eigenvalue $\lambda_1^\alpha < 0$, the eigenfunction χ_1^α being radially symmetric, whereas all Υ_q^k, $k \geq 1$, are nonempty and consist of the spheres S_k of the radius r_k growing to infinity as $k \to \infty$.

   (c) Assume that as α passes through α_2, the second negative eigenvalue $\lambda_2^\alpha > \lambda_1^\alpha$ appears, with the eigenfunction χ_2^α dependent on the angle variable as $Y_1(\,\cdot\,)$. In such a case, as $\alpha \uparrow \alpha_2$, the certain spheres S_k, $k \geq 2$, are blown up: $\lim_{\alpha \to \alpha_2} r_k = \infty$.

   In the meantime, if λ_2^α is such that χ_2^α is also radially symmetric, the picture is quite different: all Υ_q^k, $k \geq 1$, are nonempty and evolve regularly as α grows.

3.5. Comments.

- Some results of the book [1] on a system of the Schrödinger equations (3.20) with different $l \geq 0$ can be interpreted in "s-point terms." In particular, the existence of the zero energy solution of the system, which is bounded at $r = 0$, leads to a certain "nonstandard" factorization of the S-matrix that is quite analogous to the effects discussed in section 1.
- Let $x = a$ be an s-point of the potential q, and let w_a^f be a reversing wave, which satisfies

$$w_a^f|_{|x-a|<|t|} = 0\,. \tag{3.23}$$

  The Fourier transform $\widetilde{w}_a(\,\cdot\,, k) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} e^{ikt}\, w_a(\,\cdot\,, t)\, dt$ obeys

$$(-\Delta + q)\widetilde{w}_a = k^2 \widetilde{w}_a\,,$$

  so that $\widetilde{w}_a(\,\cdot\,, k)$ is a continuous spectrum eigenfunction of the Schrödinger operator H. A remarkable fact is that, by (3.23), such an eigenfunction is an *entire* function of the spectral parameter k. Historically, the existence of such eigenfunctions was a question, which has since been affirmatively answered by R. Newton. Now we see that there exists a rich family of entire continuous spectrum eigenfunctions $\{\widetilde{w}_a(\,\cdot\,, k)\}|_{a \in \Upsilon_q}$ associated with *reversing finite energy waves* and parameterized by points of the surfaces of which Υ_q consists. The concrete examples demonstrate that these surfaces may be of rather complicated shape (ovaloids, toruses, etc.). The meaning and role of such eigenfunctions in the scattering theory are not quite clear yet.
- The important question of whether the set of finite order s-points $\cup_{m=1}^{\infty} \Upsilon_q^m$ exhausts Υ_q is still open even in the case of radially symmetric potentials. Also, the conjecture (3.22) is not justified yet.

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