INVERSE SPECTRAL THEORY FOR PERIODIC
SCHRÖDINGER OPERATORS

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Abstract. This written version of my talk at the Cracovian Operator Theory Seminar in April 1996 is meant as a short introduction to the work of Eastham, Marchenko, Trubowitz et al. on the spectral theory of periodic Schrödinger operators. It was my aim to present some main results and outline the ideas of their proofs in a not too technical manner.

0. Introduction. The study of periodic differential equations and periodic differential operators has always been an important field of research: from the mathematical point of view, the analysis of periodic differential operators, which possess a large symmetry group, was possible by a beautiful interplay of techniques from analysis and group theory; moreover it turned out, that some of the notions and tools invented for the periodic case have a much wider scope. The study of Schrödinger operators with almost periodic potentials in recent times has shed light on the importance of periodic operators only once more. In solid state physics, periodic differential operators have been used in models for crystalline matter since the old days of quantum mechanics. Their spectral theory can be used to explain properties of conductors and insulators, for example.

Here, I want to focus on an aspect of the theory of one-dimensional periodic Schrödinger operators: it turns out, that their spectrum consists of a collection of infinitely many bands, which may be separated by gaps. The natural question, which configurations of bands and gaps can arise as spectra of such operators, has been answered in a quite satisfying way by results of Eastham, Marchenko, Trubowitz et al., to which I want to give a short introduction. I will try to present some essential ideas, while proofs will mostly be sketched
and can be found in detail in the references: for the proofs of the facts collected in section 1, see for example [RS4]; for the remaining sections, see especially [GT2] and [PT].

1. Direct Integral Decomposition. A basic tool in the study of periodic operators is their direct integral composition: consider \(-\Delta + V = -\sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} + V(x)\) on \(L^2(\mathbb{R}^n)\) with \(V(x)\), the potential, a measurable, real and periodic function on \(x \in \mathbb{R}^n\), i.e. there exists a lattice \(\Gamma \subset \mathbb{R}^n\), \(\Gamma = \mathbb{Z}[a_1, \ldots, a_n], \{a_1, \ldots, a_n\}\) linearly independent, such that \(V(x + \gamma) = V(x)\) for all \(x \in \mathbb{R}^n\) and \(\gamma \in \Gamma\). If \(V\) is, for simplicity, \(-\Delta\)-bounded with relative bound 0, \(-\Delta + V\) is a self-adjoint semibounded differential operator, which admits a "direct integral decomposition":

Let \(Q = \{x \in \mathbb{R}^n | x = \sum_{i=1}^{n} t_i a_i, 0 \leq t_i \leq 1\}\) denote the basic period cell of \(\Gamma\), and for \(\theta \in [0, 2\pi)^n\) let \(-\Delta_\theta\) be the operator on \(L^2(Q, d^n x) =: \mathcal{H}'\) generated by \(-\sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}\) and boundary conditions

\[
\varphi(x + a_j) = e^{i\theta_j} \varphi(x), \quad \frac{\partial \varphi}{\partial x_j}(x + a_j) = e^{i\theta_j} \frac{\partial \varphi}{\partial x_j}(x).
\]

If we set

\[
\mathcal{H} = \int_{[0,2\pi)^n} \mathcal{H}' \frac{d^n \theta}{(2\pi)^n},
\]

\(U : L^2(\mathbb{R}^n, d^n x) \to \mathcal{H}\) defined by

\[
(UF)_\theta(x) = \sum_{m \in \mathbb{Z}^n} e^{-i\theta \cdot m} f(x + \sum_{i} m_i a_i)
\]

turns out to be a unitary transformation with

\[
U(-\Delta + V)U^{-1} = \int_{[0,2\pi)^n} (-\Delta_\theta + V) \frac{d^n \theta}{(2\pi)^n}.
\]

Thus, we get a decomposition of \(-\Delta + V\) as an integral of operators whose spectra consist of eigenvalues with finite multiplicities; these eigenvalues depend continuously on \(\theta\), and their union is \(\sigma(-\Delta + V)\), the spectrum of \(-\Delta + V\). Therefore, \(\sigma(-\Delta + V)\) consists of a collection of not necessarily disjoint closed intervals called "bands" and is purely absolutely continuous under mild technical conditions. As \(-\Delta + V\) is semibounded from below, a lowest band exists; and as ist is unbounded, bands beyond any positive number exist. However, there is a remarkable difference between the cases \(n \geq 2\) and \(n = 1\):
n \geq 2$ : there exists $C \in \mathbb{R}$, such that $[C, \infty) \subset \sigma(-\Delta + V)$; in particular, for every $m \in \mathbb{N}$ there is $C(m) \in \mathbb{R}$, such that at every $r \geq C(m)$ at least $m$ bands of $-\Delta + V$ overlap;

$n = 1$ : the bands of $-\Delta + V$ may only overlap at their endpoints; if two subsequent bands do not overlap, they may be separated by an open interval not belonging to $\sigma(-\Delta + V)$, a "gap".

In the one-dimensional case, it is even possible to locate the positions of the eigenvalues of the operators constituting the direct integral fairly well: the band ends, for example, are the eigenvalues of $-\Delta_0 + V$ and $-\Delta_\pi + V$, i.e., of the operators with periodic and semiperiodic boundary conditions. Consequently, developing spectral theory and inverse spectral theory for one-dimensional Schrödinger operators, i.e., exploring the connection between periodic potentials and possible configurations of bands and gaps on the real line, has been reduced to studying the connection between potentials and certain eigenvalue problems on an interval. Some important techniques which can be used for this task and the corresponding results will now be presented for the example of Dirichlet boundary conditions.

2. The Dirichlet problem on the interval for a potential function $q \in L^2 = L^2_{\mathbb{R}}([0, 1])$, the real $L^2$-space on the interval, is constituted by the differential equation

$$-y'' + q(x)y = \lambda y, \quad 0 \leq x \leq 1, \quad \lambda \in \mathbb{R},$$

and the boundary conditions

$$y(0) = 0 = y(0).$$

The sequence of eigenvalues arising from this problem will be denoted by $(\mu_n(q))_{n \in \mathbb{N}}$, the corresponding normalized eigenfunctions by $g_n(x, q)$. The first result is

**Theorem 1.** For $q \in L^2$

$$\mu_n(q) = n^2 \pi^2 + \int_0^1 q(t) dt - \langle \cos(2\pi nx), q \rangle + O\left(\frac{1}{n}\right).$$

In particular, $\mu_n(q)$ is of the form $n^2 \pi^2 + c + \ell^2(n)$ (i.e., $(\mu_n(q) - n^2 \pi^2 - c)_{n \in \mathbb{N}} \in \ell^2$) for some constant $c \in \mathbb{R}$.

**Proof.** For the proof, we regard $-q(x)y$ in $-y'' = \lambda y - q(x)y$ as an inhomogeneity and use the Wronskian determinant to write down a solution; this
yields
\[ y(x) = a \cos(\sqrt{\lambda}x) + b \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} + \frac{1}{\sqrt{\lambda}} \int_0^x \sin(\sqrt{\lambda}(x-t))q(t)y(t)dt. \]

From this formula, the asymptotics for \( \mu_n \) can be deduced.

At this point, the question concerning the relation between potentials and spectral properties of the corresponding operators can be made precise: we can ask, whether all sequences of the form \( n^2 \pi^2 + c + \ell^2(n) \) are sequences of Dirichlet eigenvalues for some potential, and try to investigate the structure of the isospectral sets \( M(p) = \{ q \in L^2 | \mu_n(q) = \mu_n(p) \text{ for all } n \in \mathbb{N} \} \). For this purpose, one introduces
\[ S = \{(\sigma_n)_{n \in \mathbb{N}} \mid \sigma_n = n^2 \pi^2 + s + \bar{\sigma}_n, s \in \mathbb{R}, (\bar{\sigma}_n)_{n \in \mathbb{N}} \in \ell^2, \sigma_n < \sigma_{n+1} \forall n \in \mathbb{N} \} \]
and \( \mu : L^2 \to S \)
\[ q \mapsto \mu(q) = (\mu_1(q), \mu_2(q), \mu_3(q), \ldots). \]
We have to determine the image of \( \mu \) and to analyze the structure of its fibers. The identification
\[ (\sigma_n)_{n \in \mathbb{N}} \leftrightarrow (s, (\bar{s}_n)_{n \in \mathbb{N}}) \]
of \( S \) with a certain open subset of \( \mathbb{R} \times \ell^2 \) enables us to do analysis on \( S \) as if it were an open subset of a Hilbert-space. With these identification, \( \mu \) looks
\[ q \mapsto ([q], (\bar{\mu}_n(q))_{n \in \mathbb{N}}), \]
where \( [q] = \int_0^1 q(t)dt \) and \( \bar{\mu}_n = \mu_n - n^2 \pi^2 - [q] \). One gets

**Theorem 2.** \( \mu \) is real-analytic, and its derivative \( d_q \mu : L^2 \to \mathbb{R} \times \ell^2 \) at \( q \in L^2 \) is given by
\[ v \mapsto ([v], (g_n^2 - 1, v)). \]

**Proof.** The proof of the analyticity of \( \mu \) is quite technical and will be omitted; to calculate \( d_q \mu \), let us differentiate \(-g''_n + qg_n = \mu_n g_n \) in the direction of \( v \in L^2 \):
\[-d_q g''_n(v) + qd_q g_n(v) + v g_n = \mu d_q g_n(v) + d_q \mu_n(v) g_n \]
At this point, we can restrict our considerations to sufficiently regular \( q \), since they are dense in \( L^2 \), and therefore use \( d_q g''_n(v) = (d_q g_n(v))'' \); then multiplication by \( g_n \) and integration yields
\[ \langle -(d_q g_n(v))'', g_n \rangle + \langle d_q g_n(v), q g_n \rangle + \langle g_n^2, v \rangle = \mu_n \langle d_q g_n(v), g_n \rangle + d_q \mu_n(v). \]
\(-(d_q g_n(v))''(v), g_n) = (d_q g_n(v), -g_n''(v))\), so using once more the differential equation for \(g_n\) we arrive at

\[ d_q \mu_n(v) = \langle g_n^2, v \rangle, \]

which is the desired result. \(\square\)

Thus, in the simplest case, \(q \equiv 0\), \(d_0 \mu\) is given by

\[ v \mapsto ([v], -\langle \cos(2\pi nx), v \rangle); \]

if we define \(q^*(x) = q(1 - x)\), \(\ker(d_0 \mu) = \{q \in L^2 \mid q^* = -q\}\), the space of odd functions in \(L^2\), and for its orthogonal complement \(E = \{q \in L^2 \mid q^* = q\}\), the space of even functions in \(L^2\), the inverse function theorem shows that \(\mu_E = \mu|_E : E \to \mathbb{R} \times \ell^2\) is a local real-analytic isomorphism at \(0 \in E\).

The analogue of this statement can be shown to be true at every \(e \in E\), which leads to

**Theorem 3.** \(\mu_E\) is a global real-analytic isomorphism.

**Proof.** It remains to be shown that \(\mu_E\) is one-to-one globally. So suppose \(p, q \in E\) have the same Dirichlet spectrum. Cross-multiply their differential equations, subtract and integrate to get

\[ \langle q - p, g_n(q)g_n(p) \rangle = 0 \quad \text{for} \quad n \geq 1. \]

Now, the hard point is to show that \(\{1\} \cup \{g_n(q)g_n(p) - 1\}_{n \geq 1}\) forms a basis of \(E\); having done that, one only has to notice that \(\langle q - p, 1 \rangle = 0\) by the asymptotics of the \(\mu_n\), and the proof is done. \(\square\)

In order to get an isomorphic picture of the whole \(L^2\)-space, one has to introduce quantities providing additional information about \(q\): the "terminal velocities"

\[ \kappa_n(q) = \log \left| \frac{g_n'(1, q)}{g_n'(0, q)} \right|. \]

Denoting

\[ \ell^2_1 = \{(a_n)_{n \in \mathbb{N}} \mid \sum_{n=1}^{\infty} (na_n)^2 < \infty\}, \]

one has in a similar manner

**Theorem 4.** \(\kappa \times \mu : L^2 \to \ell^2_1 \times S\) is a real-analytic isomorphism.

Now what about the fibers \(M(p) = \mu^{-1}(\mu(p))\)? Obviously,

\[ M(p) = \bigcap_{n \geq 1} M_n(p), \]
where
\[ M_n(p) = \{ q \in L^2 \mid \mu_n(q) = \mu_n(p) \}. \]

\( M_n(p) \) is a real-analytic submanifold of \( L^2 \) of codimension one, since the gradient \( \frac{\partial \mu_n}{\partial q} = g_n^2 \) never vanishes. As the \( g_n^2, n \geq 1 \), are linearly independent, every \( M_1(p) \cap \ldots \cap M_n(p) \) is a real-analytic submanifold, whose normal space is spanned by \( \{ g_1^2(q), \ldots , g_n^2(q) \} \). Therefore, the following theorem, which shall not be proven here, is at least clear heuristically; to do the analysis carefully, one has to show that \( d_q \mu \) is a linear isomorphism between the orthogonal complement of its kernel and the tangent space to \( S \) at \( \mu(p) \), i. e. \( \mu(p) \) is a “regular value”.

**Theorem 4.** For all \( p \) in \( L^2 \), \( M(p) \) is a real-analytic submanifold of \( L^2 \) lying in the hyperplane of all functions with mean \([p] \). At every point \( q \) in \( M(p) \), the normal space is
\[ N_q M(p) = (\ker(d_q \mu))^\perp = \{ \eta_0 + \sum_{n \geq 1} \eta_n (g_n^2 - 1) \mid \eta \in \mathbb{R} \times \ell^2 \}, \]
and the tangent space is
\[ T_q M(p) = \ker(d_q \mu) = \{ \sum_{n \geq 1} \xi_n (2 \frac{d}{dx} g_n^2) \mid \xi \in \ell_1^2 \}. \]

Moreover, \( \kappa \) is a global coordinate system on \( M(p) \), whose derivative establishes isomorphisms \( T_q M(p) \cong T_{\kappa(q)} \ell_1^2 \cong \ell_1^2 \).

By using vectorfield techniques on \( M(p) \), it is even possible to show that \( M(p) \) is connected and simply connected.

4. **Conclusion.** As we have seen by the example of Dirichlet boundary conditions, a detailed analysis of the spectra of the operators occurring in the direct integral decomposition of section 1 is possible. In the case of an even periodic potential, periodic resp. semiperiodic boundary conditions agree with Dirichlet resp. von Neumann boundary conditions (the latter means \( y'(0) = 0 = y'(1) \)). Let \( \nu : L^2 \to S \),
\[ q \mapsto \nu(q) = (\nu_0(q), \nu_1(q), \ldots) \]
denote the sequence of von Neumann eigenvalues of \( q \in L^2 \), then this means that for
\[ E_0 = \{ q \in L^2 \mid [q] = 0, q^* = q \} \]
\( \sigma : E_0 \to \ell^2 \) with \( \sigma_n(q) = \mu_n(q) - \nu_n(q) \) is the “signed gap length”. Finally, one arrives at the following result:
Theorem 5. \( \sigma : E_0 \rightarrow \ell^2 \) is a real-analytic isomorphism between \( E_0 \) and \( \ell^2 \).

So indeed, every \( \ell^2 \)-sequence is the sequence of gap lengths of a certain \( L^2 \)-potential, which may be chosen even. A result, which is far out of reach here, but shown in [GT1], is the fact, that the band lengths and therefore the configuration of gaps and bands as a whole are determined by the sequence of gap lengths!

References


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