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LETTER TO THE EDITOR

A note on trace-class scattering amplitudes

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Abstract. A very simple proof is presented for the assumption that if the potential in the Schrödinger equation is integrable and in the Rollnik class, then for all energies the scattering amplitude is trace class. Some consequences are discussed.

The Fredholm determinant of the S matrix of the Schrödinger equation plays an important role in scattering theory, particularly in the formulation of a generalization of the Levinson theorem to higher dimensions [1–6]. This function, in its unmodified or unregularized form, is well defined as an absolutely convergent series if the scattering amplitude A is in the trace class†. A is regarded as the integral kernel of an operator $\mathscr{A}: L^2(\mathbb{S}^2) \mapsto L^2(\mathbb{S}^2)$ (where $\mathbb{S}^2$ is the unit sphere in $\mathbb{R}^3$) and defined in terms of the S matrix $\mathscr{S}$ at the fixed energy $E = k^2$ by

$$\mathscr{A} = \frac{2\pi \mathrm{i}}{k}(\mathbb{1} - \mathscr{S}).$$

If it is assumed that the potential V in the Schrödinger equation is absolutely integrable and in the Rollnik class

$$R := \left\{ V \in \mathbb{R}: \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathrm{d}x\, \mathrm{d}y \frac{|V(x)||V(y)|}{|y-x|^2} < \infty \right\}$$

then A is known to be a continuous function (see e.g. [5]) and hence $\mathscr{A}$ is Hilbert–Schmidt and thus a compact operator. Since $\mathscr{S}$ is unitary, it follows that $\mathscr{A}$ has a point spectrum only and its eigenfunctions form a complete orthonormal set, as is well known. If the eigenphase shifts δ_n are defined so that the eigenvalues of $\mathscr{S}$ are $\mathrm{e}^{2\mathrm{i}\delta_n}$ then the eigenvalues of $(k/4\pi)\,\mathscr{A}$ are $\mathrm{e}^{\mathrm{i}\delta_n} \sin \delta_n$ and the requirement that $\mathscr{A}$ be trace class is equivalent to the statement that the series $\Sigma\, \delta_n$ be absolutely convergent, i.e. that the sequence $\{\delta_n\} \in l^1$. (That it is in l^2 is already implied by the fact that $\mathscr{A}$ is Hilbert–Schmidt.)

There are several proofs in the literature that under specific conditions of V the scattering amplitude is trace class [2, 3, 7–12]. These proofs are rather complicated and abstract. I therefore consider it worthwhile to present a new and very simple proof, whose assumptions are identical to those used by Dreyfus in [2, 3].

Theorem. If the potential in the Schrödinger equation is such that $V \in L^1(\mathbb{R}^3) \cap R$ then $\mathscr{S} - \mathbb{1}$ is in the trace class for all $k \geqslant 0$.

† A reminder: an operator M is in the trace class if $\|M\|_1 := \mathrm{tr}\sqrt{M^\dagger M} < \infty$.

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Proof. In the following, dependence on the variable k, which is fixed, will not be shown. The scattering amplitude has the representation

$$A(\theta, \theta') = -\frac{1}{4\pi}\int_{\mathbb{R}^3} \mathrm{d}x \exp[-(\mathrm{i}k\theta\cdot x)]V(x)\psi(\theta, x)$$

where ψ is the scattering solution of the Schrödinger equation. We define the operators $\mathscr{A}$, $T(r)$ and $B(r)$ so that $\mathscr{A}f = g$ means

$$\int_{\mathbf{S}^2} \mathrm{d}\theta'\, A(\theta, \theta')f(\theta') = g(\theta).$$

$T(r)f = g$ means

$$-\frac{1}{4\pi}\int_{\mathbf{S}^2} \mathrm{d}\hat{x} \exp[-(\mathrm{i}kr\theta\cdot\hat{x})]|V(r\hat{x})|^{1/2}f(\hat{x}) = g(\theta)$$

and $B(r)f = g$ means

$$\int_{\mathbf{S}^2} \mathrm{d}\hat{x}\, V^{1/2}(r\hat{x})\psi(\theta, r\hat{x})f(\hat{x}) = g(\theta)$$

where $V^{1/2} := V/|V|^{1/2}$. Then we may write the representation of A in the operator form

$$\mathscr{A} = \int_0^\infty \mathrm{d}r\, r^2 K(r)$$

where $K(r) := T(r)B(r)$. Let $\|\cdot\|_1$ and $\|\cdot\|_2$ denote the trace norm and the Hilbert–Schmidt norm respectively. Then

$$\|\mathscr{A}\|_1 \leqslant \int_0^\infty \mathrm{d}r\, r^2\|K\|_1 \leqslant \int_0^\infty \mathrm{d}r\, r^2\|T(r)\|_2\|B(r)\|_2$$
$$\leqslant \left(\int_0^\infty \mathrm{d}r\, r^2\|T(r)\|_2^2\right)^{1/2}\left(\int_0^\infty \mathrm{d}r\, r^2\|B(r)\|_2^2\right)^{1/2}$$

where the first step is justified by the triangle inequality for the trace norm, the second by an abstract Schwarz inequality (see [13], equation (2.5*b*)), and the third by the Schwarz inequality for the integral. However

$$\int_0^\infty \mathrm{d}r\, r^2\|T(r)\|_2^2 = \int \mathrm{d}r\, r^2 \int_{\mathbf{S}^2\times\mathbf{S}^2} \mathrm{d}\theta\, \mathrm{d}\hat{x}|V(r\hat{x})| = 4\pi\int_{\mathbb{R}^3} \mathrm{d}x|V(x)| < \infty$$

because by assumption $V \in L^1(\mathbb{R}^3)$ and

$$\int_0^\infty \mathrm{d}r\, r^2\|B(r)\|_2^2 = \int_0^\infty \mathrm{d}r\, r^2 \int_{\mathbf{S}^2\times\mathbf{S}^2} \mathrm{d}\theta\, \mathrm{d}\hat{x}|V(r\hat{x})||\psi(\theta, \hat{x})|^2 < \infty$$

because by assumption $V \in R$ (see e.g. [5] equation (10.74)). Therefore the trace norm of $\mathscr{A}$ is finite and $\mathscr{A}$ is in the trace class. If $k = 0$ is an exceptional point of the second kind (i.e. there is a half-bound state) then A is $\mathrm{O}(k^{-1})$ and the same result holds for $\lim_{k\to 0} k\mathscr{A}$. □

This proof is easily modified to apply in the case of scattering of Bloch waves by impurities in a crystal, and the result may also be used for the generalized Levinson theorem in that case [6]. It obviously also holds if V is not multiplicative (i.e. it is non-local) but a trace-class operator [14, 15].

Even though $\mathscr{A}$ is trace class and det $\mathscr{S}$ exists, it may sometimes be useful to work with the modified Fredholm determinant

$$\det_2 \mathscr{S} = \det \mathscr{S} \exp\left[-\left(\frac{k}{2\pi} \mathrm{i}\, \mathrm{tr}\, \mathscr{A}\right)\right].$$

We note that it follows from the optical theorem (unitarity of $\mathscr{S}$) that

$$\Im\, \mathrm{tr}\, \mathscr{A} = \frac{k}{4\pi} \mathrm{tr}\, \mathscr{A}\mathscr{A}^\dagger = k\langle\sigma\rangle$$

where $\Im$ denotes the imaginary part and $\langle\sigma\rangle$ is the angle-averaged total scattering cross section. On the other hand

$$\frac{k}{2\pi} \Re\, \mathrm{tr}\, \mathscr{A} = \sum_n \sin 2\delta_n$$

where $\Re$ denotes the real part. Therefore

$$\det_2 \mathscr{S} = \exp\left(\frac{k^2}{2\pi}\langle\sigma\rangle\right) \exp(2\mathrm{i}\delta')$$

where

$$\delta' = \sum_n (\delta_n - \tfrac{1}{2}\sin 2\delta_n) \qquad (\mathrm{mod}\ \pi).$$

The series on the right converges faster than $\delta := \Sigma\, \delta_n$. Furthermore, it is known that even though each $\delta_n \to 0$ (mod π) as $k \to \infty$ (since $\|\mathscr{S} - \mathbb{1}\| \to 0$ [16]) their sum does not:

$$\delta(k) = -\frac{k}{4\pi}\langle V\rangle + \mathrm{o}(1) \qquad (\mathrm{mod}\ \pi)$$

where $\langle V\rangle = \int \mathrm{d}x\, V(x)$. But we also have

$$\sum_n \tfrac{1}{2}\sin 2\delta_n = \frac{k}{4\pi} \Re\, \mathrm{tr}\, \mathscr{A} = -\frac{k}{4\pi}\langle V\rangle + \mathrm{o}(1).$$

Therefore δ' is uniquely defined by continuity and the demand that $\lim_{k\to\infty} \delta'(k) = 0$. A generalization of Levinson's theorem [2–4] then reads

$$\delta'(0) = \pi(n + \tfrac{1}{2}\nu)$$

where n is the total number of eigenvalues (bound states) and $\nu = 1$ if there is a half-bound state; $\nu = 0$ otherwise.

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