

AN ALGEBRAIC APPROACH TO SAXON-HUTNER THEOREM

TSETSKA G. RASHKOVA and IVAILO M. MLADENOV[†]

*Department of Algebra and Geometry, A. Kanchev University of Ruse
7017 Ruse, Bulgaria*

[†]*Institute of Biophysics, Bulgarian Academy of Sciences
1113 Sofia, Bulgaria*

Abstract. Here we give some necessary and sufficient conditions for the validity of the Saxon-Hutner conjecture concerning the preservation of the energy gaps into an infinite one-dimensional lattice.

Let us consider the Schrödinger equation

$$\frac{d^2\Psi}{dx^2} + (E - U(x))\Psi = 0 \quad (1)$$

where Ψ is the wave function, the spectral parameter E is the particle energy and $U(x)$ is a known function – the potential. Quantum mechanics deals with the above equation and its generalizations. When $U(x) = 0$ we have a free particle and when $E = k^2$, two solutions are e^{ikx} and e^{-ikx} representing respectively a particle moving to the right ($k > 0$) and a particle moving to the left ($k < 0$).

We will use the standard group theory notation for the invertible matrices listed below. The Lie group of pseudo-unitary matrices of signature $(1, 1)$ (i.e., those 2×2 matrices having one positive and one negative square in their canonical form $\langle z, z \rangle = |z_1|^2 - |z_2|^2$), or what is the same – the group of all linear transformations of the complex plane preserving the above hermitian form $\langle \cdot, \cdot \rangle$ will be denoted as $U(1,1)$ while $SL(2, \mathbb{C})$ will denote the corresponding unimodular group keeping the symplectic structure $[\cdot, \cdot]$ invariant (here $[\zeta, \eta]$ is the oriented area of the parallelogram spanned on the vectors ζ, η and $GL(2, \mathbb{R})$ will denote the group of all real linear transformations. We have $\langle a, b \rangle = \frac{1}{2}[a, \bar{b}]$.

Proposition 1. *The intersection of any two groups coincides with the intersection of the three of them – it is the special $(1, 1)$ unitary group $SU(1, 1)$.*

A monodromy operator for (1) with a finite potential is a linear operator acting on the space of states of the free particle in a special way.

Proposition 2. *The matrix of the monodromy operator in the basis (e^{ikx}, e^{-ikx}) is an element of the group $SU(1, 1)$, where*

$$SU(1, 1) = \left\{ M_A = \begin{pmatrix} w_A + i\zeta_A & v_A + i\eta_A \\ v_A - i\eta_A & w_A - i\zeta_A \end{pmatrix} \in M_2(\mathbb{C}); \det(M_A) = 1 \right\}.$$

Actually, we speak about groups of operators but the matrices of these operations are elements of $SU(1, 1)$ in the considered basis (e^{ikx}, e^{-ikx}) . The matrix groups $SL(2, \mathbb{R})$ and $SU(1, 1)$ are isomorphic. We get from them one and the same group of operators. For the real basis (e_1, e_2) these matrices are in $SL(2, \mathbb{R})$ and for the complex conjugate basis (e^{ikx}, e^{-ikx}) they are elements of $SU(1, 1)$. Geometrically, going from $SL(2, \mathbb{R})$ to $SU(1, 1)$ means transforming Lobachevski's plane model in the upper half plane to a model in the unit circle.

In 1949 Saxon and Hutner [8] have announced a conjecture concerning the coupling of impurities introduced into an infinite one-dimensional crystal lattice.

Conjecture 1. *Forbidden energies that are common to the pure A crystal and the pure B crystal (with the same lattice constant) will always be forbidden in any arrangement of A and B atoms in a substitutional solid solution.*

This can be easily reformulated using the transfer-matrix formalism [4]. As the concept of the transfer matrix has been used extensively in transport theory, optics and engineering [2, 3, 7] let us remind that by its very definition the **transfer matrix** M relates the wave functions (states, amplitudes) on either side of the potential (force). The crucial point in using this formalism is the observation that real localized potentials and transfer matrices are in a one-to-one correspondence. The group nature permits defining a total transfer matrix for an arbitrary sequence of potentials as a product of their individual matrices. The **forbidden energies** for an electron propagating in a periodic lattice are given by the condition $\text{tr } M > 2$, where M is a transfer (monodromy) matrix of a unit cell. Thus we can ask:

Question 1. *Under what conditions for any arrangement $A^{r_1} B^{s_1} \dots A^{r_k} B^{s_k}$ of A and B atoms ($r_i, s_j \in \mathbb{Z}^+$) we have $\text{tr}(M_A^{r_1} M_B^{s_1} \dots M_A^{r_k} M_B^{s_k}) > 2$ provided that $\text{tr}(M_A) > 2$ and $\text{tr}(M_B) > 2$?*

Various conditions for the validity of the above statement are discussed in [4–6] and [9] in the context of one-dimensional quantum mechanics which will have in mind in this paper as well.

For convenience from now on we denote the transfer matrices by A, B . We give the following necessary and sufficient condition:

Theorem 1. *Let A and B be two elements of the group $SU(1, 1)$ such that $\text{tr } A > 2$ and $\text{tr } B > 2$. Then $\text{tr}(AB) > 2$ if and only if*

$$(w_A - w_B)^2 + (\zeta_A + \zeta_B)^2 < (\eta_A + \eta_B)^2 + (v_A + v_B)^2.$$

Proof: The condition $\text{tr}(AB) > 2$ gives

$$2w_A w_B - 2\zeta_A \zeta_B + 2v_A v_B + 2\eta_A \eta_B > 2.$$

Taking into account that $w_A^2 + \zeta_A^2 - v_A^2 - \eta_A^2 = w_B^2 + \zeta_B^2 - v_B^2 - \eta_B^2 = 1$ we get the desired inequality. \square

For $\text{tr } A = \text{tr } B$ we get $(\zeta_A + \zeta_B)^2 < (v_A + v_B)^2 + (\eta_A + \eta_B)^2$.

Remark 1. *The necessary and sufficient condition of Theorem 1 could be expressed as $\det(A + B) < \text{tr } A \text{tr } B$.*

Really $\det(A + B) = (w_A + w_B)^2 + (\zeta_A + \zeta_B)^2 - (\eta_A + \eta_B)^2 - (v_A + v_B)^2$ and thus we get $\det(A + B) < \text{tr } A \text{tr } B$.

We could formulate the following sufficient condition:

SC 1. Let $\det(A + B) < \text{tr } A \text{tr } B$ provided that $\text{tr } A > 2$ and $\text{tr } B > 2$. Then $\text{tr}(AB) > 2$.

Exchanging $\text{SU}(1, 1)$ for $\text{SL}(2, \mathbb{R})$ using the group homomorphism

$$M = \begin{pmatrix} w + i\zeta & v + i\eta \\ v - i\eta & w - i\zeta \end{pmatrix} \longrightarrow r(M) = \begin{pmatrix} w - v & \eta + \zeta \\ \eta - \zeta & w + v \end{pmatrix}$$

one could associate with any transfer matrix a complex three-dimensional vector

$$c_M = \frac{1}{w}(-i\eta, -\zeta, iv). \tag{2}$$

In [6] one could find the following

SC 2 ([6, p. 995]). The conditions $c_A \cdot c_B < 0$ and $(c_A \times c_B)^2 < 0$ are sufficient for the validity of the Saxon-Hutner theorem.

In this setting, symmetric potentials are represented by vectors, whose third component is identically zero and this implies that they can be considered as elements of a pseudo-Euclidean plane of index one. In such a plane the condition $(c_A \times c_B)^2 < 0$ is satisfied automatically and **SC2** is transformed into the inequality $\frac{1}{w_A w_B}(-\eta_A \eta_B + \zeta_A \zeta_B) < 0$, which is equivalent to the Tong and Tong [6] criterion, namely

SC 3. Let $\text{sign}(w_A w_B) = \text{sign}(\eta_A \eta_B - \zeta_A \zeta_B)$ when both $\text{tr } A > 2$ and $\text{tr } B > 2$. Then $\text{tr}(AB) > 2$.

Proposition 3. *In the symmetric case **SC2** is equivalent to **SC3**.*

Proposition 4. *In the symmetric case **SC3** is a stronger condition than **SC1**, i.e., **SC1** follows from **SC3**.*

Proof: The inequality in Theorem 1 could be rewritten as

$$w_A w_B - \zeta_A \zeta_B + \eta_A \eta_B > 1.$$

Clearly, the Tong and Tong criterion, namely $w_A w_B > 1$ and $\eta_A \eta_B - \zeta_A \zeta_B > 0$ gives $w_A w_B - \zeta_A \zeta_B + \eta_A \eta_B > 1$. \square

We look for other sufficient conditions as well.

Our next step is to consider the characteristic polynomial of the matrix $A + xB$ for arbitrary x . Classifying pairs of $n \times n$ matrices (A, B) under the simultaneous similarity (TAT^{-1}, TBT^{-1}) Friedland has shown in [1] that if $n = 2$ and U is the set of pairs (A, B) such that $|\lambda E - (A + xB)| = 0$ splits into a product of two linear factors, then U could be defined as

$$U = \{(A, B); (2 \operatorname{tr}(A^2) - \operatorname{tr}^2 A)(2 \operatorname{tr}(B^2) - \operatorname{tr}^2 B) = (2 \operatorname{tr}(AB) - \operatorname{tr} A \operatorname{tr} B)^2\}.$$

We work really in $U^* = U \cap \operatorname{SU}(1, 1)$ and can prove the following:

SC 4. Let $A, B \in \operatorname{SU}(1, 1)$ such that $\operatorname{tr} A > 2, \operatorname{tr} B > 2, \operatorname{tr} A \neq \operatorname{tr} B$ and the characteristic polynomial $|\lambda E - (A + xB)|$ is reducible over $\mathbb{C}[\lambda, x]$. Then $\operatorname{tr}(AB) > 2$.

Proof: Starting with $(\operatorname{tr} A - \operatorname{tr} B)^2 > 0$, we rewrite it as

$$\operatorname{tr} A \operatorname{tr} B - 4 > \sqrt{(\operatorname{tr}^2 A - 4)(\operatorname{tr}^2 B - 4)}. \tag{3}$$

The Cayley-Hamilton theorem gives $A^2 - \operatorname{tr} A \cdot A + E = 0$ and taking traces we get

$$\operatorname{tr}(A^2) = \operatorname{tr}^2 A - 2, \quad \text{i.e.,} \quad 2 \operatorname{tr}(A^2) - \operatorname{tr}^2 A = \operatorname{tr}^2 A - 4. \tag{4}$$

I) Let $|\lambda E - (A + xB)|$ splits into two linear factors. Thus the Friedland’s representation gives

$$\pm \sqrt{(\operatorname{tr}^2 A - 4)(\operatorname{tr}^2 B - 4)} = 2 \operatorname{tr}(AB) - \operatorname{tr} A \operatorname{tr} B.$$

Considering the sign possibilities we get:

- For the positive case $2 \operatorname{tr}(AB) = \operatorname{tr} A \operatorname{tr} B + \sqrt{(\operatorname{tr}^2 A - 4)(\operatorname{tr}^2 B - 4)}$, i.e., $\operatorname{tr}(AB) > 2$.
- In the negative one, we get respectively

$$-\sqrt{(\operatorname{tr}^2 A - 4)(\operatorname{tr}^2 B - 4)} = \operatorname{tr}(AB) - \operatorname{tr} A \operatorname{tr} B$$

which combined with the inequality

$$-\sqrt{(\operatorname{tr}^2 A - 4)(\operatorname{tr}^2 B - 4)} > 4 - \operatorname{tr} A \operatorname{tr} B$$

from (3) gives exactly $\operatorname{tr}(AB) > 2$.

II) Let $|\lambda E - (A + xB)|$ be a square of a linear factor. Friedland describes the set V of such matrices A, B as

$$V = \{(A, B); 2 \operatorname{tr}(A^2) = \operatorname{tr}^2 A, 2 \operatorname{tr}(B^2) = \operatorname{tr}^2 B, 2 \operatorname{tr}(AB) = \operatorname{tr} A \operatorname{tr} B\}.$$

This is not the case for $\operatorname{tr} A > 2$ and $\operatorname{tr} B > 2$ (because of (4) the equality $\operatorname{tr}(A^2) = \operatorname{tr}^2 A$ gives $\operatorname{tr} A = 2$, analogously $\operatorname{tr} B = 2$, a contradiction with the assumption). \square

Remark 2. For $\operatorname{tr} A = \operatorname{tr} B > 2$, the reducibility of the considered characteristic polynomial guarantees only that $\operatorname{tr}(AB) \geq 2$.

Proof: The definition of U^* gives in this case

$$(2 \operatorname{tr}(A^2) - \operatorname{tr}^2 A)^2 = (2 \operatorname{tr}(AB) - \operatorname{tr}^2 A)^2.$$

It could be written as

$$(2 \operatorname{tr}(A^2) - \operatorname{tr}^2 A - 2 \operatorname{tr}(AB) + \operatorname{tr}^2 A)(2 \operatorname{tr}(A^2) - \operatorname{tr}^2 A + 2 \operatorname{tr}(AB) - \operatorname{tr}^2 A) = 0$$

i.e., either

- a) $\operatorname{tr}(AB) = \operatorname{tr}(A^2) > 2$ or
- b) $\operatorname{tr}(AB) = \operatorname{tr}^2 A - \operatorname{tr}(A^2) = 2$ as (4) is valid.

\square

Remark 3. Using the computer algebra system Mathematica, we get the following expression for U^*

$$(\eta_A^2 + v_A^2 - \zeta_A^2)(\eta_B^2 + v_B^2 - \zeta_B^2) = (\eta_A \eta_B + v_A v_B - \zeta_A \zeta_B)^2$$

i.e.,

$$c_A^2 \cdot c_B^2 = (c_A \cdot c_B)^2.$$

As $(c_A \times c_B)^2 = c_A^2 \cdot c_B^2 - (c_A \cdot c_B)^2$, i.e., $(c_A \times c_B)^2 = 0$ we see that **SC4** does not include the symmetric case as Proposition 3 is valid.

As an example of concrete matrices A and B , let us take $w_A = \sqrt{2}$, $\zeta_A = \eta_A = v_A = 1$, $w_B = \sqrt{3}$, $\zeta_B = 0$, $\eta_B = v_B = 1$, so that $\operatorname{tr}(AB) > 2$ although the characteristic polynomial is not reducible. This proves again that the condition

$$w_A w_B - \zeta_A \zeta_B + \eta_A \eta_B > 1$$

is only a sufficient one. Nevertheless it is inequality for the three parameters only.

Another proof of SC4: We apply the canonization theory to the quadratic

$$f(x, \lambda) = |A + xB - \lambda E|$$

$$= x^2 - 2\lambda x w_B + 2x(w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B) + \lambda^2 - 2\lambda w_A + 1.$$

The characteristic equation $\begin{vmatrix} 1 - \lambda & -w_B \\ -w_B & 1 - \lambda \end{vmatrix} = 0$ gives two eigenvalues $\lambda_1 = 1 + w_B$ and $\lambda_2 = 1 - w_B$. The corresponding eigenvectors are $e_1 = \left(\frac{-\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right)$ and $e_2 = \left(\frac{-\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right)$. The transformation

$$\lambda = \frac{-\sqrt{2}}{2} (\tilde{\lambda} + \tilde{x}), \quad x = \frac{\sqrt{2}}{2} (\tilde{\lambda} - \tilde{x})$$

gives $f(\tilde{x}, \tilde{\lambda}) = \lambda_1 \tilde{\lambda}^2 + \lambda_2 \tilde{x}^2 + 2b_1 \tilde{\lambda} + 2b_2 \tilde{x} + b_3$, where $\Delta = \lambda_1 \lambda_2 < 0$ and the quadratic form represents two crossing lines when $c = 0$, where $c = b_3 - b_1^2/\tilde{\lambda} - b_2^2/\tilde{x}$.

In our case,

$$\begin{aligned} b_1 &= \frac{\sqrt{2}}{2} w_A + \frac{\sqrt{2}}{2} (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B) \\ b_2 &= \frac{\sqrt{2}}{2} w_A - \frac{\sqrt{2}}{2} (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B) \\ b_3 &= 1. \end{aligned}$$

Then

$$c = 1 - \frac{1}{(1 - w_B)^2} [w_A^2 + (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B)^2 - 2w_a w_B (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B)].$$

The condition $c = 0$ gives

$$\begin{aligned} w_A^2 + (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B)^2 \\ - 2w_a w_B (w_A w_B + \zeta_A \zeta_B - v_A v_B - \eta_A \eta_B) = 1 - w_B^2. \end{aligned}$$

This could be easily transformed to

$$(\zeta_A \zeta_B - v_A v_B - \eta_A \eta_B)^2 = (1 - w_A^2)(1 - w_B^2) = (\eta_A^2 + v_A^2 - \zeta_A^2)(\eta_B^2 + v_B^2 - \zeta_B^2)$$

which is the simplified expression for U^* as pointed out in Remark 3.

There are no other possibilities for the singularity of the considered quadratic form. The next step is to consider the arrangements $A^{r_1} B^{s_1} \dots A^{r_k} B^{s_k}$ provided that $\text{tr } A = \text{tr } B > 2$ and $\text{tr}(AB) > 2$. Direct computations in this case show that $\text{tr}(A^{r_1} B^{r_2} A^{r_3} B^{r_4}) > 2$ for $2 < r_1 + r_2 + r_3 + r_4 \leq 5$.

The main tools for proving it are:

- a) equality (4) and
- b) the equality $\text{tr}(AB) = \text{tr } A \text{tr } B - \text{tr}(BA^{-1})$ proved directly for unimodular matrices in [5, equation (23)]. For $\text{tr } A = \text{tr } B$ it gives

$$\text{tr}(AB) = \text{tr}^2 A - \text{tr}(BA^{-1}). \tag{5}$$

For the general case we could prove

Lemma 1. *Let $k \in \mathbf{N}$. Then $\operatorname{tr}(A^k) > \operatorname{tr} A$.*

Proof: For $k = 2$, (4) gives $\operatorname{tr}(A^2) = \operatorname{tr}^2 A - 2 > \operatorname{tr} A$ for $\operatorname{tr} A > 2$. Item b) above gives $\operatorname{tr}(A^3) = \operatorname{tr} A \operatorname{tr}(A^2) - \operatorname{tr} A = \operatorname{tr} A(\operatorname{tr}(A^2) - 1) > \operatorname{tr} A$ and $\operatorname{tr}(A^4) = \operatorname{tr}(A^2)^2 = \operatorname{tr}^2 A^2 - 2 > 2$, using (4) again.

Then we proceed by induction. Let $\operatorname{tr}(A^s) > \operatorname{tr} A$ for every $s < 2k + 1$. Then

$$\operatorname{tr}(A^{2k+1}) = \operatorname{tr}(A^k) \operatorname{tr}(A^{k+1}) - \operatorname{tr} A > \operatorname{tr}^2 A - \operatorname{tr} A = \operatorname{tr} A(\operatorname{tr} A - 1) > \operatorname{tr} A.$$

□

Lemma 2. *Let $\operatorname{tr} A = \operatorname{tr} B > 2$ and $\operatorname{tr} AB > 2$. Then $\operatorname{tr}(A^{2k+1}B) > \operatorname{tr}(AB)$ and $\operatorname{tr}(A^{2k}B) > \operatorname{tr} A$ for every integer k .*

Proof: For $k = 1$, $\operatorname{tr}(A^2B) = \operatorname{tr} A \operatorname{tr}(AB) - \operatorname{tr} A = \operatorname{tr} A(\operatorname{tr}(AB) - 1) > \operatorname{tr} A$.

Conditions (5), $\operatorname{tr}(AB) > 2$ and (4) give consequently

$$-\operatorname{tr}(BA^{-1}) = \operatorname{tr}(AB) - \operatorname{tr}^2 A > 2 - \operatorname{tr}^2 A = -\operatorname{tr} A^2.$$

Thus

$$\begin{aligned} \operatorname{tr}(A^3B) &= \operatorname{tr}(A^2) \operatorname{tr}(AB) - \operatorname{tr}(BA^{-1}) > \operatorname{tr}(A^2) \operatorname{tr}(AB) - \operatorname{tr}(A^2) \\ &= \operatorname{tr}(A^2)(\operatorname{tr}(AB) - 1) \\ &> 2(\operatorname{tr}(AB) - 1) > \operatorname{tr}(AB) \quad \text{as} \quad \operatorname{tr}(AB) > 2. \end{aligned}$$

Then we can proceed by induction. Let $\operatorname{tr}(A^sB) > \operatorname{tr}(AB)$ for any odd $s < 2k + 1$ (k is fixed) and $\operatorname{tr}(A^sB) > \operatorname{tr} A$ for any even $s < 2k$. Applying $\operatorname{tr}(A^2B) > \operatorname{tr} A$ for $A = A^k$ we get

$$\operatorname{tr}(A^{2k}B) = \operatorname{tr}\left((A^k)^2B\right) > \operatorname{tr}(A^k) > \operatorname{tr} A$$

as Lemma 1 is valid.

Let k be even. Then

$$\begin{aligned} \operatorname{tr}(A^{2k+1}B) &= \operatorname{tr}(A^k) \operatorname{tr}(A^{k+1}B) - \operatorname{tr}(AB) \\ &> (\operatorname{tr}^2(A^{k/2}) - 2) \operatorname{tr}(AB) - \operatorname{tr}(AB) \\ &> 2 \operatorname{tr}(AB) - \operatorname{tr}(AB) = \operatorname{tr}(AB). \end{aligned}$$

Let k be odd. Then using (5) we get

$$\begin{aligned} \operatorname{tr}(A^{2k+1}B) &= \operatorname{tr}(A^{k+1}) \operatorname{tr}(A^k B) - \operatorname{tr}(BA^{-1}) \\ &> \left(\operatorname{tr}^2\left(A^{\frac{k+1}{2}}\right) - 2\right) \operatorname{tr}(AB) + 2 - \operatorname{tr}^2 A \\ &> \left(\operatorname{tr}^2 A - 2\right) \operatorname{tr}(AB) + 2 - \operatorname{tr}^2 A \\ &= \left(\operatorname{tr}^2 A - 2\right) (\operatorname{tr}(AB) - 1) > 2(\operatorname{tr}(AB) - 1) > \operatorname{tr}(AB). \end{aligned}$$

□

Lemma 2 shows that $\operatorname{tr}(A^s B A^k) > 2$ for all s, k provided that $\operatorname{tr} A > 2$, $\operatorname{tr} B > 2$ and $\operatorname{tr}(AB) > 2$.

Remark 4. In the general case (i.e., when $\operatorname{tr} A \neq \operatorname{tr} B$ and relying on vector parametrization (2)) one can see that (5) can be rewritten in the form

$$t(AB) = t(A)t(B)(1 - \mathbf{c}_A \cdot \mathbf{c}_B), \quad t(X) = \frac{1}{2} \operatorname{tr}(M_X), \quad X = A, B, AB$$

which means that the second condition in **SC2** is actually superfluous. In the same time it is easy to prove that

$$\mathbf{c}_{A^k} = \alpha_k(\mathbf{c}_A)\mathbf{c}_A, \quad \alpha_k(\mathbf{c}_A) \in \mathbb{R}^+, \quad k = 1, 2, 3, \dots$$

so that the validity of the Saxon-Hutner conjecture for $A^m B$, AB^m , and $A^m B^n$ for $m, n \in \mathbb{N}$ is obvious.

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