Inverse theory of Schrödinger matrices

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Abstract. In this note we discuss the inverse spectral theory for Schrödinger matrices, in particular a conjecture of Gesztesy–Simon [1] on the number of distinct iso-spectral Schrödinger matrices. We consider 3 × 3 matrices and obtain counter examples to their conjecture.

Keywords. Schrödinger matrices; iso-spectral sets; inverse spectral theory.

1. Introduction

Given a point $B = (b_1, \ldots, b_n)$ in $\mathbb{R}^n$, consider the Schrödinger matrix $H(B)$ as

$$H(B) = \begin{pmatrix} b_1 & 1 & \ldots & \ldots & 0 \\ 1 & b_2 & 1 & \ldots & 0 \\ 0 & 1 & \ddots & 1 & 0 \\ 0 & \ldots & 1 & \ddots & 1 \\ 0 & \ldots & \ldots & 1 & b_n \end{pmatrix}.$$ 

This matrix has all real and distinct eigenvalues say $t_1, \ldots, t_n$. Define the map $F : \mathbb{R}^n \to \mathbb{R}^n$ as $F(B) = (t_1, \ldots, t_n)$ where $t_1 < \cdots < t_n$ are the eigenvalues of $H(B)$. Let $W_n$ denote the range of $F$, then the following conjecture is posed in [1].

**Conjecture 1.1 (Gesztesy–Simon).** Let $n$ be a positive integer and let $F$ and $W_n$ be as above. Then

1. $W_n$ is closed set in $\mathbb{R}^n$ whose interior is dense in $W_n$. For $(t_1, \ldots, t_n)$ in interior of $W_n$, $F^{-1}(t_1, \ldots, t_n)$ contains $n!$ points and for $(t_1, \ldots, t_n)$ in $\partial W_n$, $F^{-1}(t_1, \ldots, t_n)$ contains fewer than $n!$ points.
2. $F^{-1}(W_n^\text{int})$ is a disjoint union of $n!$ sets and on each of them $F$ is a diffeomorphism to $(W_n^\text{int})$.

We address (1) of the above conjectures. That $W_n$ is closed is already proved in [1] (theorem 7.4).

The case $n = 2$ is solved in the paper [1]. Now we will inspect the map $F$ for the case $n = 3$. Given a point $B \in \mathbb{R}^3$, consider the characteristic polynomial of $H(B)$, given by $\det(H(B) - tl) = 0$, viz.,

$$t^3 - (b_1 + b_2 + b_3)t^2 + (b_1b_2 + b_2b_3 + b_1b_3 - 2)t + b_1 + b_3 - b_1b_2b_3 = 0.$$ 

Observe that the characteristic polynomial is not symmetric in $b_1, b_2, b_3$. 

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Lemma 1.2. For \( T = (t_1, t_2, t_3) \in \mathbb{R}^3 \), define \( P_1 = t_1 + t_2 + t_3; \ P_2 = t_1t_2 + t_2t_3 + t_1t_3; \ P_3 = t_1t_2t_3. \) Then \( (t_1, t_2, t_3) = F(b_1, 0, b_3) = F(b_3, 0, b_1) \) iff \( (t_1, t_2, t_3) \) satisfy
\[
(P_1 - 4(2 + P_2)) \geq 0 \quad \text{and} \quad P_1 + P_3 = 0. \tag{1}
\]

Proof. Consider the characteristic polynomial of \( H(B) \) for \( B = (b_1, 0, b_3). \) Express the relations between the coefficients of that polynomial and its roots \( t_1, t_2, t_3. \) Now the lemma is a straightforward consequence. For the converse part set
\[
b_1 = \frac{P_1 \pm \sqrt{P_1^2 - 4(2 + P_2)}}{2}; \quad b_3 = \frac{P_1 \pm \sqrt{P_1^2 - 4(2 + P_2)}}{2}
\]
and again verify those relations. \( \square \)

Theorem 1.3. For \( (t_1, t_2, t_3) \in \mathbb{R}^3 \) and \( P_1, P_2, P_3 \) as defined in lemma (1.2) we have, \( (t_1, t_2, t_3) \in \text{Range}(F) \) iff the following system of equations has a real solution
\[
y^3 - P_1y^2 + (3 + P_2)y - (P_1 + P_3) = 0 \tag{2}
\]
\[
-3y^2 + 2P_1y + P_2^2 - 4(2 + P_2) \geq 0.
\]

Proof. Observe that \( (t_1, t_2, t_3) = F(b_1, b_2, b_3) \) iff
\[
(t_1 - b_2, t_2 - b_2, t_3 - b_2) = F(b_1 - b_2, 0, b_3 - b_2). \tag{3}
\]
Let
\[
\bar{P}_1 = t_1 - t_2 - t_2 + t_3 - b_2 = P_1 - 3b_2,
\]
\[
\bar{P}_2 = (t_1 - b_2)(t_2 - b_2) + (t_3 - b_2)(t_2 - b_2) + (t_1 - b_2)(t_3 - b_2)
\]
\[
= P_2 - 2P_1b_2 + 3b_2^2,
\]
\[
\bar{P}_3 = (t_1 - b_2)(t_2 - b_2)(t_3 - b_2) = P_3 - P_2b_2 + P_1b_2^2 - b_3^2.
\]
By lemma (1.2), eq. (3) holds iff \( (t_1, t_2, t_3) \) satisfy
\[
(\bar{P}_1^2 - 4(2 + \bar{P}_2)) \geq 0 \quad \text{and} \quad \bar{P}_1 + \bar{P}_3 = 0. \tag{4}
\]
The conditions (4) for \( \bar{P}_1, \bar{P}_2, \bar{P}_3 \) translate into
\[
b_2^3 - P_1b_2^2 + (3 + P_2)b_2 - (P_1 + P_3) = 0, \tag{5}
\]
\[
-3b_2^2 + 2P_1b_2 + P_2^2 - 4(2 + P_2) \geq 0. \tag{6}
\]
If \( (t_1, t_2, t_3) = F(b_1, b_2, b_3) \) then clearly \( b_2 \) satisfies eqs (5) and (6) and hence is the solution of the system of equations (2).
Conversely if the system of equations (2) has a solution \( y = y_0, \) then set \( b_2 = y_0. \)
Therefore \( (t_1 - b_2, t_2 - b_2, t_3 - b_2) \) satisfies equations (4). Now set
\[
b_1 = b_2 + \frac{\bar{P}_1 - \sqrt{\bar{P}_1^2 - 4(2 + \bar{P}_2)}}{2}
\]
and
\[
b_3 = b_2 + \frac{\bar{P}_1 - \sqrt{\bar{P}_1^2 - 4(2 + \bar{P}_2)}}{2}
\]
This gives \( (t_1, t_2, t_3) = F(b_1, b_2, b_3) \) i.e. \( (t_1, t_2, t_3) \in \text{Range}(F). \) \( \square \)
By observing lemma (1.2) we get that there are two pre-images of \((t_1, t_2, t_3)\) for every value of \(b_2\) satisfying the system of equations (2). We are now interested in finding the conditions under which the system of equations (2) has exactly one real solution.

Consider the general cubic equation with real coefficients
\[
x^3 + a_2x^2 + a_1x + a_0 = 0. \tag{7}
\]
Let \(q_1, q_2\) denote the complex cube roots of unity, \(Q = a_2^2 - 3a_1, R = -2a_2^3 + 9a_1a_2 - 27a_0\). Define \(u, v, w\) as
\[
u = \frac{3(R + \sqrt{R^2 - 4Q^3})}{2}, \quad w = \frac{3(R - \sqrt{R^2 - 4Q^3})}{2}. \tag{8}
\]

Then referring to \([2]\) the solutions of eq. (7) are \(x_1 = u + v + w; \ x_2 = u + q_1v + q_2w; \ x_3 = u + q_2v + q_1w\).

**Lemma 1.4.** The equation (7) has exactly 1 real root iff \(R^2 - 4Q^3 > 0\).

**Proof.** Using the expressions given above, one can easily verify that eq. (7) has 3 real roots iff \(v = w\), which happens iff \(R^2 - 4Q^3 < 0\). The lemma now follows by negating these statements appropriately. \(\square\)

For \(T = (t_1, t_2, t_3) \in R^3\), consider the cubic equation (5) given by
\[
b_2^3 - P_1b_2^2 + (3 + P_2)b_2 - (P_1 + P_3) = 0.
\]

Here
\[
a_2 = -P_1, \ a_1 = 3 + P_2, \ a_0 = -(P_1 + P_3),
\]
\[
Q = a_2^2 - 3a_1 = P_1^2 - 3(3 + P_2)
\]
\[
= t_1^2 + t_2^2 + t_3^2 - (t_1t_2 + t_2t_3 + t_1t_3) - 9, \tag{9}
\]
\[
R = -2a_2^3 + 9a_1a_2 - 27a_0 = 2P_1^3 - 9P_1P_2 + 27P_3
\]
\[
= 2(t_1^2 + t_2^2 + t_3^2) - 3[t_1(t_2 + t_3) + t_2(t_1 + t_3) + t_3(t_1 + t_2)] + 12t_1t_2t_3. \tag{10}
\]

**Lemma 1.5.** If \(Q, R\) as in eqs (9), (10) respectively and \(v, w\) are given by eq. (8), then the system of equations (2) has exactly 1 real solution iff \(R^2 - 4Q^3 > 0\) and \(4P_1^2 - 12(2 + P_2) \geq 9(v + w)^2\).

**Proof.** By lemma (1.4), the cubic equation (5) has exactly 1 real root iff \(R^2 - 4Q^3 > 0\). Moreover this root must satisfy the equation (6) so that \((t_1, t_2, t_3) \in \text{Range } F\). In this case the only real root is given by \(x_1 = u + v + w = P_1/3 + v + w\). Substituting the value of \(b_2 = x_1\) in eq. (6) and simplifying gives
\[
4P_1^2 - 12(2 + P_2) \geq 9(v + w)^2. \tag{11}
\]

**COROLLARY 1.6**

Let
\[
D = \{T \in R^3 | R^2 - 4Q^3 > 0\} \cap \{T \in R^3 | 4P_1^2 - 12(2 + P_2) > 9(v + w)^2\}.
\]

Then \(D \subset (\text{Range } F)^{\text{int}}\).
Proof. Theorem (1.3) and lemma (1.5) implies that \( D \subset (\text{Ran} \ F) \). Moreover \( D \) is intersection of 2 open sets and therefore \( D \subset (\text{Ran} \ F)^{\text{int}} \).

COROLLARY 1.7

Let \( C = \{(-\sqrt{2 + t^2}, 0, \sqrt{2 + t^2}) | t \in (-1, 1); t \neq 0 \} \). Then \( C \subset (\text{Ran} \ F)^{\text{int}} \).

Proof. Let \( T = (-\sqrt{2 + t^2}, 0, \sqrt{2 + t^2}) \in C \), for such points \( T \) we have, \( P_1 = 0, P_2 = -2 - t^2, P_3 = 0, R = 2P_1^3 - 9P_1P_2 + 27P_3 = 0 \) and \( Q = P_2^2 - 3(3 + P_2) = -3(1 - t^2) \). Therefore, \( R^2 - 4Q^3 = 108(1 - t^2)^3 > 0 \ \forall \ t \in (-1, 1) \). Also, \( P_1^2 - 12(2 + P_2) = 12t^2 \) and \( 9(v + w)^3 = 0 \). So by Corollary (1.6), \( C \subset D \) and hence \( C \subset (\text{Ran} \ F)^{\text{int}} \). Observe that by lemma (1.5), \( F^{-1}(T) = \{(-t, 0, t), (t, 0, -t)\} \).

Thus, there are points in the interior of \( W_3 = \text{Range}(F) \) which have only two pre-images under the map \( F \), i.e. for each point in the family \( C \) there exist only two isospectral Schrödinger matrices whose spectrum is that point of \( C \). This gives a counterexample to the Conjecture (1.1) (1).

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References