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The determination of one-dimensional bands by fibres

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Abstract. It is shown that the bands $\{\epsilon_m(k)|m=1,\ldots,\infty, k\in[-\pi,\pi)\}$ of one-dimensional Bloch Hamiltonians $H=p^n+V(x)$, $n\geqslant 2$, V periodic, are uniquely determined by $n-1$ fibres $\{\epsilon_m(k_i)|m=1,\ldots,\infty, i=1,\ldots,n-1\}$. This extends known results on Hill's equation.

We follow an idea of Hill (see Magnus and Winkler 1966) for determining the eigenvalue equation of infinite determinants, coupled with properties of integral functions, to show that the band spectrum $\{\epsilon_m(k)|m=1,\ldots,\infty, k\in[-\pi,\pi)\}$ for one-dimensional Bloch Hamiltonians:

$$H=p^n+V(x), \qquad V(x+1)=V(x), n\geqslant 2, \tag{1}$$

$V(x)$ real periodic, is uniquely determined by $n-1$ fibres $\{\epsilon_m(k_i)|m=1,\ldots,\infty, i=1,\ldots,m-1\}$. For notation and terminology on Bloch Hamiltonians see Avron *et al* (1974, 1976).

For $n=2$, equation (1) is the important case of Hill's equation. By methods of differential equations it is known that for V continuous the periodic spectrum ($k=0$) determines uniquely the antiperiodic spectrum ($k=\pi$). The equation for the discriminant (the trace of the monodromy matrix) determines the spectrum for all $k\in[-\pi,\pi]$. Our approach is via infinite determinants. It extends the results for Hill's equation to unbounded V and enables general n in equation (1).

Define the reduced Bloch Hamiltonian, H_k, in $l^2(\mathbb{Z})$ by (Avron *et al* 1974):

$$H_k\psi(j)=(2\pi j+k)^n\psi(j)+(\hat{V}*\psi)(j)\equiv(T_k+\hat{V})\psi \tag{2}$$

$\hat{V}$ is the Fourier series of V. Since $\Sigma_j|2\pi j+k|^{-\alpha}<\infty$, $\alpha>1$, $|T_k|^{\alpha/n}$ has a trace class resolvent. Furthermore, let $1/\alpha+1/\alpha'=1$, $\alpha' n>2$, $\alpha\leqslant 2$ then

$$\left\|\hat{V}\frac{1}{T_k+\lambda}\right\|\leqslant\|\hat{V}\|_\alpha\left\|\frac{1}{p^n+\lambda}\right\|_{\alpha'}<1$$

provided $|\mathrm{Im}\,\lambda|$ is large enough. It follows from the resolvent equation that $H_k=T_k+\hat{V}$ has a trace class resolvent. In addition

$$B(k,\lambda)=(T_k+1)^{-1}(\hat{V}-\lambda-1) \tag{3}$$

$$C(k,\lambda)=(T_k-\lambda)^{-1}\hat{V} \tag{4}$$

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are trace class whenever well defined. Note that

$$\frac{1+C(k,\lambda)}{1+B(k,\lambda)}=\frac{T_k+1}{T_k-\lambda}. \tag{5}$$

Since $B(k,\lambda)$, $C(k,\lambda)$ are trace class:

$$b(k,\lambda)=\det(1+B(k,\lambda)) \tag{6}$$

$$c(k,\lambda)=\det(1+C(k,\lambda)) \tag{7}$$

are well defined (Simon 1976, Gohberg and Krein 1969).

The zeros of $b(k,\lambda)$ and $c(k,\lambda)$ are the band functions (Gohberg and Krein 1969). Properties of b and c are summarized as follows.

Proposition 1

(a) $b(k,\lambda)$ and $c(k,\lambda)$ are periodic in k with period 2π.

(b) Let $\hat{V}\in l^p(\mathbb{Z})$, $1\leqslant p<2$ (λ in compacts) then $b(k,\lambda)$ and $c(k,\lambda)$ converge to unity as $\operatorname{Im} k\to\pm\infty$.

(c) Let n be even. $\bar{c}(k,\lambda)=c(-\bar{k},\bar{\lambda})$, $\bar{b}(k,\lambda)=b(-\bar{k},\bar{\lambda})$.

(d) Let e_m be the mth root of unity. Then $b(k,\lambda)$ has simple poles for $k=\mathrm{e}^{\mathrm{i}\pi/n}e_m+2\pi j$, $m\in\{1,\ldots,n\}$, $j\in\mathbb{Z}$. Similarly $c(k,\lambda)$ has its poles at $k=|\lambda|^{1/n}e_m+2\pi j$, $m\in\{1,\ldots,n\}$, $j\in\mathbb{Z}$.

Proof

(a) $B(k,\lambda)$ is unitarily equivalent to $B(k+2\pi,\lambda)$ by the shift $U\psi(j)=\psi(j-1)$.

(b) $\operatorname{Tr}|T_k+\lambda|^{-q}\to 0$, $\operatorname{Im} k\to\pm\infty$, $q>1/n$. Let $q'=1-q$:

$$\|\hat{V}(T_k+\lambda)^{-q'}\|\leqslant\|\hat{V}\|_p\|(T_k+\lambda)^{-q'}\|_r\leqslant c<\infty, \tag{8}$$

$1/p+1/r=\frac{3}{2}$, p, $r\geqslant 1$, $r>1/nq'>1/n-1$. Hence $C(k,\lambda)\to 0$ in the trace norm and $c(k,\lambda)\to 1$.

(c) This is time reversal.

(d) This is evident for finite matrices. The result follows by taking limits.

Theorem 2 gives a generalized version of Hill's equation (Whittaker and Watson 1927).

Theorem 2. Let $\hat{V}$ be as in the previous proposition. Then:

$$c(k,\lambda)=1+\sum_{j=1}^{n}F_j(\lambda)\cot[\tfrac{1}{2}(k-|\lambda|^{1/n}e_j)] \tag{9}$$

where

$$\sum_{j=1}^{n}F_j(\lambda)=0. \tag{10}$$

If n is even:

$$F_j(\bar{\lambda})+\bar{F}_{n-j+1}(\lambda)=0. \tag{11}$$

Proof. By proposition 1(a), (b), (d) the poles of $c(k,\lambda)$ are generated by the translation of n poles. $\cot x$ has a periodic array of poles and converges to a constant as $\operatorname{Im} x\to\pm\infty$. It follows from Liouville's theorem that:

$$c(k,\lambda)=\sum_{j=1}^{n}F_j(\lambda)\cot[\tfrac{1}{2}(k-\lambda^{1/n}e_j)]+F_0(\lambda). \tag{12}$$

Using (b) for $\operatorname{Im} k \to \pm\infty$:

$$\begin{aligned} 1 &= \sum_{j=0}^{n} F_j(\lambda) \\ 1 &= F_0(\lambda) - \sum_{j=1}^{n} F_j(\lambda). \end{aligned} \tag{13}$$

(11) follows from (c).

The bands are therefore uniquely determined once the $n-1$ functions $\{F_j(\lambda) | j = 1, \ldots, n-1\}$ are. As we shall see, these may be determined by $n-1$ fibres of bands $\{\epsilon_m(k_i) | m = 1, \ldots, \infty, i = 1, \ldots, n-1\}$.

Theorem 3

$$c(k, \lambda) = \prod_m \left(1 - \frac{\lambda}{\epsilon_m(k)}\right) \prod_j \frac{(2\pi j + k)^n}{(2\pi j + k)^n - \lambda}. \tag{14}$$

(The infinite product in (14) for $n = 2$ can be expressed in terms of trigonometric functions.)

Proof. $b(k, \lambda)$ is an integral function of λ of order less than unity and so is uniquely determined by its zeros (Titchmarsh 1939):

$$b(k, \lambda) = \gamma(k) \prod_m \left(1 - \frac{\lambda}{\epsilon_m(k)}\right). \tag{15}$$

The infinite product is absolutely convergent since H_k has trace class resolvent, i.e. $\Sigma |\epsilon_m(k)|^{-1} < \infty$ (for simplicity we assume $\epsilon_m(k) \neq 0$):

$$\gamma(k) \prod_j \frac{(2\pi j + k)^n + 1}{(2\pi j + k)^n} = 1 \tag{16}$$

and the result follows.

Combining theorems 2 and 3 one sees that the n functions $F_j(\lambda)$ are determined by $n-1$ fibres $\epsilon_m(k_j)$ provided the determinant $\Delta = \det(d_{ij}) \neq 0$:

$$\begin{aligned} d_{ij} &= \cot[\tfrac{1}{2}(k_i - |\lambda|^{1/n} e_j)], \qquad j = 1, \ldots, n, i = 1, \ldots, n-1 \\ d_{ni} &= 1. \end{aligned} \tag{17}$$

In conclusion, let us make the following comments.

First, the bands are uniquely determined even though the potential V is in general not uniquely determined. In fact the Korteweg–de Vries equation generates an isospectral family of potentials for Hill's equation (Gardner *et al* 1967, Perelomov 1976). For the n-band problem (i.e. Hill's equation with n gaps in the spectrum) this family is a certain class of Abelian functions (McKean and Van Moerbeke 1975).

Second, one would obviously like to see how much of the above analysis extends to three dimensions. The first difficulty is that one needs to consider regularized determinants (Gohberg and Krein 1969) rather than the usual ones. The more serious problem is the loss of simple structure of singularities for the determinant which prevents an easy generalization of theorem 2. This is still an open problem.

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