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On a Generalization of Rouché's Theorem for Trace Ideals with Applications for Resonances of Schrödinger Operators

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1. Introduction

Given an operator A on a complex Hilbert space $\mathscr{H}$ in applications the question of determining the spectrum of A, i.e., its localization in the complex plane, often arises. For selfadjoint operators a variety of methods for obtaining upper and lower bounds on the eigenvalues exists (see, e.g., Collatz [1]). For nonnormal operators, $AA^* \neq A^*A$, most of these bounds are not applicable since they either require the spectrum to be real or use in the proof the spectral theorem as an essential ingredient. Exceptions are the method in [2] and the bound of Gershgorin [3]. In the case of finite dimensional $\mathscr{H}$ it localizes the spectrum in some circles of the complex plane (for a similar result see Brauer [4]). Its generalization to the finite dimensional case, however, excludes only spectral points in certain regions of the complex plane, sharing this feature with [2], leaving open the question of where in the complement of these regions the spectrum actually lies and whether the operator has spectrum at all.

We shall pursue this question with a particular example of a nonnormal operator, the complex dilated Hamiltonian $H(\theta) = -\Delta e^{-2\theta} + V(e^{\theta}r)$ (θ a complex parameter) which is used for describing quantum mechanical resonances (see, e.g., Reed and Simon [5, pp. 51 ff and 183 ff]). Obtaining bounds on the width of a resonance which is proportional to the inverse of the imaginary part of the corresponding complex eigenvalue of $H(\theta)$ has

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been an open problem for a long time (see Simon [6, open problem B], Reinhardt [7], and Junkers [8] for more recent overviews).

In the second section we prove a generalization of an earlier result of Algazin [9]. As an essential tool (regularized) Fredholm determinants are used. In the third section we show how these results apply to the complex dilation formalism described above and certain variants thereof.

2. Rouché's Theorem for Operators in $1+\mathscr{I}_p$

Let $\mathscr{I}_p$ denote the trace ideal of order p, i.e., all bounded operators A on $\mathscr{H}$ the p-trace norm $\|A\|_p = (\mathrm{tr}\,|A|^p)^{1/p}$ of which is finite. For $p=1$, the trace class operators, the Fredholm determinant may be defined by

$$\det(1+\mu A) := \exp(\mathrm{tr}(\log(1+\mu A))) \tag{1}$$

for μ small enough. By analytic continuation in μ, the left-hand side is defined for all μ.

Now, by observing that for $A \in \mathscr{I}_p$ $(p>1)$ only the traces of the first $p-1$ terms of the power series expansion of $\log(1+\mu A)$ can diverge, we can define a regularized determinant (Simon [10]) as

$$\det_p(1+A) := \det(1+R_p(A)) \tag{2}$$

with

$$R_p(A) = (1+A)\exp\left(\sum_{j=1}^{p-1} (-1)^j j^{-1} A^j\right) - 1. \tag{3}$$

We can now formulate the theorem:

Theorem. *Let Γ be a simply connected domain enclosed by the curve γ; let $f(z) := 1+F(z)$ and $g(z) := 1+G(z)$ where F and G are meromorphic $\mathscr{I}_p$-valued functions on Γ, analytic on its boundary. Furthermore let*

$$\max_{z\in\gamma} \|f(z)\,g(z)-1\|_p < 1. \tag{4}$$

Then

$$\frac{1}{2\pi i}\,\mathrm{tr}\oint_\gamma f'(z)\,f(z)^{-1}\,dz = -\frac{1}{2\pi i}\,\mathrm{tr}\oint_\gamma g'(z)\,g(z)^{-1}\,dz. \tag{5}$$

In particular, if F is analytic in Γ then

$$N_\Gamma(F) = \text{number of eigenvalues } (-1) \text{ of } F(z) \text{ counted according to their algebraic multiplicity with } z \in \Gamma$$

$$= \frac{-1}{2\pi i} \operatorname{tr} \oint_\gamma g'(z)\, g(z)^{-1}\, dz.$$

Proof. We first claim that $(1/2\pi i) \operatorname{tr} \oint_\gamma h'(z)\, h(z)^{-1}\, dz$ is an integer provided h fulfills the analyticity hypothesis of f and g and is invertible on γ. Assume $h(z) = 1 + H(z)$ with $H(z) \in \mathscr{I}_1$. We have

$$\mathbb{Z} \ni \frac{1}{2\pi i} \oint_\gamma \frac{d}{dz} \log \det\nolimits_p h(z)$$

$$= \frac{1}{2\pi i} \oint_\gamma \frac{d}{dz} \log \exp \operatorname{tr} \log[1 + R_p(H)(z))]\, dz$$

$$= \frac{1}{2\pi i} \oint_\gamma \operatorname{tr} \frac{d}{dz} \log[1 + R_p(H(z))]\, dz$$

$$= \frac{1}{2\pi i} \oint_\gamma \operatorname{tr} \frac{d}{dz} \left[(1 + H(z)) \exp\left(\sum_{j=1}^{p-1} (-1)^j j^{-1} (H(z))^j \right) \right]$$

$$\times \left[(1 + (H(z)) \exp\left(\sum_{j=1}^{p-1} (-1)^j j^{-1} (H(z))^j \right) \right]^{-1} dz$$

$$= \frac{1}{2\pi i} \operatorname{tr} \oint_\gamma H'(z)(1 + H(z))^{-1} + \frac{d}{dz} \left(\sum_{j=1}^{p-1} (-1)^j \frac{1}{j} (H(z))^j \right) dz$$

$$= \frac{1}{2\pi i} \operatorname{tr} \oint_\gamma H'(z)(1 + H(z))^{-1}\, dz.$$

The general case follows now by an approximation argument. We remark that $\operatorname{tr} \oint_\gamma h'(z)\, h(z)^{-1}\, dz$ is finite for any $h(z) = 1 + H(z)$ with $H(z) \in \mathscr{I}_p$:

$$\operatorname{tr} \oint_\gamma H'(z)(1 + H(z))^{-1}\, dz$$

$$= \operatorname{tr} \oint_\gamma H'(z) \left[\sum_{\nu=0}^{p-1} (-1)^\nu H(z)^\nu + (-1)^p H(z)^p (1 + H(z))^{-1} \right]$$

$$\leq \oint_\gamma \| H'(z)\, H(z)^p (1 + H(z))^{-1} \|_p\, dz$$

$$\leq \oint_\gamma \| (1 + H(z))^{-1} H'(z) \|_\infty \| H(z)^p \|_1\, dz < \infty.$$

Let the $H_n(z)$ be a sequence converging uniformly in $\|\cdot\|_p$-norm to $H(z)$; e.g., if e_ν is an orthonormal basis of $\mathscr{H}$, define $H_n(z)$ by

$$H_n(z)e_\nu := \begin{cases} H(z)e_\nu & \text{for } \nu \le n \\ 0 & \phantom{\text{for }} \nu > n. \end{cases}$$

Then for $h_n(z) = 1 + H_n(z)$

$$\frac{1}{2\pi i} \operatorname{tr} \oint_\gamma h'(z)\, h(z)^{-1}\, dz = \frac{1}{2\pi i} \lim_{n\to\infty} \operatorname{tr} \oint_\gamma h_n'(z)\, h_n(z)^{-1}\, dz.$$

Thus the left-hand side is an integer as claimed.

Second, we show that the left-hand and right-hand sides can be continuously deformed into each other: Define on γ

$$h_\kappa = f(z)^{-1} + \kappa(g(z) - f(z)^{-1})$$

which is well defined since, because of (4), $f(z)$ is invertible on γ.

We have

$$\operatorname{tr} \oint_\gamma h_0'(z)\, h_0(z)^{-1}\, dz = -\operatorname{tr} \oint_\gamma f'(z)\, f(z)^{-1}\, dz$$

which is formally obvious. For the actual proof, however, an approximation argument like that in the first step is needed to justify that $f'(z)$ commutes with $f(z)^{-1}$ under $\operatorname{tr} \oint$. We do not repeat the argument since it is completely analogous. Furthermore

$$h_1'(z)\, h_1(z)^{-1} = g'(z)\, g(z)^{-1}.$$

Now we can connect both sides of (5) by an analytic function in κ by writing the Neumann series

$$\begin{aligned} h_\kappa(z)^{-1} &= \sum_{\nu=0}^{\infty} \{f(z)[g(z) - f(z)^{-1}]\}^\nu f(z)(-\kappa)^\nu \\ &= \sum_{\nu=0}^{\infty} (f(z)\, g(z) - 1)^\nu f(z)(-\kappa)^\nu \end{aligned}$$

which converges because of (4) in $\|\cdot\|_p$-norm. ∎

We remark that this theorem generalizes an earlier result of Algazin [9] who proved it for the case where $f(z)$ is the resolvent of some operator A and $g(z) = B - z$. Algazin [9] did not require that A and B be in some trace ideal. For the applications we will discuss, this is not essential. We shall see that even for the unbounded operators $H(\theta)$, the complex scaled Hamiltonians, spectral values can be localized by (5). It will, however, prove to be essential that we do not restrict ourselves to the case of resolvents for f or g.

3. Localization of Resonances

In order to define resonances for a Schrödinger operator $H = -\Delta + V$, we require that the potential V be exterior dilation analytic, i.e.:

(i) V is a symmetric form with $Q(V) \supset Q(-\Delta)$, where $Q(V)$ and $Q(-\Delta)$ are the form domains of the potential and the Laplacian, respectively.

(ii) $(-\Delta+1)^{-1/2} V(-\Delta+1)^{-1/2}$ is compact.

(iii) There are R, $\alpha > 0$ such that

$$F(\theta) = (-\Delta+1)^{-1/2} (u_R(\theta) V u_R(\theta)^{-1})(-\Delta+1)^{-1/2}$$

which is defined for real θ as an extension to an analytic bounded operator-valued function into the strip $B_\alpha = \{\theta \mid |\mathrm{Im}\,\theta| < \alpha\}$, where $u_R(\theta)$ is the unitary transformation

$$(u_R(\theta) f)(x) = \left[\det \frac{\partial(S(\theta, R)x)}{\partial x}\right]^{1/2} f(S(\theta, R)x)$$

with

$$S(\theta, R)x = \begin{cases} x & \text{for } |x| \leqslant R \\ [R + e^\theta(|x| - R)](x/|x|) & \phantom{\text{for }} |x| > R. \end{cases}$$

A point in the discrete spectrum $\sigma_d(H_\theta)$ of $H(\theta) = u(\theta)(-\Delta + V)\, u(\theta)^{-1}$, the exterior dilated Schrödinger operator with exterior dilation analytic potential V, is called a resonance of H if its imaginary part is nonzero, and a bound state otherwise. For further details of the exterior dilation analytic formalism we refer to [11–13]. Here we need only the fact that $E \in \sigma_d(H_\theta)$ iff the complex dilated Rollnik kernel

$$W_{R,\theta,E} = |V(R, \theta)|^{1/2}\, G_0(R, \theta, E)\, V^{1/2}(R, \theta)$$

has the eigenvalue one and its multiplicities are the same ($G_0(R, \theta, E)$ is the exterior dilated free resolvent $(E+\Delta)^{-1}$, and $V(R, \theta)$ is the exterior dilated potential) for $E \notin e^{-2\theta}\mathbb{R}_+$. We observe that $W_{R,\theta,E}$ is analytic as a function of E in this region.

In order to apply the above theorem, we need not only compactness but some lower trace ideal property of the Rollnik kernel. For short range potentials the Rollnik kernel is Hilbert–Schmidt, and for longer range potentials a higher trace ideal must be considered. (For a more detailed discussion see [2].) Assuming such a trace ideal property, we may choose in (4)

$$f(E) = 1 - W_{R,\theta,E}$$

and, e.g.,

$$g(E) = 1 + \alpha W_{R,\theta,E} + \beta W_{R,\theta,E} + \cdots$$

with E dependent meromorphic functions α, β, ...

As shown in [14, 15] there can be no eigenvalue one and thus no resonance or bound state at E if $\|f(E)\, g(E) - 1\|_p$ is less than one. Therefore $W_{R,\theta,E}$ can have eigenvalues only where this quantity is greater than or equal to one; i.e., if the contourline $\phi(E) = 1$ is closed, the resonances and bound states with E "above" the cut $e^{-2\theta}\mathbb{R}_+$ are enclosed by this contourline. In [14, 15], however, the existence or nonexistence of resonances within this contourline is not discussed. By application of the above theorem we get the exact number of resonances and bound states within this region. We shall demonstrate this for the exactly solvable example used in [15] to exclude resonances, the δ-shell potential $V = -c\delta_a(|x|)$ where δ_a is the (one-dimensional) Dirac distribution. Because of the spherical symmetry of the problem we may look at each angular momentum subspace l, m separetely. The corresponding radial equation is one-dimensional. The δ-potential can be treated as a form perturbation. The whole Schrödinger operator may then be defined as a direct product of these radial operators. The Rollník operator $W_{l,m,R,\theta,W}$ projected onto the space with fixed angular momentum l, m has an explicit "integral kernel" (sequence of kernels with potentials concentrated around $|x| = a$) in terms of Bessel functions

$$W_{l,m,R,\theta,E} = -|V|^{1/2}(r)\, K_{l+1/2}(\sqrt{-E}r_>)\, I_{l+1/2}(\sqrt{-E}r_<)\, V^{1/2}(r')(r \cdot r')^{1/2}$$

($r_> = \max(r, r')$ and $r_< = \min(r, r')$) which does not depend on R and θ since the potential has compact support. We may then apply the theorem with

$$f(E) = 1 - W_E,$$

where we have suppressed all indices except E; for g we choose

$$g(E) = 1 + \frac{-1}{\mathrm{tr}(W_E - 1)}\, W_E.$$

We observe that $g(E)$ is an analytic function in E as long as $E \notin e^{-2\theta}\mathbb{R}_+$

and one avoids the zeros of $\operatorname{tr}(W_E - 1)$. Furthermore a straightforward calculation shows that with this choice of g in the complement of these E

$$\|f(E)\, g(E) - 1\|_2^2 = 0$$

in the limit of the δ-potential. Thus, for each curve δ surrounding a zero of $\operatorname{tr}(W_E - 1)$, hypothesis (4) is fulfilled.

Now g has a singularity where $\operatorname{tr}(W_E - 1) = 0$. Thus

$$-\frac{1}{2\pi i} \operatorname{tr} \oint_\gamma dz\, g'(z)\, g(z)^{-1} \neq 0,$$

showing the existence of resonances at these points.

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