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The extraordinary spectral properties of radially periodic Schrödinger operators

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Abstract. Since it became clear that the band structure of the spectrum of periodic Sturm–Liouville operators $t = -(\mathrm{d}^2/\mathrm{d}r^2) + q(r)$ does not survive a spherically symmetric extension to Schrödinger operators $T = -\Delta + V$ with $V(x) = q(|x|)$ for $x \in \mathbb{R}^d$, $d \in \mathbb{N}\setminus\{1\}$, a wealth of detailed information about the spectrum of such operators has been acquired. The observation of eigenvalues embedded in the essential spectrum $[\mu_0, \infty[$ of T with exponentially decaying eigenfunctions provided evidence for the existence of intervals of dense point spectrum, eventually proved by spherical separation into perturbed Sturm–Liouville operators $t_c = t + (c/r^2)$. Subsequently, a numerical approach was employed to investigate the distribution of eigenvalues of T more closely. An eigenvalue was discovered below the essential spectrum in the case $d = 2$, and it turned out that there are in fact infinitely many, accumulating at μ_0. Moreover, a method based on oscillation theory made it possible to count eigenvalues of t_c contributing to an interval of dense point spectrum of T. We gained evidence that an asymptotic formula, valid for $c \to \infty$, does in fact produce correct numbers even for small values of the coupling constant, such that a rather precise picture of the spectrum of radially periodic Schrödinger operators has now been obtained.

Keywords. Schrödinger operator; self-adjointness; embedded eigenvalue; exponential decay; dense point spectrum.

0. Introduction and preliminaries

The Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t, x) = (-\triangle + V(x))\ \Psi(t, x)$$

may certainly be counted among the most important pieces of physics *and* mathematics in the twentieth century. The mathematical interest associated with it and the corresponding operator $-\triangle + V$ can be characterized either by topical issues or by considering variants of the operator itself.

Early on it became clear by the work of J von Neumann and M H Stone that the unique solvability of the Schrödinger equation with the initial state $\Psi(0, \cdot)$ given amounts to prove that the Schrödinger operator as defined in L_2 on the set of test functions (smooth and with bounded support) is *essentially self-adjoint*, i.e. has a unique self-adjoint extension. Ever since, the question of (essential) self-adjointness has been central in the theory. Although this problem was essentially settled by the early 1970s (cf. ([18], Chapter 3), ([34], Chapter III)), we will discuss some less acknowledged aspects of it in § 0.1. Started in the early 1950s by È È Shnol', the interest in the connections between the *spectrum* of Schrödinger operators and the *asymptotic behavior of eigensolutions*, to which we will refer in § 0.2, reached its peak in the 1970s and early 1980s (cf. ([18], Chapter 4), ([34], Chapter IV)) with the now famous *Kato class* (named after T Kato, the 'father of the modern theory of Schrödinger operators ([34], p. 3523)') emerging as the most natural home for *potential functions* V. This was accompanied by the development of semigroup techniques and scattering theory, which led to a more thorough investigation into the fine structure of the spectrum these last twenty years. The discovery of peculiar spectral phenomena, like e.g. embedded eigenvalues, dense point spectrum and singular continuous spectrum, formed a motivation to consider magnetic (cf. ([34], Chapter X)), random (cf. ([34], Chapter VII)) and in particular one-dimensional (cf. ([34], Chapter V)) Schrödinger operators as well as Dirac operators. Originally just a mathematical curiosity, there is now some evidence that embedded eigenvalues can actually be observed experimentally (cf. [5]), thus adding to the revived interest in these questions.

In this survey we do not attempt to give a historical overview of all these developments; see the article [34] and its vast bibliography. We want to collect, correct, rearrange and refine some of the old and more recent results of the theory. We will concentrate on a class of operators which may not have received the attention it deserves, namely *spherically symmetric* Schrödinger operators (§ 1). It turns out that they live a life in between their one-dimensional and general higher dimensional brethren. On one hand, their spectra are qualitatively different from the spectra of the corresponding Sturm–Liouville operators; on the other hand the emergence of phenomena like embedded eigenvalues and dense point spectrum, or *localization* as it has become to be called, can be obtained by recourse to the one-dimensional theory. The spectral properties especially of *radially periodic* Schrödinger operators (§ 2) are therefore extra-ordinary in every sense of the word. For the same reason, spherically symmetric Schrödinger operators can be approached by numerical methods too, and we will report on an example of a numerical investigation into the distribution of eigenvalues in intervals of dense point spectrum in § 3. We hope that the elementary character of the cases treated in this article will contribute to the understanding of non-orthodox patterns in the spectral theory of differential operators.

0.1 *Self-adjointness*

A Schrödinger operator in $\mathrm{L}_2\left(\mathbb{R}^d\right)$, $d \in \mathbb{N}$, is of the form $-\Delta + V$ with a real-valued potential $V \in \mathrm{L}_{2,\mathrm{loc}}\left(\mathbb{R}^d\right)$. It is symmetric on a natural domain like $\mathrm{C}_0^\infty\left(\mathbb{R}^d\right)$, but this domain will be too small to make the operator self-adjoint. For the sake of definiteness it is therefore necessary to prove essential self-adjointness. A sufficient condition for a densely defined operator T in a Hilbert space H to possess a unique self-adjoint extension is the self-adjointness of its closure $\overline{T}$, because then for any self-adjoint extension S of T, we have $\overline{T} \subset S = S^* \subset \overline{T}^* = \overline{T}$, whence $S = \overline{T}$. So we have at our disposal all the classical criteria for self-adjointness as applied to $\overline{T}$. In practice, this turns out to be not too easy, but it is unavoidable, since self-adjointness of $\overline{T}$ happens to be also necessary for T to be essentially self-adjoint (cf., e.g., ([19], Theorem 1.2.7)).

The problem to show that $\overline{-\Delta + V \restriction \mathrm{C}_0^\infty\left(\mathbb{R}^d\right)}$ is self-adjoint in $\mathrm{L}_2\left(\mathbb{R}^d\right)$ has a long and winding history (cf. ([18], Chapter 3)). Unfortunately, there is no handy assumption on V which would be both sufficient and necessary. If the operator is bounded from below, it turns out that we only need a local condition on the negative part $V_- := \max\{0, -V\}$ of V, namely the *local Kato condition*.

DEFINITION 0.1

$K(\mathbb{R}^d)$ is the set of all measurable functions f on $\mathbb{R}^d$ with

$$\lim_{r\to 0}\sup_{x\in\mathbb{R}^d}\int_{|x-y|<r} s_d(x-y)\,|f(y)|\,\mathrm{d}y = 0,$$

where $s_d(z) = (1/\omega_d)\int_1^{|z|^{-1}} \rho^{d-3}\,\mathrm{d}\rho$, with ω_d the area of the unit sphere in $\mathbb{R}^d$. $\mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$ is the set of all functions f on $\mathbb{R}^d$ with $f\circ\chi_\Omega \in \mathrm{K}\left(\mathbb{R}^d\right)$ for every bounded, open $\Omega\subset\mathbb{R}^d$.

With this definition, the following result holds.

Theorem 0.1. *If $T := -\triangle + V\restriction C_0^\infty\left(\mathbb{R}^d\right)$ is bounded from below and $V_- \in \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$, then T is essentially self-adjoint in $\mathrm{L}_2\left(\mathbb{R}^d\right)$.*

The *proof* can be based upon the criterion that a positive operator T is essentially self-adjoint, iff its range is dense in H, i.e. iff T^* is injective. The latter can be shown as soon as one knows that every *eigensolution* for T and $\lambda\in\mathbb{R}$, i.e. $u\in \mathrm{L}_{1,\mathrm{loc}}\left(\mathbb{R}^d\right)\setminus\{0\}$ with $\forall\varphi \in C_0^\infty\left(\mathbb{R}^d\right) : \int u\,T\varphi = \lambda\int u\,\varphi$, is locally bounded, which is the case if $V_-\in \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$ (([1], Theorem 1.5), ([18], Corollary 2.8)).

Remark. The local Kato condition is not necessary for essential self-adjointness, as can be seen from the example $V(x) = -c\,|x|^{-2}$ in $\mathbb{R}^6$, where $V_-\notin \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^6\right)$ (cf. ([18], Example 1.7)), but T is bounded from below iff $c\le 4$ and essentially self-adjoint iff $c\le 3$ (cf. ([12], VII Proposition 4.1)).

There are a couple of applications of Theorem 0.1. First of all, boundedness from below T can be guaranteed by the assumption $V_-\in\mathrm{K}\left(\mathbb{R}^d\right)$ due to relative form boundedness with respect to $-\triangle$ (cf. ([18], Corollary 3.3)). Moreover, by truncating the negative part of the potential, we may even use Theorem 0.1 to obtain essential self-adjointness of Schrödinger operators which are not bounded from below, namely allowing for a behavior of the potential like $-\mathrm{O}\left(|x|^2\right)$ at infinity (cf. ([18], Theorem 3.4); see also [21]).

COROLLARY 0.1

If $V_-\in\mathrm{K}\left(\mathbb{R}^d\right)+\mathrm{O}\left(|x|^2\right)$, then $-\triangle + V\restriction C_0^\infty\left(\mathbb{R}^d\right)$ is essentially self-adjoint in $\mathrm{L}_2\left(\mathbb{R}^d\right)$.

Let us mention that the same approach allows to treat magnetic Schrödinger operators as well, i.e. $T := -(\nabla - i\,b)^2 + V\restriction C_0^\infty\left(\mathbb{R}^d\right)$, as long as b is continuously differentiable as a function from $\mathbb{R}^d$ to $\mathbb{R}^d$; if one employs the method of H Leinfelder and C Simader, one can even cover the most general case where $b\in\left(\mathrm{L}_{4,\mathrm{loc}}\left(\mathbb{R}^d\right)\right)^d$ and $\nabla\cdot b\in \mathrm{L}_{2,\mathrm{loc}}\left(\mathbb{R}^d\right)$ (cf. ([19], Theorem 2.5)).

The big open question about essential self-adjointness of Schrödinger operators is conjecture of K Jörgens (1972), where no progress seems to have occurred since twenty years (cf. [7]).

Conjecture. If $-\triangle + V\restriction C_0^\infty\left(\mathbb{R}^d\right)$ is bounded from below and essentially self-adjoint in $\mathrm{L}_2\left(\mathbb{R}^d\right)$ and if $W\in\mathrm{L}_{2,\mathrm{loc}}\left(\mathbb{R}^d\right)$ with $W\ge V$, then $-\triangle + W\restriction C_0^\infty\left(\mathbb{R}^d\right)$ is essentially self-adjoint in $\mathrm{L}_2\left(\mathbb{R}^d\right)$.

By Theorem 0.1 this is open for dimensions $d\ge 4$, because $\mathrm{L}_{2,\mathrm{loc}}\left(\mathbb{R}^d\right)\subset \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$ for $d\le 3$.

0.2 *Asymptotic behavior of eigensolutions and the spectrum*

Once the essential self-adjointness of $-\Delta + V \restriction C_0^\infty\left(\mathbb{R}^d\right)$ being established, the *spectrum* σ of T, by which we will from now on denote the self-adjoint closure of this operator, and its parts are well-defined. We will consider the decompositions

$$\sigma_{\mathrm{e}}(T) \,\dot\cup\, \sigma_{\mathrm{d}}(T) = \sigma(T) = \sigma_{\mathrm{c}}(T) \cup \overline{\sigma_{\mathrm{p}}(T)},$$

where σ_{p} is the *point spectrum*, i.e. the set of eigenvalues, σ_{d} is the *discrete spectrum*, i.e. the set of eigenvalues of finite multiplicity which are isolated from other elements of the spectrum, with the *essential spectrum* σ_{e} being its complement in σ, and σ_{c} denotes the *continuous spectrum*. A further decomposition of the latter into an *absolutely continuous* and a *singular continuous* part, useful in scattering theory, will not be pursued here.

There are a couple of tools to investigate the essential spectrum which are specific for Schrödinger operators and show that it depends mainly on the behavior of V at ∞. The most important are the following, which go back to ideas of Glazman ([13], p. 59ff, 71ff) Shnol' ([33], p. 121) and Persson ([24], Theorem 2.1).

Theorem 0.2. *Let* $T := \overline{-\Delta + V \restriction C_0^\infty\left(\mathbb{R}^d\right)}$ *be self-adjoint and* $V_- \in \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$. *Then*

(a) $\quad \lambda \in \sigma_{\mathrm{e}}(T) \Leftrightarrow \exists\, \varphi_n \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_n\right),\ \|\varphi_n\| = 1 : (T-\lambda)\varphi_n \to 0,\ n \to \infty.$

If T *is bounded from below, then*

(b) $\quad \inf \sigma_{\mathrm{e}}(T) = \sup\limits_{n\in\mathbb{N}} \inf \left\{(T\varphi, \varphi);\ \varphi \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_n\right),\ \|\varphi\| = 1\right\}.$

Here $\overline{\mathrm{B}}_n := \left\{x \in \mathbb{R}^d;\ \|x\| \le n\right\}$.

Proof. A simple proof of statement (a) in this general form can be found in ([15], p. 199f). If $\sigma_{\mathrm{e}}(T) \ne \emptyset$ in (b), then $\inf \sigma_{\mathrm{e}}(T) \in \sigma_{\mathrm{e}}(T)$, since T is bounded from below, and '$\ge$' follows easily from (a).

For '$\le$' in (b), we may assume $T \ge 1$. Let $0 \le \mu < \inf \sigma_{\mathrm{e}}(T)$. Then we have

$$\exists\, K \in \mathbb{N}_0\, \exists\, \psi_k \in \mathrm{L}_2\left(\mathbb{R}^d\right),\ \|\psi_k\| = 1\, \forall\, f \in \mathrm{L}_2\left(\mathbb{R}^d\right) :\ E_\mu f = \sum_{k=1}^{K} (f, \psi_k)\, \psi_k,$$

where $(E_\lambda)_{\lambda\in\mathbb{R}}$ denotes the spectral family of T. Hence

$$\forall\, \varphi \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_n\right) :\ \left\|E_\mu \varphi\right\| \le \sum_{k=1}^{K} \left(\int_{\mathbb{R}^n \setminus \overline{\mathrm{B}}_n} |\psi_k|^2\right)^{1/2} \|\varphi\|.$$

Now let $0 < \varepsilon < 1$; then there is an $n_\varepsilon \in \mathbb{N}$ such that $\forall\, \varphi \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_{n_\varepsilon}\right) :\ \left\|E_\mu\varphi\right\| \le \varepsilon\, \|\varphi\|$, whence

$$\begin{aligned}(T\varphi, \varphi) &= \left(T\left(1 - E_\mu\right)\varphi, \varphi\right) + \left(T E_\mu \varphi, \varphi\right) \ge \mu\, \left\|\left(1 - E_\mu\right)\varphi\right\|^2 \\ &\ge \mu\, \left(\|\varphi\| - \left\|E_\mu\varphi\right\|\right)^2 \ge \mu\,(1-\varepsilon)^2\, \|\varphi\|^2.\end{aligned}$$

Therefore $\inf \left\{(T\varphi, \varphi);\ \varphi \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_{n_\varepsilon}\right),\ \|\varphi\| = 1\right\} \ge \mu\,(1-\varepsilon)^2$ and letting $\varepsilon \to 0$, we arrive at $\sup\limits_{n\in\mathbb{N}} \inf \left\{(T\varphi, \varphi);\ \varphi \in C_0^\infty\left(\mathbb{R}^d \setminus \overline{\mathrm{B}}_n\right),\ \|\varphi\| = 1\right\} \ge \mu$.

There are intimate relations between the different parts of the spectrum and the asymptotic behavior of eigensolutions at infinity, the obvious one being

$$\lambda \in \sigma_{\mathrm{p}}(T) \Leftrightarrow \exists \text{ eigensolution } u \in \mathrm{L}_2\left(\mathbb{R}^d\right);$$

such eigensolutions in $\mathrm{L}_2\left(\mathbb{R}^d\right)$ are called *eigenfunctions*. The general idea is that $\lambda \in \sigma$ is associated with bounded eigensolutions and that eigenfunctions for discrete eigenvalues do decay exponentially. The precise statements, however, depend on the behavior of the potential V at infinity. They read as follows:

PROPOSITION 0.1

If $V_- \in \mathrm{K}\left(\mathbb{R}^d\right) + \mathrm{o}\left(|x|^2\right)$, *then*

$$\sigma(T) = \overline{\left\{\lambda \in \mathbb{R};\ \exists\, \gamma > 0\, \exists \textit{ eigensolution } u \textit{ for } T \textit{ and } \lambda:\ (1 + |\cdot|)^{-\gamma}\, u \in \mathrm{L}_\infty\left(\mathbb{R}^d\right)\right\}}.$$

This follows from ([19], Main Theorem), where a magnetic potential b is allowed for too. There are two obvious questions, namely if it is utterly necessary to take the closure on the right-hand side and if $\gamma = 0$ would suffice for the inclusion '$\subset$'.

PROPOSITION 0.2

If $V_- \in \mathrm{K}\left(\mathbb{R}^d\right) + \mathrm{o}\left(|x|^2\right)$, *then every eigenfunction of* T *for* $\lambda \in \sigma_{\mathrm{d}}(T)$ *decays faster than any inverse polynomial*; *if* $V_- \in \mathrm{K}\left(\mathbb{R}^d\right)$, *then the decay is faster than* $\exp(-\mu|x|)$ *for some* $\mu > 0$.

This can be found in ([18], Corollary 4.5).

The case where V_- behaves like $\mathrm{O}\left(|x|^2\right)$ at infinity is open for dimensions $d \geq 2$. An example of G Halvorsen for $d = 1$, where there is a $\lambda \in \mathbb{R} \setminus \sigma(T)$ with a bounded eigensolution and an eigenfunction for a discrete eigenvalue which decays only polynomially, indicates that both Propositions 0.1 and 0.2 may fail for these potentials in any dimension (cf. the discussion in ([18], Chapter 5)).

More explicit bounds on eigenfunctions are known for the standard case of a potential which tends to some constant at infinity (cf. ([18], § 4.1)).

PROPOSITION 0.3.

Let $V \in \mathrm{K}_{\mathrm{loc}}\left(\mathbb{R}^d\right)$ *with* $V(x) \to V_0 \in \mathbb{R} \cup \{\infty\}$, *as* $|x| \to \infty$. *Then for every eigenfunction* u *for* $\lambda \in \sigma_{\mathrm{p}}$ *and any* $\mu < \sqrt{\operatorname{dist}(\lambda, \sigma_{\mathrm{e}})}$: $u(x) = \mathrm{O}(\exp(-\mu|x|))$; *if* $u > 0$, *then* $(\ln(u(x))/|x|) \to -\sqrt{\operatorname{dist}(\lambda, \sigma_{\mathrm{e}})}$, as $|x| \to \infty$. *Moreover,* $\sigma_{\mathrm{e}}(T) = [V_0, \infty[$.

If $V(x) \geq V_0 - c\,|x|^{-1-\varepsilon}$ outside a compact set for some $c > 0$ and $\varepsilon > 0$, i.e. in particular for *short range* potentials, we even get, by subharmonic comparison, $u(x) = \mathrm{O}\left(|x|^{-((d-1)/2)} \exp(-\sqrt{\operatorname{dist}(\lambda, \sigma_{\mathrm{e}})}\, |x|)\right)$ (cf. ([6], Theorem 2) or ([17], Theorem 2) in conjunction with ([16], Lemma 10)).

The lower bound for positive u suggests that the exponential decay rate given in Proposition 0.3 is optimal in general. Two cases are of interest: eigenvalues below the essential spectrum, as in Proposition 0.3, and eigenvalues in gaps of the essential spectrum, whose existence has been proved in ([22], Theorem (2.2)) and [10] (cf. also [16]). We will approach this question in the following section.

1. Spherical symmetry

We now come to the investigation of the spectrum of *spherically symmetric* Schrödinger operators, where $d \in \mathbb{N} \setminus \{1\}$, and the potential is of the form $V(x) = q(r)$ with some $q : [0, \infty[\to \mathbb{R}$, $r := |x|$. They have been used to demonstrate statements (cf., e.g., ([35], Problem 8)) or to provide (counter-)examples in spectral theory and also in the scattering theory (cf. ([2], Chapter 11)). We will start with some basic examples leading to classical types of spectra and then turn to the phenomenon of *embedded eigenvalues*, i.e. $\lambda \in \sigma_{\mathrm{p}}(T) \cap \sigma_{\mathrm{e}}(T)$. All examples will be in $\mathbb{R}^3$.

1.1 *Some basic examples*

Classical types of spectra are a *purely continuous spectrum*, as in the case of the free particle, where $q = 0$ and $\sigma_{\mathrm{e}}(T) = \sigma(T) = \sigma_{\mathrm{c}}(T) = [0, \infty[$, $\sigma_{\mathrm{p}}(T) = \emptyset$, or a *purely discrete spectrum*, as for the harmonic oscillator with $q(r) = r^2$ and $\sigma(T) = \sigma_{\mathrm{d}}(T) = \{3 + 2k;\ k \in \mathbb{N}_0\}$.

The hydrogen atom, where $q(r) = -(1/r)$, has a *combined discrete/continuous spectrum*

$$\sigma_{\mathrm{p}}(T) = \sigma_{\mathrm{d}}(T) = \left\{-\frac{1}{4(k+1)^2};\ k \in \mathbb{N}_0\right\}, \sigma_{\mathrm{e}}(T) = \sigma_{\mathrm{c}}(T) = [0, \infty[\,.$$

The function $u(x) = \exp(-(r/2))$ is a *ground state* eigenfunction, i.e. for the lowest point $\lambda = -(1/4)$ of the spectrum. Eigenfunctions which do not change sign are always associated with the lowest point of the spectrum. More general, we have the following:

Theorem 1.1. *Let $-\Delta + V \restriction \mathrm{C}_0^\infty(\mathbb{R}^d)$ be bounded from below and $V \in \mathrm{K}_{\mathrm{loc}}(\mathbb{R}^d)$. If there exists a positive eigensolution u for $\lambda \in \mathbb{R}$ and $T := \overline{-\Delta + V \restriction \mathrm{C}_0^\infty(\mathbb{R}^d)}$, then $\lambda \le \min \sigma(T)$.*

Proof. Let $\varphi \in \mathrm{C}_0^\infty(\mathbb{R}^d)$ be real-valued. Since $u \in \mathrm{C}(\mathbb{R}^d) \cap \mathrm{W}^1_{2,\mathrm{loc}}(\mathbb{R}^d)$ (cf. ([18], Corollaries 2.8 and 2.9)), we may replace $\psi \in C_0^\infty(\mathbb{R}^d)$ in

$$0 = -\int u\,\Delta\psi + \int u\,(V - \lambda)\psi = \int \nabla u \cdot \nabla\psi + \int u\,(V - \lambda)\psi$$

by φ^2/u, whence after some calculation we get

$$0 = \int |\nabla\varphi|^2 - \int u^2 \left|\nabla\left(\frac{\varphi}{u}\right)\right|^2 + \int u\,(V - \lambda)\frac{\varphi^2}{u},$$

that is

$$((T - \lambda)\varphi, \varphi) = \int u^2 \left|\nabla\left(\frac{\varphi}{u}\right)\right|^2 \ge 0.$$

As T and λ are real, we arrive at $\forall\,\varphi \in \mathrm{C}_0^\infty(\mathbb{R}^d) : \lambda\,\|\varphi\|^2 \le (T\varphi, \varphi)$, whence $\lambda \le \min \sigma(T)$, because T is self-adjoint by Theorem 0.1.

Ground state eigenfunctions can have a faster decay rate than the one expected in view of Proposition 0.3. Here is an example.

Example 1. With $\alpha(r) = r + (1/6)\sin(3r)$ let

$$q(r) = \alpha'(r)^2 \left(1 - \frac{2}{\cosh(\alpha(r))^2}\right) - \left(\alpha''(r) + \frac{2}{r}\alpha'(r)\right)\tanh(\alpha(r)) .$$

Then $0 \in \sigma_{\mathrm{d}}(T)$ with eigenfunction $u(x) = 1/\cosh(\alpha(r))$ and $\sigma_{\mathrm{e}}(T) = [\mu_0, \infty[$, where $\mu_0 < 1$ ($\mu_0 \approx 0.9466$).

The *proof* for Example 1 depends on the following theorem, where

$$t = \overline{-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + q(r)\restriction C_0^\infty(\mathbb{R})}$$

in $L_2(\mathbb{R})$ ($q(-r) = q(r)$).

Theorem 1.2. *Let* $q \in C([0, \infty[)$, *with*

$$\frac{1}{r}\sup\left\{\frac{|q(r) - q(s)|}{|r - s|};\ 0 < |r - s| < 1\right\} \to 0,\ \text{as } r \to \infty,$$

and such that t *and* T *are self-adjoint. Then* $]\inf \sigma_{\mathrm{e}}(t), \infty[\ \subset \sigma_{\mathrm{e}}(T)$. *If* q_- *is bounded, then* $[\inf \sigma_{\mathrm{e}}(t), \infty[\ = \sigma_{\mathrm{e}}(T)$.

The *proof* of the first statement (cf. ([15], Corollary 1)) is based on rectangular separation and Theorem 0.2(a). (The same fundamental ideas have been employed in [27] to study the corresponding question for three-dimensional spherically symmetric Dirac operators.) If $q_- \in K(\mathbb{R})$ (and consequently $V_- \in K(\mathbb{R}^d)$; cf. ([18], Lemma 1.6)), we can prove $[\inf \sigma_{\mathrm{e}}(t), \infty[\ \subset \sigma_{\mathrm{e}}(T)$ without any further local assumption on q, based on spherical separation and the construction of singular sequences by cutting off eigensolutions (cf. ([15], Proposition 2)). (For an alternative proof of this inclusion, see [40].) Under the same assumption on q and making use of Theorem 0.2(b), it is possible to show that $\inf \sigma_{\mathrm{e}}(t) \le \inf \sigma_{\mathrm{e}}(T)$ (cf. ([15], Proposition 1)), with the second statement of Theorem 1.2 as an immediate consequence. We refer to [15], where details on the determination of μ_0 in Example 1 can be found as well.

Theorem 1.2 limits the possibilities to construct an example of an *isolated eigenvalue* λ of T *of infinite multiplicity*, i.e.

$$\exists\, \varepsilon > 0 :\ E_{\lambda-\varepsilon} = E_{\lambda-},\ E_\lambda = E_{\lambda+\varepsilon},\ \dim\,(E_\lambda - E_{\lambda-})\, L_2\left(\mathbb{R}^d\right) = \infty.$$

On the other hand, the results of this section yield many other eigenvalues in the essential spectrum.

1.2 *Embedded eigenvalues*

Theorem 1.1 allows us to construct an example of an *eigenvalue at the bottom of the* (*essential*) *spectrum*.

Example 2. Let $q(r) = 2((r^2 - 3)/(1 + r^2)^2)$. Then $0 \in \sigma_{\mathrm{p}}(T)$, $\sigma_{\mathrm{d}}(T) = \emptyset$, $\sigma_{\mathrm{e}}(T) = [0, \infty[$.

Proof. $u(x) = (1/(1+r^2))$ is an eigenfunction for $\lambda = 0$. The rest follows from Theorem 1.1 and Proposition 0.3.

As mentioned in the introduction, there is now a revived interest in eigenvalues which are *strictly* embedded in the essential spectrum (cf. also [37]). The example which produced the first scandal is due to J von Neumann and E Wigner (cf. [23]; note that the source of this reference is often cited inaccurately); here is a slightly corrected and simplified version.

Example 3 (*von Neumann and Wigner*). With $\alpha(r) = 2\,r - \sin(2\,r)$ let

$$q(r) = -1 - \frac{8\,\sin(2r)}{1+\alpha(r)} + \frac{32\,\sin(r)^4}{(1+\alpha(r))^2}.$$

Then $0 \in \sigma_{\rm p}(T)$, $\sigma_{\rm e}(T) = [-1, \infty[$.

Proof. $u(x) = \sin(r)/(r(1+\alpha(r)))$ is an eigenfunction for $\lambda = 0$. The rest follows from Proposition 0.3. □

As in Example 2, the eigenfunction in the von Neumann/Wigner example decays only polynomially. With Theorem 1.2 on hand, we are now able to produce an *embedded eigenvalue with an exponentially decaying eigenfunction*.

Example 4. Let $q(r) = -1 + (1/25)\,\sin(r)^4 - (2/5)\,\sin(2r)$. Then $\sigma_{\rm e}(T) \supset [-(14/25), \infty[$, and $0 \in \sigma_{\rm p}(T)$, with eigenfunction

$$u(x) = (\sin(r)/r)\exp(-(1/10)\,(r - (1/2)\sin(2r))).$$

For the *proof* we only have to observe that by Theorem 0.2(b), $\min \sigma_{\rm e}(t) \le \max q(r) \le -(14/25)$ and use Theorem 1.2.

Example 4 seems to be the only existing example where both an embedded eigenvalue and its exponentially decaying eigenfunction are known explicitly. It puts an end to efforts to provide lower bounds for eigenfunctions, even for spherical means, for large classes of Schrödinger operators and opens one path to the phenomenon which has now become known as *localization*, i.e. the existence of dense point spectrum associated with exponentially decaying eigenfunctions (cf. [38]).

2. Radial periodicity

Examples 1 and 4 suggest a further investigation into spherically symmetric Schrödinger operators which are *radially periodic*, i.e. where q is a *periodic* (even) function; we also assume q to be bounded, throughout. To fix notation, we remark the following: for $f \in \mathrm{L}_{1,\mathrm{loc}}(\mathbb{R})$, let $P_f := \{\alpha \in \mathbb{R};\ f = f_\alpha\}$, where $f_\alpha \in \mathrm{L}_{1,\mathrm{loc}}(\mathbb{R})$ is given by $\forall\, r \in \mathbb{R}:\ f_\alpha(r) = f(r+\alpha)$, and define $\alpha_f := \inf\left\{\alpha \in P_f;\ \alpha > 0\right\}$.

Lemma 2.1. *If* $f \in \mathrm{L}_{1,\mathrm{loc}}(\mathbb{R})$, *then*

$$0 < \alpha_f < \infty \Leftrightarrow P_f = \mathbb{Z}\alpha_f$$
$$\alpha_f = 0 \Leftrightarrow f \ \ is\ \ constant.$$

Proof. P_f is a subgroup of $(\mathbb{R}, +)$, such that it is either trivial, non-trivial and discrete or dense in $\mathbb{R}$, with $\alpha_f = \infty$, $P_f = \mathbb{Z}\alpha_f$, $\alpha_f = 0$, respectively. In the latter case there is a sequence $(\alpha_n)_{n\in\mathbb{N}} \subset P_f$ with $0 < \alpha_n \to 0$ as $n \to \infty$. Let $\varphi \in C_0^\infty(\mathbb{R})$ be real-valued. Then

$$\int f\,\varphi' = \lim_{n\to\infty} \int f\,\frac{\varphi - \varphi_{-\alpha_n}}{\alpha_n} = \lim_{n\to\infty} \int \frac{f - f_{\alpha_n}}{\alpha_n}\,\varphi = 0,$$

whence f is constant by the Lemma of DuBois–Reymond. □

Now the following definition makes sense.

DEFINITION 2.1

$f \in L_{1,\mathrm{loc}}(\mathbb{R})$ is called periodic with (principal) period α_f, iff $0 < \alpha_f < \infty$.

Remark. It is easy to extend this notion of periodicity and period to distributions.

Typically, the spectrum of a one-dimensional periodic Schrödinger operator has band structure (cf., e.g., ([11], § 5.3), ([39], § 12)), as for instance in the prototype case of the *Mathieu operator*, where $q = \cos$; here

$$\sigma(t) = \sigma_{\mathrm{e}}(t) = \bigcup_{k=1}^{\infty} \left[\mu_{k-1}, M_k\right],\ \sigma_{\mathrm{p}}(t) = \emptyset,$$

with $\mu_{k-1} < M_k < \mu_k \to \infty$, as $k \to \infty$ ($\mu_0 \approx -0.3785,\ M_1 \approx -0.3477,\ \mu_1 \approx 0.5948,\ M_2 \approx 0.9181,\ \mu_2 \approx 1.293, \ldots$). By Theorem 1.2, this is not so for radially periodic Schrödinger operators, their essential spectrum being a half-line.

2.1 *Dense point spectrum*

A spherically symmetric extension of t could possibly produce any kind of spectrum of T in spectral gaps of t: (absolutely or singular) continuous or dense point spectrum or even a mixture of these. In order to characterize the quality of the spectrum of T in the gaps of the spectrum of a periodic t, we note the following. By spherical separation,

$$\sigma_{\mathrm{c}}(T) = \overline{\bigcup_{l=0}^{\infty} \sigma_{\mathrm{c}}(t_{c_l})}, \tag{1}$$

where for $c \geq -(1/4)$, t_c is the Friedrichs extension in $L_2(]0,\infty[)$ of $-(\mathrm{d}^2/\mathrm{d}r^2) + q(r) + (c/r^2)$ on $C_0^\infty(]0,\infty[)$; $c_l = l(l+d-2) + (1/4)(d-1)(d-3),\ l \in \mathbb{N}_0$. Since the difference of resolvents for t_0 and t_c is compact (cf. ([14], Lemma 1)) and the essential spectra of t_0 and t are the same by virtue of Glazman's decomposition principle (cf. ([13], Chapter I, Theorem 23)), we have $\sigma_{\mathrm{e}}(t_c) = \sigma_{\mathrm{e}}(t)$. Combining this with (1), we arrive at $\sigma_{\mathrm{c}}(T) \subset \sigma_{\mathrm{e}}(t)$. Together with Theorem 1.2, this yields the following result.

Theorem 2.1. *Let q be bounded. If* $\min \sigma_{\mathrm{e}}(t) \leq \lambda_1 < \lambda_2$ *with* $]\lambda_1, \lambda_2[\cap \sigma_{\mathrm{e}}(t) = \emptyset$, *then*

$$]\lambda_1, \lambda_2[\ \cap\ \sigma_{\mathrm{c}}(T) = \emptyset,\ [\lambda_1, \lambda_2] \subset \overline{\sigma_{\mathrm{p}}(T)}.$$

For more details of the *proof*, see ([14], §1).

For every such q with a gap in the essential spectrum of the corresponding one-dimensional operator t we therefore have an *interval of dense point spectrum* for T.

Example 5. Let $q = \cos$, then

$$\sigma_{\mathrm{c}}(T) = \bigcup_{k=1}^{\infty} \left[\mu_{k-1}, M_k\right], \ \{\mu_0\} \cup \overline{\sigma_{\mathrm{p}}(T)} = \sigma_{\mathrm{d}}(T) \cup \{\mu_0\} \cup \bigcup_{k=1}^{\infty} [M_k, \mu_k].$$

If $d \geq 3$, then $\sigma_{\mathrm{d}}(T) = \emptyset$ and $\mu_0 \notin \overline{\sigma_{\mathrm{p}}(\mathrm{T})}$.

Proof. The first two results follow from Theorem 2.1, together with the fact that $\sigma_{\mathrm{p}}(t_c) \cap]\mu_{k-1}, M_k[= \emptyset$ (cf. ([14], Corollary 1)). For the last result we note that $c_l \geq 0$ for $d \geq 3$.

We have thus obtained a very elementary example of a Schrödinger operator with a spectrum consisting of alternating intervals of (absolutely, cf. ([14], Theorem 2)) continuous and dense point spectrum. The presence of intervals of dense point spectrum had been known for magnetic Schrödinger operators since the example of K Miller and B Simon (cf. ([8], §6.2)). Their construction, together with the ideas presented above also formed the basis for a more general investigation into the spectrum of two-dimensional magnetic Schrödinger operators with radial periodicity of both, the electric potential $V(x) = q(r)$ and the magnetic field, i.e. $(\partial b_2/\partial x_1)(x) - (\partial b_1/\partial x_2)(x) = B(r)$ with B and q periodic with period α (cf. [20]). It turns out that here too there are alternating intervals of absolutely continuous spectrum and dense point spectrum, provided that $\int_0^{\alpha} B(r)\mathrm{d}r = 0$, and that otherwise the essential spectrum consists entirely of dense point spectrum. Moreover, intervals filled with dense point spectrum can also be observed for spherically symmetric Dirac operators; cf. [28]. For localization in random Schrödinger operators we refer to [38] and the literature cited there. We also do not want to go into the one-dimensional case, for which we point to [25]. The construction of one-dimensional Dirac operators with a prescribed dense set of eigenvalues can be found in [29].

An interesting question is the persistence of dense point spectrum in our radially periodic examples under a compact support perturbation, say.

2.2 *Welsh eigenvalues*

In Example 5 the question of existence of discrete eigenvalues and the status of the lowest point μ_0 of the essential spectrum of T remained open for $d = 2$. As in connection with Example 1, where we constructed an admissible function for which the value of a quadratic form associated with t is strictly less than 1, thus showing that $\min \sigma_{\mathrm{e}}(T) = \min \sigma_{\mathrm{e}}(t) < 1$, we now produced a function in the form domain of t_0 with a value of the form strictly less than μ_0, such that for $q = \cos$ and $d = 2$, we have $\sigma_{\mathrm{d}}(T) \neq \emptyset$ (cf. [3]). Numerical calculations, based on the SLEIGN2 code to find eigenvalues of t_0 as restricted to functions defined on $]a, b[\subset]0, \infty[$ with $0 < a < b < \infty$, revealed the ground state, which was baptized the *Welsh eigenvalue* and denoted by $\lambda\!\lambda$ for its place of discovery, at about -0.4016. The question if the *lower spectrum*, i.e. the discrete spectrum below the essential spectrum, is finite or not is a delicate one, because the perturbation $-1/(4r^2)$ represents a borderline case which had not been studied before with sufficient thoroughness. The following can be shown by oscillation theory (cf. ([30], Theorem 2)).

PROPOSITION 2.1

Let $q \in \mathrm{L}_{2,\mathrm{loc}}(\mathbb{R})$ *be periodic with* $q_- \in \mathrm{L}_\infty(\mathbb{R})$; $d = 2$. *Then* $|\sigma_{\mathrm{d}}(T)| = \infty$ *and* $\min \sigma_{\mathrm{e}}(T) \in \overline{\sigma_{\mathrm{p}}(T)}$.

3. Numerical analysis

The preceding results suggest to look at the contribution of t_{c_l} for $l \in \mathbb{N}_0$ to $\sigma_p(T) \cap]M_k, \mu_k[$ for $k \in \mathbb{N}$ as well, if this gap in the spectrum of t is not empty, as in Example 5. For l fixed and k large enough, $|\sigma_p\left(t_{c_l}\right) \cap]M_k, \mu_k[\,| < \infty$ (cf. ([26], Corollary 3)). However, if we look into a fixed interval $]M_k, \mu_k[$, we get a similar result as in Proposition 2.1, at least for sufficiently large l.

PROPOSITION 3.1

Let $q \in \mathrm{L}_{2,\mathrm{loc}}(\mathbb{R})$ be periodic. If $c > c_{\mathrm{crit}} = (\alpha^2/(4|D|'(\mathrm{M}_k)))$, where $D(\mu)$ is the discriminant of $-u'' + q\,u = \mu\,u$, then $|\sigma_p\,(t_c) \cap]\mathrm{M}_k, \mu_k[\,| = \infty$, with eigenvalues accumulating at M_k like $(\sqrt{(c/c_{\mathrm{crit}}) - 1})/(4\pi)|\ln(\lambda - \mathrm{M}_k)\,|$ and no accumulation of eigenvalues at μ_k.

For the *proof* we refer to the article [31], an extension of which to periodic Dirac systems is given in [32].

Note that $c_{\mathrm{crit}} > 0$ in Proposition 3.1, so it applies to positive c only. In the sole case where $c_l < 0$, namely $d = 2$ and $l = 0$, there is no accumulation at the left end of a gap, but may be at the right end, as in Proposition 2.1.

To obtain further insight inside the gaps of $\sigma(t)$, we employed a numerical analysis to count eigenvalues of t_c in a closed subinterval of $]\mathrm{M}_k, \mu_k[$. The analytic foundation for our method to calculate $N(\lambda_1, \lambda_2; c) := |\sigma_p\,(t_c) \cap [\lambda_1, \lambda_2]\,|$ is the following result based on relative oscillation theory of Sturm–Liouville operators (cf. ([4], Proposition 1)).

PROPOSITION 3.2

Let $q \in \mathrm{L}_{2,\mathrm{loc}}(\mathbb{R})$ be periodic with period α. Let $c \geq 3/4$, $[\lambda_1, \lambda_2] \subset]\mathrm{M}_k, \mu_k[$, $k \in \mathbb{N}$. Choose constants $a > 0$, $m_1, m_2 \in \mathbb{N}$ such that $\inf\limits_{r \in]0,a[} \left\{q(r) + (c/r^2)\right\} > \lambda_2$, and $\left|(c/r^2)\right| \leq \operatorname{dist}\left(\lambda_j, \sigma(t)\right)$ for $r \geq m_j\alpha$ and $j \in \{1, 2\}$. Denote by n_j the number of zeros in $\left]a, m_j\alpha\right[$ of a non-trivial real-valued solution u_j of

$$-u''(r) + \left(q(r) - \lambda_j + \frac{c}{r^2}\right)u(r) = 0$$

satisfying the boundary condition $u_j(a) = 0$.

Then $N(\lambda_1, \lambda_2; c) - (n_2 - n_1 + (m_1 - m_2)k) \in \{-4, \ldots, 3\}$.

Remark. The restriction to $c \geq 3/4$ has been made for technical reasons only. It does not effect but the case $d = 2$ and $l = 0$.

With Proposition 3.2 in hand, the problem is therefore reduced to count zeros of solutions in finite intervals. This counting is particularly simple, if the solutions are piecewise trigonometric or hyperbolic functions, which is the case for piecewise constant coefficients in the equations. Such calculations have been performed in ([4], § 2). The results suggest a formula

$$N(\lambda_1, \lambda_2; c) \approx \sqrt{c} \int_{\lambda_1}^{\lambda_2} f(\lambda)\,\mathrm{d}\lambda$$

with some density function f depending on q and k only.

This compares to an asymptotic formula for $c \to \infty$ (cf. ([36], (1.8) and Theorem 3.8)

$$N(\lambda_1, \lambda_2; c) \sim \frac{\sqrt{c}}{\pi\alpha} \int\int \chi_{\lambda_1,\lambda_2}(\lambda, r)\, \mathrm{d}\kappa(\lambda)\, \mathrm{d}r; \tag{2}$$

here $\chi_{\lambda_1,\lambda_2}$ is the characteristic function of the set $\{(\lambda, r) \in \mathbb{R} \times]0, \infty[\,;\ \lambda + (1/r^2) \in [\lambda_1, \lambda_2]\}$, and κ is related to the discriminant D of t by $D(\lambda) = 2\cos(\kappa(\lambda))$ for λ inside the spectral bands, and it is constant in the spectral gaps of t.

For instance, if $k = 1$, we have $\mu_0 \leq \lambda(\kappa) = D^{-1}(2\cos(\kappa)) \leq \mathrm{M}_1 < \lambda_1 < \lambda_2 < \mu_1$, whence (2) can be written as

$$N(\lambda_1, \lambda_2; c) \sim \frac{\sqrt{c}}{\pi\alpha} \int_0^\pi \left(\frac{1}{\sqrt{\lambda_1 - \lambda(\kappa)}} - \frac{1}{\sqrt{\lambda_2 - \lambda(\kappa)}} \right) \mathrm{d}\kappa,$$

i.e. $f = F'$, where $F(\lambda) = -(1/(\pi\alpha)) \int_0^\pi (\mathrm{d}\kappa/(\sqrt{\lambda - \lambda(\kappa)}))$, which behaves like $((\sqrt{|D'(\mathrm{M}_1)|})/(2\pi\alpha))\ \ln(\lambda - \mathrm{M}_1)$ as $\lambda \to \mathrm{M}_1$, in perfect accordance with Proposition 3.1 for large c. Together with the numerical attestation (cf. ([4], § 3)) this provides strong evidence for formula (2) to hold already for small values of the coupling constant c.

Such an inference is an example of the great potential which lies in *numerical spectral analysis* to obtain insight into the unexpected spectral behavior of differential operators where non-asymptotic analytical methods seem to fail. A possible field of investigation would be the decay of eigenfunctions for embedded eigenvalues. Spherically symmetric (radially periodic) Schrödinger operators with their neither typically higher-dimensional nor simply one-dimensional spectral characteristics can serve as lodestars for further discoveries.

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