Saxon-Hutner-Luttinger theorem in various physical models in one dimension

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The Saxon-Hutner-Luttinger theorem is proved herein by using a very simple mathematical scheme within the transfer-matrix method for one-dimensional Schrödinger operators in various types of physical models. This theorem is extended to that for the regular and the disordered chain systems, where binary types of regularity and disorder are assumed throughout the paper. This scheme is very general and does not depend upon the explicit forms of transfer matrices in the models. Clarified is the relationship between Anderson localization and the Saxon-Hutner-Luttinger theorem.

I. INTRODUCTION

Disordered systems have been attracting much interest of physicists for a long time.[1,2] Even in one-dimensional (1D) disordered lattices there are many deep physical problems such as Anderson localization[3] and Saxon-Hutner-Luttinger (SHL) theorem.[4,5] These are believed to provide a foundation of 1D disordered lattices.

On the one hand, the Anderson localization problem has been studied by many authors for several decades.[2] Up to now, the physics of Anderson localization is well understood by these efforts, and its ground is widely established.[6-11] Especially in 1D, there is the theorem that all the states in the spectrum belong to localized states.[1,6-11] On the other hand, the SHL theorem was once intensively studied a long time ago.[1] Using the transfer-matrix method in the Kronig-Penny (KP) model,[12] Saxon and Hutner[4] first conjectured a theorem that, in the case of a 1D diatomic mixed chain, the interval that corresponds to a spectral gap for both of the pure chains remains to give a gap for a mixed chain also; in other words, the common band gaps in the spectra for the pure chains remain forever as band gaps for a mixed crystal chain as well. Soon, this conjecture was rigorously proved by Luttinger.[5]

Later, this theorem was clarified by many authors[13-15] in order to generalize the proof to other physical models such as the tight-binding model and the phonon model, etc.[1] Around that time the spectrum of these systems was intensively studied in order to prove the existence of a gap in the optical band of a 1D disordered mixed crystal such as $AB_{1-x}C_x$, etc.[16-18] However, the proof of Luttinger is restricted to the disordered diatomic chains. There has been no generalization to the polyatomic chain systems. And also the relationships of the SHL theorem between the different models and systems are not so clear up to now. Thus, its ground still seems mysterious.

Recently there have been considerable developments in the so-called *quasiperiodic* and *aperiodic lattices*.[19,20] These theoretical efforts are motivated by the recent discovery of *quasicrystals*[21] and their 1D modelings.[22] In this problem the systems are 1D nonperiodic lattices that are uniquely generated by a deterministic substitution scheme of letters, where letters denote the distinct species of atoms. Therefore, the systems are classified in between periodic and disordered lattices, where we use the words "quasiperiodic" and "aperiodic" for the systems constructed by deterministic substitutions and "disordered" for the usual systems constructed by an ensemble average over randomness. And one would like to obtain the spectrum as well as the wave function in the system. This has been successfully performed by using the so-called *trace map* on the transfer matrices.[23]

In spite of these many efforts the systems that have been considered were restricted to the systems that letters describe only *monatoms*. In other words, it has been assumed that there is no inner structure of unit elements (i.e., bases) represented by letters. However, letters may represent and stand for a polyatomic structure of the unit elements (i.e., *molecules*) in the system, such that the system is constructed as a quasiperiodic or an aperiodic arrangement of molecules. In this case, a regular chain of molecules may provide a spectrum with a finite number of spectral gaps. Therefore, one would like to know whether or not common spectral gaps exist for the quasiperiodic and aperiodic chains of molecules as well. Thus, one encounters a situation similar to that when the SHL theorem is considered for disordered diatomic chains. Therefore, the relationship between quasiperiodicity (or aperiodicity) and the SHL theorem will be worth investigating.

In this paper we are going to present a simple but a very general proof of the SHL theorem. In this proof it is necessary to require not the explicit details but the more general mathematical properties of physical models. And the relationship between the proofs for different physical models will be clarified.

To ease the reference we first state the main result. The SHL theorem is mathematically described as follows: Denote the two transfer matrices by $\underline{P}$ and $\underline{Q}$ belonging to $SL(2,\mathbf{R})$. Consider a matrix product of $\underline{P}$ and $\underline{Q}$:

$$\underline{M}(N_k)=\underline{P}^{r_k}\underline{Q}^{s_k}\underline{P}^{r_{k-1}}\underline{Q}^{s_{k-1}}\cdots\underline{P}^{r_1}\underline{Q}^{s_1}\ , \tag{1.1}$$

where r_k's and s_k's are all positive integers. The total number N_k of sites in the unit cell is given by

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$N_k = \sum_{j=1}^{k}(r_j + s_j)$ and the density of Q in the system by

$$x = \frac{\sum_{j=1}^{k} s_j}{\sum_{j=1}^{k}(r_j + s_j)} . \tag{1.2}$$

Then the SHL theorem is equivalent to the following theorem.

Theorem: Suppose the condition $|\mathrm{Tr}(\underline{P}\underline{Q})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})| > 2$ and $|\mathrm{Tr}(\underline{Q})| > 2$, then $|\mathrm{Tr}\underline{M}(N_k)| > 2$.

This is a consequence of the following lemma.

Lemma: (a) Suppose $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q}) > 0$. If $|\mathrm{Tr}(\underline{P}\underline{Q})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{P}\underline{Q}) = |\mathrm{Tr}(\underline{P}\underline{Q})|$, and if $|\mathrm{Tr}(\underline{P}\underline{Q})| < |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{P}^{-1}\underline{Q}) = |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. (b) Suppose $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q}) < 0$. If $|\mathrm{Tr}(\underline{P}\underline{Q})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{P}\underline{Q}) = -|\mathrm{Tr}(\underline{P}\underline{Q})| = -|\mathrm{Tr}(\underline{P}\underline{Q})|$, and if $|\mathrm{Tr}(\underline{P}\underline{Q})| < |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ then $\mathrm{Tr}(\underline{P}^{-1}\underline{Q}) = -|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$.

This lemma will be proved in Sec. III.

The organization of the present paper is the following. In Sec. II, the physical models are summarized for later purposes. In Sec. III, several lemmas will be proved as a basic tool for the proof of the SHL theorem. In Sec. IV, by means of the above lemmas, the SHL theorem for the discrete Schrödinger equation with a single band gap is proved in the various physical systems—the regular and disordered binary chains. The powerful effectiveness of the lemmas will be demonstrated. And the SHL theorem will be extended to the system of the discrete Schrödinger equation with many band gaps and to the system of the continuous Schrödinger equation, where an infinite number of band gaps appear in the spectrum. In Sec. V, the relationship between Anderson localization and the SHL theorem will be discussed. And a summary will be made.

II. PHYSICAL MODELS

There are mainly two types of physical models that have been studied for a long time.[1] One is the *discrete models* such as the discrete (i.e., the tight-binding) Schrödinger equation for an electron and the lattice vibration on a 1D lattice. The other is the *continuum models* such as the KP model[7] and Hill's equation,[24] etc. These are the one-body problems in one dimension. Throughout this paper we restrict ourselves to investigate only these models.

The most important thing is that all the above physical models are written in the same manner as the transfer-matrix form in 1D:

$$\Psi_{n+1} = \underline{T}(n)\Psi_n , \tag{2.1}$$

where the transfer matrix $\underline{T}(n) \in SL(2,\mathbf{R})$ and Ψ_n is given as a 2D column vector at site n. The discrete Schrödinger equation is given by

$$T_{n+1}\psi_{n+1} + T_n\psi_{n-1} + V_n\psi_n = E\psi_n , \tag{2.2}$$

where T_n is the hopping integral between the nth and the $(n-1)$th sites and V_n the on-site potential at site n, respectively.[1] The above equation can be converted into the following transfer matrix:

$$\underline{T}(n) \equiv \begin{bmatrix} \dfrac{E-V_n}{T_{n+1}} & -\dfrac{T_n}{T_{n+1}} \\ 1 & 0 \end{bmatrix} \qquad \Psi_n \equiv \begin{bmatrix} \psi_n \\ \psi_{n-1} \end{bmatrix} . \tag{2.3}$$

We note the following. There are two typical models: The *on-site model* of $T_n = 1$ and the *off-diagonal model* of $V_n = 0$. In the former, obviously $\underline{T}(n) \in SL(2,\mathbf{R})$. But in the latter, it is not apparently so. However, if one considers a product of the N transfer matrices:

$$\underline{M}(N) = \underline{T}(N)\underline{T}(N-1) \cdots \underline{T}(1) , \tag{2.4}$$

through the lattice where N is the number of the unit cell, then $\mathrm{Det}\underline{M}(N) = 1$ such that $\underline{M}(N) \in SL(2,\mathbf{R})$. Thus, what is important here is that each transfer matrix does not belong to $SL(2,\mathbf{R})$ but the product of the N transfer matrices belongs to $SL(2,\mathbf{R})$.

In the continuum models, the Schrödinger equation (i.e., Hill's equation[24]) is given by

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x) , \tag{2.5}$$

where the potential is given by a sum of atomic potentials. Therefore, the whole x region of $-\infty < x < \infty$, is divided into the regions (i.e., the cells), $x_{n-1} \leq x < x_n$, $n \in \mathbf{Z}$, and define $\xi_n \equiv x_n - x_{n-1}$. For example, in the δ-function KP model, the potential is given by

$$V(x) = \sum_n \gamma_n \delta(x - x_n) . \tag{2.6}$$

Therefore, the wave function is defined as

$$\psi_n(x) = \psi_n \cos kx + \psi_n' \frac{\sin kx}{k} , \tag{2.7}$$

for the region $x_{n-1} \leq x < x_n$, where $k \equiv \sqrt{2mE/\hbar^2}$. The boundary condition satisfies

$$\begin{aligned} &\psi_{n+1}(0) = \psi_n(\xi_n) , \\ &\frac{d\psi_{n+1}}{dx}(0) - \frac{d\psi_n}{dx}(\xi_n) = \delta_n \psi_n(0) , \end{aligned} \tag{2.8}$$

where $\delta_n \equiv 2m\gamma_n/\hbar^2$, and then the transfer matrix and Ψ_n are given by

$$\underline{T}(n) \equiv \begin{bmatrix} \cos(k\xi_n) & \sin(k\xi_n)/k \\ -k\sin(k\xi_n) + \delta_n\cos(k\xi_n) & \cos(k\xi_n) + \delta_n\sin(k\xi_n)/k \end{bmatrix} \qquad \Psi_n \equiv \begin{bmatrix} \psi_n \\ \psi_n' \end{bmatrix} , \tag{2.9}$$

with $\mathrm{Det}\underline{T}(n)=1$, respectively.

In the above the various types of physical models are introduced. These will be used in Sec. IV in order to prove the SHL theorem by means of the mathematical tools that will be discussed in the next section.

III. BASIC TOOLS

Let us introduce several mathematical theorems as a basic tool in order to prove the SHL theorem. These will be addressed as lemmas 1, 2, and 3, and especially lemmas 2 and 3 will be used in the preceding sections.

Let $\underline{P}$ and $\underline{Q}$ belong to $SL(2,\mathbf{R})$. Then, there exist identities which are known as the *Fricke identities*:[25]

$$\mathrm{Tr}(\underline{PQ})+\mathrm{Tr}(\underline{P}^{-1}\underline{Q})=\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})\ , \tag{3.1}$$

$$\begin{aligned}\Lambda&\equiv\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{-1}\underline{PQ})\\&=[\mathrm{Tr}(\underline{P})]^2+[\mathrm{Tr}(\underline{Q})]^2+[\mathrm{Tr}(\underline{PQ})]^2\\&\quad-\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})\mathrm{Tr}(\underline{PQ})-2\ .\end{aligned} \tag{3.2}$$

From Eq. (3.1) one finds the following lemma.

Lemma 1: (a) Suppose $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})>0$. If $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{PQ})=|\mathrm{Tr}(\underline{PQ})|$, and if $|\mathrm{Tr}(\underline{PQ})|<|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{P}^{-1}\underline{Q})=|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. (b) Suppose $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})<0$. If $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{PQ})=-|\mathrm{Tr}(\underline{PQ})|$, and if $|\mathrm{Tr}(\underline{PQ})|<|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, then $\mathrm{Tr}(\underline{P}^{-1}\underline{Q})=-|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$.

Proof of Lemma 1: Let us denote a and b by $a=\mathrm{Tr}(\underline{PQ})$ and $b=\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$. (a) Let $a+b=s>0$, where $s=\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})$. If $|a|\geq|b|$, then $a^2\geq b^2$. From this, $a^2-b^2=(a-b)(a+b)=(a-b)s\geq 0$. So, if $s>0$, then $a-b\geq 0$. Therefore, from $a-b\geq 0$ together with $a+b=s>0$, one can conclude that $a=|a|\geq|b|$. In the same way, if $|a|<|b|$, then $b=|b|>|a|$. (b) Let $a+b=s<0$. If $|a|\geq|b|$, then $a^2-b^2=(a-b)(a+b)=(a-b)s\geq 0$. So, if $s<0$, then $a-b\leq 0$. Therefore, from $a-b\leq 0$ together with $a+b=s<0$, one can conclude that $a=-|a|\leq-|b|$. In the same way, if $|a|<|b|$, then $b=-|b|<-|a|$. Q.E.D.

Lemma 2: (a) Suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})>2$ or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})<-2$. If $\mathrm{Tr}(\underline{PQ})\geq\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$, then $\mathrm{Tr}(\underline{PQ})>2$. (b) Suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})<-2$ or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})>2$. If $\mathrm{Tr}(\underline{PQ})<\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$, $\mathrm{Tr}(\underline{PQ})<-2$.

Proof of Lemma 2: Use the same notations in the proof of lemma 1. (a) Suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})>2$ or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})<-2$. Then, $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})=s>4$. Now, from lemma 1(a), if $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ (i.e., $|a|\geq|b|$), then $a>b$ and $a=|a|$. Therefore, if $a>b$ and $a+b=s>4$, then $a>2$. That is $\mathrm{Tr}(\underline{PQ})>2$. (b) Suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})<-2$ or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})>2$. Then, $\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})=s<-4$. Now, from lemma 1(b), if $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ (i.e., $|a|\geq|b|$), then $a<b$ and $a=-|a|$. Therefore, if $a<b$ and $a+b=s<-4$, then $a<-2$. That is $\mathrm{Tr}(\underline{PQ})<-2$. Q.E.D.

Lemma 2 can be rewritten compactly as the following lemma.

Lemma 3: Suppose $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})|>2$, $|\mathrm{Tr}(\underline{Q})|>2$, then $|\mathrm{Tr}(\underline{PQ})|>2$.

Remark 1 (on the condition, $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$): In the above lemmas we always assume the condition, $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. The reason is the following: As we will see later in Sec. IV, in most physical models the condition $|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|\geq 2$ is satisfied. So, once $|\mathrm{Tr}(\underline{P})|>2$, $|\mathrm{Tr}(\underline{Q})|>2$, and $|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|\geq 2$ are supposed, then $|\mathrm{Tr}(\underline{PQ})|>2$ seems to be trivially obtained. However, there is a counterexample for this case,[26] where even if $|\mathrm{Tr}(\underline{P})|>2$, $|\mathrm{Tr}(\underline{Q})|>2$, and $|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|\geq 2$ are supposed, then $|\mathrm{Tr}(\underline{PQ})|\leq 2$. Thus, if the condition $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ cannot hold, then the lemmas become false as a general statement. To avoid this case one has to impose the condition, $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. Once this condition is supposed, then the lemmas seem trivial. However, it is not so even in this case. Because this condition includes information of the physical models and depends upon the parameters in the models such as energy and potentials. Therefore, this holds only for the certain range of the parameters.

Remark 2: Lemmas 1, 2, and 3 are free from the specific details of $\underline{P}$ and $\underline{Q}$. They are just a consequence of the $SL(2,\mathbf{R})$ character of $\underline{P}$ and $\underline{Q}$, and hold for the case where $\underline{P}$ is replaced by $\underline{P}^{-1}$ as well.

IV. THE SHL THEOREM IN VARIOUS PHYSICAL MODELS

In this section, we are going to prove the SHL theorem for various types of physical systems such as the regular and disordered chains. Here regularity and disorder are based upon the *binary* systems, respectively. We first discuss the SHL theorem in the discrete Schrödinger equation with a single band gap, which will be considered as a prototype for later purposes. Later, we discuss the SHL theorem to other physical models such as the discrete Schrödinger equation with many band gaps and the continuous Schrödinger equation.

A. Schrödinger equation with a single band gap for the regular binary chains

Consider a 1D binary alloy system and P and Q, represented by a chemical formula, $P_{1-x}Q_x$ $(0\leq x\leq 1)$, where x is the density of Q in the system. If we regard P (Q) as a monatom $P\equiv A$ $(Q\equiv B)$, then this expression describes the usual binary chain system of $A_{1-x}B_x$. And if we regard $P(Q)$ as a diatomic molecule, $P\equiv AB$ $(Q\equiv AC)$, then it turns out to be the ternary chain system of $AB_{1-x}C_x$.[27]

The latter system will be investigated for our purpose here. If $x=0$, then the system is a regular AB chain, which means a chain made by two atoms of A and B such that the system is an infinite chain constructed by an infinite repetition of the unit cell AB. If $x=1$, then the system is a regular AC chain. And if $0<x<1$, then the system is a mixed crystal characterized by a fraction x. So, in this system the local coordination is either AB or AC. Let us assume that the parameters in the model take on only three values associated with the three types of atoms, A, B, and C in the chain. Throughout this section only the off-diagonal model is studied for simplicity.

According to the configuration in the chain, one can assign the corresponding transfer matrices as

$$\underline{P}\equiv\underline{AB}=\begin{pmatrix} \frac{E^2}{T_aT_b}-\frac{T_b}{T_a} & -\frac{E}{T_b} \\ \frac{E}{T_b} & -\frac{T_a}{T_b} \end{pmatrix}$$

and (4.1)

$$\underline{Q}\equiv\underline{AC}=\begin{pmatrix} \frac{E^2}{T_aT_c}-\frac{T_c}{T_a} & -\frac{E}{T_c} \\ \frac{E}{T_c} & -\frac{T_a}{T_c} \end{pmatrix} .$$

From these one gets the traces as

$$\mathrm{Tr}(\underline{Q})/2=\frac{1}{2}\left[\frac{E^2}{T_aT_c}-\frac{T_a}{T_c}-\frac{T_c}{T_a}\right]\equiv X_0 , \tag{4.2}$$

$$\mathrm{Tr}(\underline{P})/2=\frac{1}{2}\left[\frac{E^2}{T_aT_b}-\frac{T_a}{T_b}-\frac{T_b}{T_a}\right]\equiv Y_0 , \tag{4.3}$$

$$\mathrm{Tr}(\underline{PQ})/2=\frac{1}{2}\left[\frac{E^4-(2T_a^2+T_b^2+T_c^2)E^2}{T_a^2T_bT_c}+\frac{T_a^2}{T_bT_c}+\frac{T_bT_c}{T_a^2}\right]\equiv Z_0 , \tag{4.4}$$

$$\mathrm{Tr}(\underline{P}^{-1}\underline{Q})/2=\frac{1}{2}\left[\frac{T_c}{T_b}+\frac{T_b}{T_c}\right]\equiv Z_0' . \tag{4.5}$$

Since X_0 and Y_0 are quadratic functions of E, the conditions $|X_0|>1$ and $|Y_0|>1$ provide one band gap in the spectra, respectively. Thus, in this model the regular AB and AC chains consist of only one band gap, respectively.

Theorem 1: The common band gap in the spectra for the regular AB and AC chains remains as a gap for the regular $ABAC$ chain as well.

Proof of theorem 1: For the regular AC chain case, from Eq. (4.2) we have

$$X_0=\mathrm{Tr}(\underline{Q})/2=[E^2/(T_aT_c)-T_a/T_c-T_c/T_a]/2 .$$

If $X_0>1$, the energy lies outside the band. If $X_0<-1$, then the energy lies in the band gap. This gives the band gap $\Delta_{ac}\equiv2|T_a-T_c|$ around $E=0$. Similarly, from Eq. (4.3), if $Y_0<-1$, one obtains the band gap $\Delta_{ab}\equiv2|T_a-T_b|$ around $E=0$ for the regular AB chain. To see how lemma 1 works in this problem, let us first consider the regular $ABAC$ chain. From Eq. (4.4), one has $\mathrm{Tr}(\underline{PQ})/2=2X_0Y_0-Z_0'$, where

$$Z_0'\equiv\mathrm{Tr}(\underline{P}^{-1}\underline{Q})/2=(T_b/T_c+T_c/T_b)/2$$

[Eq. (4.5)]. Consider an energy such that $X_0<-1$ and $Y_0<-1$, which then defines the common band gap $\Delta_0\equiv\min[\Delta_{ab},\Delta_{ac}]$. And $X_0Y_0=\mathrm{Tr}(\underline{P})\mathrm{Tr}(\underline{Q})/4>0$. Now, one can use lemma 1. If

$$|Z_0|=|\mathrm{Tr}(\underline{PQ})/2|\ge|Z_0'|=|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})/2| ,$$

then $Z_0=|Z_0|$. Therefore, $Z_0=|Z_0|\ge|Z_0'|>1$, unless $T_b=T_c$. In this way, the common band gap between the spectra for the regular AB and AC chains remains as a gap for the regular $ABAC$ chain as well. Q.E.D.

Theorem 2: The common band gap in the spectra for the regular AB, AC, and $ABAC$ chains remains as a gap for the regular $ABACAB$ chain as well.

Proof of theorem 2: Consider a bit complicated case of the regular $ABACAB$ chain. Then, one needs treat $\mathrm{Tr}(\underline{PQP})=\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})-\mathrm{Tr}(\underline{Q})$. Consider an energy such that $|\mathrm{Tr}(\underline{P})|>2$ and $|\mathrm{Tr}(\underline{Q})|>2$. This lies in the common gap between the regular AB and AC chains. Suppose the condition $|\mathrm{Tr}(\underline{PQ})|\ge|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. Then from Eqs. (4.2)–(4.5) one gets $|\mathrm{Tr}(\underline{PQ})|>2$, since $|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|=|T_b/T_c+T_c/T_b|>2$ unless $T_b=T_c$. Since $\mathrm{Tr}(\underline{PQ})$ is a fourth-order polynomial of E, there appear three band gaps in the spectrum for the regular $ABAC$ chain, where one center gap is given by $\mathrm{Tr}(\underline{PQ})>2$ and the other two gaps are given by $\mathrm{Tr}(\underline{PQ})<-2$. Thus, when one wants to find the common gap for the regular $ABACAB$ chain, one needs consider the case of $\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})<0$ as well as that of $\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})>0$. Regard $\underline{P}'=\underline{PQ}$ and $\underline{Q}'=\underline{P}$. If $|\mathrm{Tr}(P'Q')|\ge|\mathrm{Tr}(P'^{-1}Q')|$ [i.e., $|\mathrm{Tr}(\underline{PQP})|\ge|\mathrm{Tr}(\underline{Q})|$], then lemma 3 can be used. This condition is proved as follows:

$$|\mathrm{Tr}(\underline{PQP})|=|\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})-\mathrm{Tr}(\underline{Q})|$$
$$\ge|\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})|-|\mathrm{Tr}(\underline{Q})| .$$

So,

$$|\mathrm{Tr}(\underline{PQP})|-|\mathrm{Tr}(\underline{Q})|\ge|\mathrm{Tr}(\underline{PQ})\mathrm{Tr}(\underline{P})|-2|\mathrm{Tr}(\underline{Q})|$$
$$>2\{|\mathrm{Tr}(\underline{PQ})|-|\mathrm{Tr}(\underline{Q})|\} .$$

And,

$$|\mathrm{Tr}(\underline{PQ})|-|\mathrm{Tr}(\underline{Q})|=|\mathrm{Tr}(\underline{PQ})|-|\{\mathrm{Tr}(\underline{PQ})+\mathrm{Tr}(\underline{P}^{-1}\underline{Q})\}/\mathrm{Tr}(\underline{P})|$$
$$>|\mathrm{Tr}(\underline{PQ})|-\{|\mathrm{Tr}(\underline{PQ})|+|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|\}/2=\{|\mathrm{Tr}(\underline{PQ})|-|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|\}/2\ge0$$

from the assumption. Therefore, $|\mathrm{Tr}(P'Q')|\ge|\mathrm{Tr}(P'^{-1}Q')|$. Thus, from lemma 3, one finds $|\mathrm{Tr}(\underline{PQP})|=|\mathrm{Tr}(\underline{P'Q'})|>2$. Q.E.D.

Theorem 3: The common band gap in the spectra for the regular AB and AC chains remains as a gap for the regular $(AB)^nAC$ chain as well.

Proof of theorem 3: Let $\underline{P}=\underline{AB}$ and $\underline{Q}=\underline{AC}$. Then, for the regular $(AB)^nAC$ chain one needs consider a trace of $\mathrm{Tr}(\underline{P}^n\underline{Q})$. Since there is the Cayley-Hamilton identity,

$$\underline{P}^2=\mathrm{Tr}(\underline{P})\underline{P}-\underline{I} , \tag{4.6}$$

one finds

$$\underline{P}^{n+1}=\mathrm{Tr}(\underline{P})\underline{P}^n-\underline{P}^{n-1} . \tag{4.7}$$

Multiplying by $\underline{Q}$ from the right, one finds $\underline{P}^{n+1}\underline{Q}=\mathrm{Tr}(\underline{P})\underline{P}^{n}\underline{Q}-\underline{P}^{n-1}\underline{Q}$. Taking the trace for both sides, one gets

$$K_{n+1}=2Y_0K_n-K_{n-1}\ , \tag{4.8}$$

where $K_n\equiv\mathrm{Tr}(\underline{P}^n\underline{Q})/2$ and $Y_0=\mathrm{Tr}(\underline{P})/2$. From this, K_n is the nth Chebyshev polynomial of the second kind[28] with respect to Y_0, with the initial condition $K_{-1}=\mathrm{Tr}(\underline{P}^{-1}\underline{Q})/2=2X_0Y_0-Z_0$, $K_0=\mathrm{Tr}(\underline{Q})/2=X_0$, and $K_1=\mathrm{Tr}(\underline{PQ})/2=Z_0$. Consider an energy such that $|K_{n-1}|>1$, $|K_n|>1$, and $|Y_0|>1$ [i.e., $|\mathrm{Tr}(\underline{P}^{n-1}\underline{Q})|>2$, $|\mathrm{Tr}(\underline{P}^n\underline{Q})|>2$, and $|\mathrm{Tr}(\underline{P})|>2$]. This provides the energy in the common band gap of the regular AB, $(AB)^{n-1}AC$, and $(AB)^nAC$ chains. But for the cases of $n=1$ and 2 are already proved as theorems 1 and 2. Consider $|K_{n+1}|$. From Eq. (4.8),

$$\begin{aligned}|K_{n+1}|&=|2Y_0K_n-K_{n-1}|\\&\geq|2Y_0K_n|-|K_{n-1}|\\&>|2K_n|-|K_{n-1}|\\&=|K_n|+\{|K_n|-|K_{n-1}|\}\ .\end{aligned}$$

So, if $|K_n|-|K_{n-1}|>0$, then $|K_{n+1}|-|K_n|>0$. Hence, by induction together with lemma 3, $|K_{n+1}|>|K_n|>\cdots>|K_1|>1$. Thus, theorem 3 is proved. Q.E.D.

B. Schrödinger equation with a single band gap for the disordered binary chains

Let us consider the disordered binary chains of P and Q. This system was studied long time ago first by Saxon and Hutner.[4] Later, Luttinger[5] gave the first rigorous proof for the Saxon-Hutner conjecture. So, let us follow Luttinger's argument for the moment.

Consider the matrix product of transfer matrices of Eq. (1.1). We are now able to state the SHL theorem for the disordered binary chain systems.

Theorem 4: The common band gap in the spectra for the regular AB and AC chains remains as a gap for the disordered chains as well.

Proving this theorem is obviously equivalent to proving the following theorem.

Theorem 5: Suppose $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})|>2$ and $|\mathrm{Tr}(\underline{Q})|>2$, then $|\mathrm{Tr}\underline{M}(N_k)|>2$.

Before going to prove theorem 5, let us prove the following lemmas first, which are relevant to the proof. These lemmas come from the lemmas in the previous section.

Lemma 5: Suppose $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})|>2$ and $|\mathrm{Tr}(\underline{Q})|>2$, then $|\mathrm{Tr}(\underline{P}^m\underline{Q}^n)|>2$.

Lemma 6: Suppose $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})|>2$ and $|\mathrm{Tr}(\underline{Q})|>2$, then $|\mathrm{Tr}(\underline{P}^{r_2}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})|>2$.

Lemma 7: Suppose $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. If $|\mathrm{Tr}(\underline{P})|>2$ and $|\mathrm{Tr}(\underline{Q})|>2$, then $|\mathrm{Tr}(\underline{P}^{r_3}\underline{Q}^{s_3}\underline{P}^{r_2}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})|>2$.

Proofs of lemmas 5, 6 and 7: We only show the proof of lemma 6 in Appendix A. Since the proof of lemma 5 is included in it as a special case and by a similar argument one can prove lemma 7. So, the proofs of lemmas 5 and 7 are omitted here. See Iguchi and Yoshikawa.[29] Q.E.D.

Now, one can prove theorem 5 immediately.

Proof of theorem 5: Recursively using lemmas 5, 6, and 7, or by using a similar argument to that in the proofs of the lemmas, theorem 5 is proved no matter what value of k. Q.E.D.

Remark 3: An alternative and a more general proof of theorem 5 is given by Iguchi and Yoshikawa.[29]

Next, we are going to extend the SHL theorem to other physical models such as the discrete Schrödinger equation with many band gaps and to the continuous Schrödinger equation. To do so, one must ask whether or not the condition $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ is automatically satisfied for these models, respectively. Once this is established, then the proof of the SHL theorem remains the same for these models as well.

C. Discrete Schrödinger equation with many band gaps

Let us first consider the SHL theorem in the discrete Schrödinger equation with many band gaps. In order to have many band gaps in the spectra for the two independent pure P and Q systems, one can assume the transfer matrices as

$$\underline{P}\equiv\underline{P}_1\underline{P}_2\cdots\underline{P}_p\ , \tag{4.9}$$

$$\underline{Q}\equiv\underline{Q}_1\underline{Q}_2\cdots\underline{Q}_q\ , \tag{4.10}$$

where the distinct transfer matrices $\underline{P}_i$ $(i=1,\ldots,p)$ and $\underline{Q}_j$ $(j=1,\ldots,q)$ are given by Eq. (2.3) such that $\underline{P},\underline{Q}\in SL(2,\mathbf{R})$. This means that $\underline{P}$ represents a molecule with p atoms and $\underline{Q}$ a molecule with q atoms. So, the regular P lattice means that there is a regular lattice of the molecule P, and so does the regular Q lattice. If $|\mathrm{Tr}(\underline{P})|>2$, then an energy lies in a band gap. Therefore, the spectrum of the regular P lattice consists of the $p-1$ band gaps unless T_n (and V_n) are identical. Similarly, the spectrum of the regular Q lattice system consists of the $q-1$ band gaps in general.

Now, let us ask whether or not the condition $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ is automatically satisfied in this model. $\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$ is given by

$$\begin{aligned}\mathrm{Tr}(\underline{P}^{-1}\underline{Q})&=\mathrm{Tr}[(\underline{P}_1\underline{P}_2\cdots\underline{P}_p)^{-1}\underline{Q}_1\underline{Q}_2\cdots\underline{Q}_q]\\&=\mathrm{Tr}[(\underline{P}_2\cdots\underline{P}_{p-1})^{-1}(\underline{P}_1^{-1}\underline{Q}_1)\\&\quad\times(\underline{Q}_2\cdots\underline{Q}_{q-1})(\underline{Q}_q\underline{P}_p^{-1})]\ .\end{aligned}$$

So, in this case it is not that simple to find the condition $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. For this reason, instead of supposing that $|\mathrm{Tr}(\underline{P})|>2$, $|\mathrm{Tr}(\underline{Q})|>2$ with $|\mathrm{Tr}(\underline{PQ})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$, suppose that $|\mathrm{Tr}(\underline{PQ})|>2$, $|\mathrm{Tr}(\underline{P})|>2$, and $|\mathrm{Tr}(\underline{Q})|>2$ with $|\mathrm{Tr}(\underline{PQP})|\geq|\mathrm{Tr}(\underline{Q})|$. Here, $|\mathrm{Tr}(\underline{PQ})|>2$ provides in general the $(p+q-1)$ band gaps in the spectrum of the regular PQ chain. Then, find the common band gaps in the spectra of the Q system, the P system, and the PQ chain system. In other words, one would like to regard $\underline{P}$, $\underline{Q}$, and $\underline{P}^{-1}\underline{Q}$ as $\underline{P}'=\underline{PQ}$, $\underline{Q}'=\underline{P}$, and $\underline{P}'^{-1}\underline{Q}'=\underline{Q}^{-1}\underline{P}^{-1}\underline{P}=\underline{Q}^{-1}$ such that $\mathrm{Tr}(\underline{P}')=\mathrm{Tr}(\underline{PQ})$, $\mathrm{Tr}(\underline{Q}')=\mathrm{Tr}(\underline{P})$, and $\mathrm{Tr}(\underline{P}'^{-1}\underline{Q}')$

$=\mathrm{Tr}(\underline{Q})$. Then, the condition $|\mathrm{Tr}(\underline{P}'\underline{Q}')| \geq |\mathrm{Tr}(\underline{P}'^{-1}\underline{Q}')|$ turns out to be the trivial relation $|\mathrm{Tr}(\underline{P}'\underline{Q}')| \geq 2$. So, one can use lemma 3 for $\underline{P}'$ and $\underline{Q}'$.

We can then state the SHL theorem in this model as follows.

Theorem 6: The common band gaps in the spectra for the regular Q, P, and PQ lattice systems in the discrete Schrödinger equation with many band gaps remain as the band gaps for the regular and the disordered PQ lattice systems as well.

Proof of theorem 6: Since the condition $|\mathrm{Tr}(\underline{PQ})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ is automatically satisfied in this model, the proofs for the regular PQ chains are the same as those of theorems 1, 2, and 3, and the proof for the disordered PQ chains is the same as that of theorem 5 for the disordered PQ alloys, respectively. Q.E.D.

D. Continuous Schrödinger equation

Let us now consider the SHL theorem in the continuous Schrödinger equation. In the KP model,[1,2,12] the transfer matrix is given by Eq. (2.9). So, to distinguish the two different transfer matrices, $\underline{P}$ and $\underline{Q}$, for the two independent pure systems, let us define that either ξ_n or δ_n takes only two values such that $\xi_n = a$ or b, and $\delta_n = \delta_a$ or δ_b. Thus, the transfer matrices are given by

$$\underline{P} \equiv \begin{bmatrix} \cos(ka) & \sin(ka)/k \\ -k\sin(ka)+\delta_a\cos(ka) & \cos(ka)+\delta_a\sin(ka)/k \end{bmatrix}, \tag{4.11}$$

$$\underline{Q} \equiv \begin{bmatrix} \cos(kb) & \sin(kb)/k \\ -k\sin(kb)+\delta_b\cos(kb) & \cos(kb)+\delta_b\sin(kb)/k \end{bmatrix}. \tag{4.12}$$

Taking the trace of $\underline{P}$ and $\underline{Q}$, one finds

$$\mathrm{Tr}(\underline{P}) = 2\cos(ka)+\delta_a\sin(ka)/k\ , \tag{4.13}$$

$$\mathrm{Tr}(\underline{Q}) = 2\cos(kb)+\delta_b\sin(kb)/k\ . \tag{4.14}$$

If $|\mathrm{Tr}(\underline{P})| > 2$, then an energy lies in a band gap. Therefore, Eq. (4.13) provides an infinite set of energy bands and band gaps for the regular P lattice system, and so does Eq. (4.14) for the regular Q lattice system. But there is the exception: When $k_n = \pi n/a$ (n integer), $\sin(k_n a) = 0$ such that $\mathrm{Tr}(\underline{P}) = 2(-1)^n$, i.e., $|\mathrm{Tr}(\underline{P})| = 2$. Therefore, these energies $E_n = \hbar^2 k_n^2/2m$, lie in the upper band edges of the energy bands.

Now, let us ask whether or not the condition $|\mathrm{Tr}(\underline{PQ})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ is automatically satisfied in this model. To do so, consider $\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$. One now finds

$$\mathrm{Tr}(\underline{P}^{-1}\underline{Q}) = 2\cos[k(a-b)] + (\delta_a - \delta_b)\sin[k(a-b)]/k\ . \tag{4.15}$$

It is not difficult to see this point by a direct calculation.[29] However, for our purpose here, we may only assume that the scattering potentials are equally spacing, i.e., $a=b$. This leads us to $\mathrm{Tr}(\underline{P}^{-1}\underline{Q}) = 2$. Therefore, in this particular case, the condition $|\mathrm{Tr}(\underline{PQ})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ becomes the trivial relation, $|\mathrm{Tr}(\underline{PQ})| \geq 2$. Suppose that there exists a wave number k (i.e., an energy, $E = \hbar^2 k^2/2m$) such that $|\mathrm{Tr}(\underline{P})| > 2$, $|\mathrm{Tr}(\underline{Q})| > 2$, and $|\mathrm{Tr}(\underline{PQ})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. Thus, we can state the SHL theorem in the KP model.

Theorem 7: The common band gaps in the spectra for the regular P and Q lattice systems in the continuum Schrödinger equation remain as the band gaps for the regular and disordered PQ lattice systems as well.

Proof of theorem 7: Since the condition $|\mathrm{Tr}(\underline{PQ})| \geq |\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$ is automatically satisfied in this model, the proof is the same as theorem 6. Q.E.D.

In the same way, the SHL theorem can be immediately established for the model of Hill's equation.[24]

Remark 4: The KP model[12] has been applied to the quasiperiodic binary chains such as the Fibonacci lattice and the results show numerically the validity of the SHL theorem in the spectrum.[30–32] Thus, the above theorem provides a foundation for their numerical results.

V. DISCUSSION AND CONCLUSION

Now, we are going to discuss the relationship between Anderson localization and the SHL theorem. As is discussed in Sec. IV, we have shown the SHL theorem holds valid for the regular and disordered chains in the various types of physical models. It has been shown that the SHL theorem states not the spectrum itself but the location of band gaps in the spectrum. On the other hand, there is the famous Anderson theorem in 1D disordered lattices: all the states in the spectrum belong to localized states, where the spectrum is point spectrum (i.e., discrete levels) and the states are exponentially localized.[1] Usually this theorem is proved for the system with a single band. However, it should work for the system with a number of the band gaps as well. Thus, the Anderson theorem states not the location of band gaps but the spectrum itself. In this way, one can understand that both theorems can be compatible with one another and their roles are complimentary in the 1D systems, and thus, they are dual theorems to one another.

In conclusion, the SHL theorem has been extended to the various types of physical models. First, the SHL theorem has been discussed in the discrete Schrödinger equation for the system of $AB_{1-x}C_x$, where the spectra of the two regular AB and AC chain systems consist of only one band gap, respectively. In this system, it has been rigorously proved that the SHL theorem is valid for the regular and disordered binary chains. Second, the SHL theorem has been extend to those for the discrete Schrödinger equation with many band gaps and the continuous Schrödinger equation such as the KP model.[12]

Finally we would like to mention that the SHL theorem for the 1D quasiperiodic and aperiodic systems constructed by a deterministic substitution scheme with many letters[33–38] and for the disordered polyatomic chains will be worth investigating for further research.

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APPENDIX A: PROOF OF LEMMA 6

Let $K(r_2,s_2;r_1,s_1)\equiv \mathrm{Tr}(\underline{P}^{r_2}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})/2$, where r_2, r_1, s_2, and s_1 are all positive integers. From the Cayley-Hamilton identity, one finds

$$K(r_2+1,s_2;r_1,s_1)=\mathrm{Tr}(\underline{P})K(r_2,s_2;r_1,s_2)-K(r_2-1,s_2;r_1,s_1)\ . \quad \text{(A1)}$$

From this, one can have

$$|K(r_2+1,s_2;r_1,s_2)|>|K(r_2,s_2;r_1,s_1)| \quad \text{(A2)}$$

if $|K(1,s_2;r_1,s_1)|>|K(-1,s_2;r_1,s_1)|$. This is proved as follows:

$$\begin{aligned}|K(r_2+1,s_2;r_1,s_1)|&=|\mathrm{Tr}(\underline{P})K(r_2,s_2;r_1,s_1)-K(r_2-1,s_2;r_1,s_1)|\\ &\geq|\mathrm{Tr}(\underline{P})K(r_2,s_2;r_1,s_1)|-|K(r_2-1,s_2;r_1,s_1)|\\ &>2|K(r_2,s_2;r_1,s_1)|-|K(r_2-1,s_2;r_1,s_1)|\\ &=|K(r_2,s_2;r_1,s_1)|+\{|K(r_2,s_2;r_1,s_1)|-|K(r_2-1,s_2;r_1,s_1)|\}\ .\end{aligned}$$

Therefore, if $|K(1,s_2;r_1,s_1)|>|K(0,s_2;r_1,s_1)|$, then by induction it is proved. And we know

$$\begin{aligned}|K(1,s_2;r_1,s_1)|-|K(0,s_2;r_1,s_1)|&=|K(1,s_2;r_1,s_1)|-|\{K(1,s_2;r_1,s_1)+K(-1,s_2;r_1,s_1)\}/\mathrm{Tr}(\underline{P})|\\ &>|K(1,s_2;r_1,s_1)|-|\{K(1,s_2;r_1,s_1)+K(-1,s_2;r_1,s_1)\}/2|\\ &>|K(1,s_2;r_1,s_1)|-\{|K(1,s_2;r_1,s_1)|+|K(-1,s_2;r_1,s_1)|\}/2\\ &=\{|K(1,s_2;r_1,s_1)|-|K(-1,s_2;r_1,s_1)|\}/2\ .\end{aligned}$$

Therefore, it is equivalent to prove $|K(1,s_2;r_1,s_1)|-|K(-1,s_2;r_1,s_1)|>0$ or $|\mathrm{Tr}(\underline{P}\underline{A})|>|\mathrm{Tr}(\underline{P}^{-1}\underline{A})|$, where $\underline{A}=\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1}$ and

$$|\mathrm{Tr}(\underline{A})|=|\mathrm{Tr}(\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})|=|\mathrm{Tr}(\underline{P}^{r_1}\underline{Q}^{s_1+s_2})|>2\ .$$

To prove this condition, consider $K(1,s_2;r_1,s_1)=\mathrm{Tr}(\underline{P}\underline{A})$ and $K(-1,s_2;r_1,s_1)=\mathrm{Tr}(\underline{P}^{-1}\underline{A})$. (i) Now, suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})>2$ [or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})<-2$], and $|\mathrm{Tr}(\underline{P}\underline{Q})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. Then one finds $\mathrm{Tr}(\underline{P}\underline{Q})>\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$ and $\mathrm{Tr}(\underline{A})>2$. In this case it is sufficient to prove $\mathrm{Tr}(\underline{P}\underline{A})>\mathrm{Tr}(\underline{P}^{-1}\underline{A})$. For the case of $s_1\geq s_2$, from the Fricke identity

$$\begin{aligned}\mathrm{Tr}(\underline{P}\underline{A})&=\mathrm{Tr}(\underline{P}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})\\ &=\mathrm{Tr}(\underline{P}\underline{Q}^{s_2})\mathrm{Tr}(\underline{P}^{r_1}\underline{Q}^{s_1})-\mathrm{Tr}(\underline{P}^{r_1-1}\underline{Q}^{s_1-s_2})\end{aligned}$$

and

$$\begin{aligned}\mathrm{Tr}(\underline{P}^{-1}\underline{A})&=\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})\\ &=\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{s_2})\mathrm{Tr}(\underline{P}^{r_1}\underline{Q}^{s_2})-\mathrm{Tr}(\underline{P}^{r_1+1}\underline{Q}^{s_1-s_2})\ .\end{aligned}$$

So,

$$\mathrm{Tr}(\underline{P}\underline{A})-\mathrm{Tr}(\underline{P}^{-1}\underline{A})=[\mathrm{Tr}(\underline{P}\underline{Q}^{s_2})-\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{s_2})]\cdot\mathrm{Tr}(\underline{P}^{r_1}\underline{Q}^{s_1})-[\mathrm{Tr}(\underline{P}^{r_1-1}\underline{Q}^{s_1-s_2})-\mathrm{Tr}(\underline{P}^{r_1+1}\underline{Q}^{s_1-s_2})]\ .$$

Since $\mathrm{Tr}(\underline{P}\underline{Q}^{s_2})-\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{s_2})>0$ and

$$\mathrm{Tr}(\underline{P}^{r_1-1}\underline{Q}^{s_1-s_2})-\mathrm{Tr}(\underline{P}^{r_1+1}\underline{Q}^{s_1-s_2})<0\ ,$$

one can conclude $\mathrm{Tr}(\underline{P}\underline{A})-\mathrm{Tr}(\underline{P}^{-1}\underline{A})>0$. For the case of $s_2>s_1$,

$$\begin{aligned}\mathrm{Tr}(\underline{P}\underline{A})&=\mathrm{Tr}(\underline{Q}^{s_1}\underline{P}\underline{Q}^{s_2}\underline{P}^{r_1})\\ &=\mathrm{Tr}(\underline{Q}^{s_1}\underline{P})\mathrm{Tr}(\underline{Q}^{s_2}\underline{P}^{r_1})-\mathrm{Tr}(\underline{P}^{r_1-1}\underline{Q}^{s_2-s_1})\end{aligned}$$

and

$$\begin{aligned}\mathrm{Tr}(\underline{P}^{-1}\underline{A})&=\mathrm{Tr}(\underline{Q}^{s_1}\underline{P}^{-1}\underline{Q}^{s_2}\underline{P}^{r_1})\\ &=\mathrm{Tr}(\underline{Q}^{s_1}\underline{P}^{-1})\mathrm{Tr}(\underline{Q}^{s_2}\underline{P}^{r_1})\\ &\quad-\mathrm{Tr}(\underline{P}^{r_1+1}\underline{Q}^{s_2-s_1})\ .\end{aligned}$$

Therefore,

$$\mathrm{Tr}(\underline{P}\underline{A})-\mathrm{Tr}(\underline{P}^{-1}\underline{A})=[\mathrm{Tr}(\underline{P}\underline{Q}^{s_1})-\mathrm{Tr}(\underline{P}^{-1}\underline{Q}^{s_1})]\cdot\mathrm{Tr}(\underline{P}^{r_1}\underline{Q}^{s_2})-[\mathrm{Tr}(\underline{P}^{r_1-1}\underline{Q}^{s_2-s_1})-\mathrm{Tr}(\underline{P}^{r_1+1}\underline{Q}^{s_2-s_1})]\ .$$

Thus, by the same reason one can conclude that $\mathrm{tr}(\underline{P}\underline{A})-\mathrm{tr}(\underline{P}^{-1}\underline{A})>0$.

(ii) Suppose $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q})<-2$ [or $\mathrm{Tr}(\underline{P})<-2$, $\mathrm{Tr}(\underline{Q})>2$], and $|\mathrm{Tr}(\underline{P}\underline{Q})|\geq|\mathrm{Tr}(\underline{P}^{-1}\underline{Q})|$. Then one finds

$\mathrm{Tr}(\underline{P}\underline{Q})<\mathrm{Tr}(\underline{P}^{-1}\underline{Q})$. This case turns out to be equivalent to case (i) by a replacement of $\underline{Q}'=-\underline{Q}$ since now we have $\mathrm{Tr}(\underline{P})>2$, $\mathrm{Tr}(\underline{Q}')>2$, and $\mathrm{Tr}(\underline{P}\underline{Q}')>\mathrm{Tr}(\underline{P}^{-1}\underline{Q}')$. But here one has

$$K(r_2,s_2;r_1,s_2)\equiv\mathrm{Tr}(\underline{P}^{r_2}\underline{Q}^{s_2}\underline{P}^{r_1}\underline{Q}^{s_1})/2$$
$$=(-1)^{s_2+s_1}\mathrm{Tr}(\underline{P}^{r_2}\underline{Q}'^{s_2}\underline{P}^{r_1}\underline{Q}'^{s_1})/2\ .$$

Therefore, apart from the sign this case is exactly the same as case (i) as long as one considers the absolute value of $K(r_2,s_2;r_1,s_1)$. Thus, the relation (A2) is proved.

Similar relations hold for s_2, r_1, s_1 as well, since the trace is invariant under cyclic permutation. Using these relations we are able to obtain

$$|K(r_2+1,s_2+1;r_1+1,s_1+1)|>[|K(r_2+1,s_2;r_1,s_1)|+|K(r_2,s_2+1;r_1,s_1)|$$
$$+K(r_2,s_2;r_1+1,s_1)|+|K(r_2,s_2;r_1,s_1+1)|]/4>|K(r_2,s_2;r_1,s_1)|\ .$$

So, by induction one can conclude the following fact:

$$|K(r_2,s_2;r_1,s_1)|\geq|K(r_2',s_2';r_1',s_1')|$$

if $r_2\geq r_2'$, $s_2\geq s_2'$, $r_1\geq r_1'$, $s_1\geq s_1'$, where equality holds if and only if $r_2=r_2'$, $s_2=s_2'$, $r_1=r_1'$, $s_1=s_1'$. From this fact, one obtains

$$|K(r_2,s_2;r_1,s_1)|>\cdots>|K(1,1;1,1)|$$
$$=|\mathrm{Tr}(\underline{P}\underline{Q}\underline{P}\underline{Q})/2|>\cdots>|\mathrm{Tr}(\underline{P}\underline{Q})/2|>1\ .$$

Thus, lemma 6 is proved. Q.E.D.

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$$\underline{P}=\begin{bmatrix} s\cos\alpha & \sin\alpha/2 \\ -2\sin\alpha & \cos\alpha/2 \end{bmatrix},\quad \underline{Q}=\begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{bmatrix},$$

where we assume that α is sufficiently close to 0. Then, $|\mathrm{tr}(\underline{P})|\cong\frac{5}{2}>2$, $\mathrm{tr}(\underline{Q})>\frac{5}{2}>2$. And we obtain

$$\underline{P}^{-1}\underline{Q}=\begin{bmatrix} \cos\alpha/2 & -\sin\alpha/2 \\ 2\sin\alpha & 2\cos\alpha \end{bmatrix},\quad \underline{P}\underline{Q}=\begin{bmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{bmatrix}.$$

Therefore, $\mathrm{tr}(\underline{P}^{-1}\underline{Q})\cong\frac{5}{2}>2$ but $|\mathrm{tr}(\underline{P}\underline{Q})|=|2\cos\alpha|\leq 2$.

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