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ON SPECTRAL PROBLEMS OF DISCRETE SCHRÖDINGER OPERATORS

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Abstract. A special type of Jacobi matrices, discrete Schrödinger operators, is found to play an important role in quantum physics. In this paper, we show that given the spectrum of a discrete Schrödinger operator and the spectrum of the operator obtained by deleting the first row and the first column of it can determine the discrete Schrödinger operator uniquely, even though one eigenvalue of the latter is missing. Moreover, we find the forms of the discrete Schrödinger operators when their smallest and largest eigenvalues attain the extrema under certain constraints by use of the notion of generalized directional derivative and the method of Lagrange multiplier.

Keywords: discrete Schrödinger operator

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1. Introduction

Sturm-Liouville eigenvalue problem arises throughout many regions of applied mathematics. For example, they describe the vibrations of a string or the energy eigenfunctions of a quantum mechanical oscillator, in which case the eigenvalues correspond to the resonant frequencies of vibration or energy levels. Schrödinger equation is a type of Sturm-Liouville eigenvalue problem, coming from the idea that the discrete energy levels observed in atomic systems could be obtained as the eigenvalues of a differential operator.

One of well-known studies of Schrödinger operator is the Anderson model which was proposed by Anderson in [2] to explain the absence of diffusion of quantum waves in disordered lattices. He observed that the presence of impurities in the environment, coming from either the composition of the atoms or the space distribution of the nuclei in the atomic structure, was, under certain conditions, enough to suppress the propagation of electrons, turning the material into an insulator.

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There is an enormous literature on inverse spectral problem of Schrödinger operator ([1], [6], [13], [14] and references therein), but considerably less of its discrete analog ([3], [5], [15]). The special type of Jacobi matrix, whose off-diagonal terms all equal to 1, originates from the discretization of the Sturm-Liouville equation, Gesztesy and Simon called them the discrete Schrödinger operators in their paper [7]. The purpose of this paper is to solve some elementary eigenvalue problems for discrete Schrödinger operators.

In Section 2, we work on solving the eigenvalue problems of Jacobi matrices. In 1946, Borg proved that if $q(x)$ is even in $[0, \pi]$, namely $q(x) = q(\pi - x)$, then the spectrum of the equation

$$\begin{cases} y''(x) + [\lambda - q(x)]y(x) = 0, & 0 \leqslant x \leqslant \pi, \\ y'(0) = 0, & y'(\pi) = 0, \end{cases}$$

or

$$\begin{cases} y''(x) + [\lambda - q(x)]y(x) = 0, & 0 \leqslant x \leqslant \pi, \\ y(0) = 0, & y(\pi) = 0, \end{cases}$$

determines $q(x)$ uniquely (see [4]). This result motivated Hochstadt to study whether the eigenvalues determine persymmetric Jacobi matrices uniquely (see [10]), which can be regarded as the "even" case of Jacobi matrices. Because the uniqueness has been proven (see [10]), the existence of a persymmetric Jacobi matrix with the given eigenvalues is the next topic we wish to address. Using the recurrence relation of characteristic polynomials of Jacobi matrices, we prove the existence of an irreducible persymmetric Jacobi matrix with the given eigenvalues. When combined with the uniqueness theorem for persymmetric Jacobi matrices (see [10]), the theory of the eigenvalue problems of the irreducible persymmetric Jacobi matrices becomes more complete.

Sections 3 and 4 focus on the discrete Schrödinger operators. Section 3 is based on a result reported by Levinson in his paper [12] and proved by Hochstadt in [11]. Let $\sigma_{ND}(q)$ denote the spectrum of the eigenvalue problem

$$\begin{cases} y''(x) + [\lambda - q(x)]y(x) = 0, & 0 \leqslant x \leqslant 1, \\ y'(0) = 0, & y(1) = 0, \end{cases}$$

and let $\sigma_N(q)$ denote the spectrum of the eigenvalue problem

$$\begin{cases} z''(x) + [\mu - q(x)]z(x) = 0, & 0 \leqslant x \leqslant 1, \\ z'(0) = 0, & z'(1) = 0. \end{cases}$$

If (i) $\sigma_{ND}(q) = \sigma_{ND}(\tilde{q})$, (ii) $\sigma_N(q) \backslash \{\mu_1(q)\} = \sigma_N(\tilde{q}) \backslash \{\mu_1(\tilde{q})\}$, where $\mu_1(q)$ (or $\mu_1(\tilde{q})$) is the first eigenvalue in $\sigma_N(q)$ (or $\sigma_N(\tilde{q})$), then Levinson concluded that $q \equiv \tilde{q}$.

Because the discrete Schrödinger operators can be regarded as the discrete version of the Sturm-Liouville equation, a similar argument should be valid for them. We prove Levinson's theorem for the discrete Schrödinger operators (Theorem 3.3) and find a generalization of it (Corollary 3.4) in this section.

In Section 4, by using the notion of generalized directional derivative developed by Trubowitz [16] and the Lagrange multiplier method under certain constraints, we identify the forms of the discrete Schrödinger operators when their smallest and largest eigenvalues attain the extrema. The main result we obtained in this section is as follows.

Theorem 1.1. *For $n \times n$ discrete Schrödinger operators with a square sum of diagonal elements equal to one, the largest (smallest) eigenvalue attains the minimum (maximum) when the discrete Schrödinger operator is persymmetric.*

2. The existence theorem of the persymmetric Jacobi matrices

Definition 2.1. A symmetric matrix $\mathcal{M} = [m_{ij}]_{i,j=1}^{n}$ satisfying $m_{ij} = 0$ for all $|i-j| \geqslant 2$ is called a Jacobi matrix. Let

$$\mathcal{M} = \begin{bmatrix} a_1 & b_1 & 0 & \dots & 0 \\ b_1 & a_2 & b_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & b_{n-1} \\ 0 & \dots & 0 & b_{n-1} & a_n \end{bmatrix}.$$

Then we denote $\mathcal{M}$ by $\mathcal{J}[a_1, \dots, a_n; b_1, \dots, b_{n-1}]$. Moreover, if $b_j \neq 0$ for all $j = 1, 2, \dots, n-1$, then the Jacobi matrix $\mathcal{M}$ is said to be *irreducible.*

For $1 \leqslant k \leqslant l \leqslant n$, let $J_{k,l} = \mathcal{J}[a_k, \dots, a_l; b_k, \dots, b_{l-1}]$, and denote the characteristic polynomial of $J_{k,l}$ by $P_{k,l}(x)$. Then for irreducible Jacobi matrices there is a well-known result:

Theorem 2.2. *Suppose $J_{1,n}$ is an $n \times n$ irreducible Jacobi matrix with positive off-diagonal elements. Then*

(i) *the zeros of $P_{1,n}(x)$ are simple,*
(ii) *the zeros of $P_{k,n}(x)$ and $P_{k+1,n}(x)$ are interlacing, $1 \leqslant k \leqslant n-1$,*
(iii) *$P_{1,n}(x)$ and $P_{2,n}(x)$ determine $J_{1,n}$ uniquely.*

Proof. See [8], Chapter 3. □

Definition 2.3. Let $J_{1,n}$ be an $n \times n$ Jacobi matrix. Thus, $J_{1,n}$ is said to be *persymmetric* if $a_i = a_{n+1-i}$, $b_j = b_{n-j}$, where $1 \leqslant i \leqslant n$, $1 \leqslant j \leqslant n-1$.

Let $\mathcal{S}_n = [s_{ij}]_{n\times n}$, where

$$s_{ij} = \begin{cases} 1 & \text{if } i+j = n+1, \\ 0 & \text{otherwise.} \end{cases}$$

Denote $\mathcal{S}_n J_{1,n} \mathcal{S}_n$ by $\tilde{J}_{1,n}$. According to the definition of a characteristic polynomial of $J_{k,l}$, we have $P_{1,n}(x) = \widetilde{P}_{1,n}(x)$ and $P_{2,n}(x) = \widetilde{P}_{1,n-1}(x)$. Definition 2.3 clearly indicates that an $n \times n$ Jacobi matrix $J_{1,n}$ is persymmetric if and only if $J_{1,n} = \mathcal{S}_n J_{1,n} \mathcal{S}_n$, i.e. $J_{1,n} = \tilde{J}_{1,n}$. Hence, we have the following lemma:

Lemma 2.4. *An $n \times n$ Jacobi matrix $J_{1,n}$ is persymmetric if and only if $P_{1,n-1}(x) = P_{2,n}(x)$.*

Definition 2.5. The *spectrum of a matrix T*, denoted by $\sigma(T)$, is the set which consists of the eigenvalues of T.

In [10], Hochstadt proved the following result:

Theorem 2.6. *Let*

$$J = \mathcal{J}[a_1, \ldots, a_n; b_1, \ldots, b_{n-1}]$$

and

$$\tilde{J} = \mathcal{J}[\tilde{a}_1, \ldots, \tilde{a}_n; \tilde{b}_1, \ldots, \tilde{b}_{n-1}]$$

be two irreducible persymmetric Jacobi matrices with positive off-diagonal elements. Suppose the spectra of J and $\tilde{J}$are the same. Then $J = \tilde{J}$.

Hence, given $\lambda_1 < \lambda_2 < \ldots < \lambda_n$, Theorem 2.6 implies that there can only be one *irreducible persymmetric* Jacobi matrix with $\sigma(T) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. In this section, we solve the existence problem of *persymmetric Jacobi matrices*. For our purpose, we must obtain the following result:

Theorem 2.7. *Denote by $\lambda_1 < \lambda_2 < \ldots < \lambda_n$ the eigenvalues of an irreducible Jacobi matrix $J = \mathcal{J}[a_1, \ldots, a_n; b_1, \ldots, b_{n-1}]$. Then J is persymmetric if and only if*

$$P_{1,n-1}(\lambda_j) = (-1)^{n-j} b_1 b_2 \ldots b_{n-1}. \tag{2.1}$$

P r o o f. By the definition of $P_{k,n}(x)$, $1 \leqslant k \leqslant n$, we have for $n \geqslant 3$,

$$P_{k,n}(x) = (x - a_k)P_{k+1,n}(x) - b_k^2 P_{k+2,n}(x) \quad \forall\, 1 \leqslant k \leqslant n-2. \tag{2.2}$$

Using (2.2), it is obtained that for $1 \leqslant k \leqslant n-3$,

$$\begin{aligned} &P_{k,n}(x)P_{k+1,n-1}(x) - P_{k,n-1}(x)P_{k+1,n}(x) \\ &\quad = [(x-a_k)P_{k+1,n}(x) - b_k^2 P_{k+2,n}(x)]P_{k+1,n-1}(x) \\ &\qquad - [(x-a_k)P_{k+1,n-1}(x) - b_k^2 P_{k+2,n-1}(x)]P_{k+1,n}(x) \\ &\quad = b_k^2(P_{k+1,n}(x)P_{k+2,n-1}(x) - P_{k+1,n-1}(x)P_{k+2,n}(x)). \end{aligned} \tag{2.3}$$

Applying (2.3) repeatedly, we get

$$\begin{aligned} &P_{1,n}(x)P_{2,n-1}(x) - P_{1,n-1}(x)P_{2,n}(x) \\ &\quad = b_1^2 b_2^2 \ldots b_{n-3}^2 (P_{n-2,n}(x)P_{n-1,n-1}(x) - P_{n-2,n-1}(x)P_{n-1,n}(x)) \\ &\quad = -\, b_1^2 b_2^2 \ldots b_{n-1}^2. \end{aligned} \tag{2.4}$$

Because $P_{1,n}(\lambda_j) = 0$ for all $1 \leqslant j \leqslant n$, (2.4) leads to

$$P_{1,n-1}(\lambda_j)P_{2,n}(\lambda_j) = b_1^2 b_2^2 \ldots b_{n-1}^2, \quad 1 \leqslant j \leqslant n. \tag{2.5}$$

Suppose J is *persymmetric*, then according to Lemma 2.4, we have

$$P_{1,n-1}(x) = P_{2,n}(x).$$

Hence, (2.5) implies

$$P_{1,n-1}^2(\lambda_j) = b_1^2 b_2^2 \ldots b_{n-1}^2.$$

Note that the zeros of $P_{1,n}(x)$ and $P_{1,n-1}(x)$ are interlacing; thus,

$$\operatorname{Sgn} P_{1,n-1}(\lambda_j) = (-1)^{n-j}, \quad 1 \leqslant j \leqslant n,$$

which implies that

$$P_{1,n-1}(\lambda_j) = (-1)^{n-j} b_1 b_2 \ldots b_{n-1}, \quad 1 \leqslant j \leqslant n.$$

By contrast, if

$$P_{1,n-1}(\lambda_j) = (-1)^{n-j} b_1 b_2 \ldots b_{n-1}, \quad 1 \leqslant j \leqslant n,$$

then by using (2.5),

$$P_{2,n}(\lambda_j) = (-1)^{n-j} b_1 b_2 \ldots b_{n-1}, \quad 1 \leqslant j \leqslant n.$$

Because $P_{1,n-1}(x)$ and $P_{2,n}(x)$ are monic polynomials of degree $n-1$ and coincide at n points, we conclude that

$$P_{1,n-1}(x) = P_{2,n}(x).$$

By using Lemma 2.4, we complete the proof. $\square$

From Theorem 2.6, the question that we pose is answerable if and only if there exists a monic polynomial $P_{n-1}(x)$ with degree $n-1$ such that $P_{n-1}(\lambda_j) = (-1)^{n-j}c$ with an unknown nonzero constant c, where $1 \leqslant j \leqslant n$. For our purpose, we consider the following system of equations:

$$\begin{cases} \lambda_1^{n-1} + a_{n-2}\lambda_1^{n-2} + \ldots + a_0 = (-1)^{n-1}c, \\ \lambda_2^{n-1} + a_{n-2}\lambda_2^{n-2} + \ldots + a_0 = (-1)^{n-2}c, \\ \vdots \\ \lambda_n^{n-1} + a_{n-2}\lambda_n^{n-2} + \ldots + a_0 = c. \end{cases} \tag{2.6}$$

To achieve our goal, we must determine whether the system of equations (2.6) can be solved. For solving $a_0, \ldots, a_{n-2}$, and c, we change (2.6) into

$$\begin{cases} a_{n-2}\lambda_1^{n-2} + \ldots + a_0 + (-1)^n c = -\lambda_1^{n-1}, \\ a_{n-2}\lambda_2^{n-2} + \ldots + a_0 + (-1)^{n-1} c = -\lambda_2^{n-1}, \\ \vdots \\ a_{n-2}\lambda_n^{n-2} + \ldots + a_0 - c = -\lambda_n^{n-1}. \end{cases} \tag{2.7}$$

Thus, (2.6) is solvable if and only if the coeffcient determinant of (2.7) is not equal to zero. For this purpose we prove:

Lemma 2.8. *Let* $(n \geqslant 3)$. *For* $\lambda_1 < \lambda_2 < \ldots < \lambda_n$, *we have*

$$\det \begin{bmatrix} \lambda_1^{n-2} & \lambda_1^{n-3} & \ldots & 1 & (-1)^n \\ \lambda_2^{n-2} & \ddots & \ddots & 1 & (-1)^{n-1} \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \ldots & \ldots & 1 & -1 \end{bmatrix} \neq 0.$$

P r o o f. Let

$$A = \begin{bmatrix} \lambda_1^{n-2} & \lambda_1^{n-3} & \dots & 1 & (-1)^n \\ \lambda_2^{n-2} & \ddots & \ddots & 1 & (-1)^{n-1} \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \dots & \dots & 1 & -1 \end{bmatrix}$$

and use $\hat{A}_{ij}$ to denote the matrix obtained by deleting the ith row and the jth column of A. By multiplying the $(n-1)$th column of A by $(-1)^n$ and adding it to the nth column of A, we find that

$$\begin{aligned} \det A &= \det \begin{bmatrix} \lambda_1^{n-2} & \lambda_1^{n-3} & \dots & 1 & 2(-1)^n \\ \lambda_2^{n-2} & \ddots & \ddots & 1 & 0 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \dots & \dots & 1 & (-1)+(-1)^n \end{bmatrix} \\ &= 2(-1)^n(\det \hat{A}_{1n} + \det \hat{A}_{3n} + \ldots + \det \hat{A}_{2[(n+1)/2]-1,n}). \end{aligned}$$

Note that

$$\det \hat{A}_{in} = \det \begin{bmatrix} \lambda_1^{n-2} & \lambda_1^{n-3} & \dots & \lambda_1 & 1 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \lambda_{i-1}^{n-2} & \ddots & \ddots & \lambda_{i-1} & \vdots \\ \lambda_{i+1}^{n-2} & \ddots & \ddots & \lambda_{i+1} & \vdots \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \dots & \dots & \lambda_n & 1 \end{bmatrix},$$

which is of the form of the *Vandermonde determinant.* Hence $\hat{A}_{in} \neq 0$ and

$$\det \hat{A}_{in} = (-1)^{(n-1)(n-2)/2} \prod_{\substack{1 \leqslant k < l \leqslant n \\ k,l \neq i}} (\lambda_l - \lambda_k). \tag{2.8}$$

Because $\operatorname{Sgn} \hat{A}_{in} = (-1)^{(n-1)(n-2)/2}$, $1 \leqslant i \leqslant n$, $\det A \neq 0$. This completes the proof. □

By using Lemma 2.8, we find there exists a monic polynomial $P_{n-1}(x)$ of degree $n-1$ such that

$$P_{n-1}(\lambda_j) = (-1)^{n-j} c,$$

where

$$c = \det \begin{bmatrix} \lambda_1^{n-2} & \dots & 1 & -\lambda_1^{n-1} \\ \vdots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \dots & 1 & -\lambda_n^{n-1} \end{bmatrix} \Bigg/ \det \begin{bmatrix} \lambda_1^{n-2} & \dots & 1 & (-1)^n \\ \lambda_2^{n-2} & \ddots & 1 & (-1)^{n-1} \\ \vdots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \vdots & \vdots \\ \lambda_n^{n-2} & \dots & 1 & -1 \end{bmatrix}.$$

The numerator of c is of the form of the *Vandermonde determinant* with $\lambda_i \neq \lambda_j$ for $i \neq j$. Hence $c \neq 0$.

By summarizing the previous arguments, we obtain the following result:

Theorem 2.9. *Given any n distinct real numbers, $\lambda_1, \lambda_2, \dots, \lambda_n$. There exists an irreducible persymmetric Jacobi matrix J such that $\sigma(J) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$.*

3. Levinson's theorem for the discrete Schrödinger operators

Definition 3.1. A Jacobi matrix in which all off-diagonal terms equal 1 is called a *discrete Schrödinger operator.*

The eigenvalue problem for the discrete Schrödinger operators may be considered a discrete version of the Sturm-Liouville equation

$$y''(x) + [\lambda - q(x)]y(x) = 0.$$

Let $\sigma_{ND}(q)$ denote the spectrum of the eigenvalue problem

$$\begin{cases} y''(x) + [\lambda - q(x)]y(x) = 0, & 0 \leqslant x \leqslant 1, \\ y'(0) = 0, & y(1) = 0, \end{cases}$$

and let $\sigma_N(q)$ denote the spectrum of the eigenvalue problem

$$\begin{cases} z''(x) + [\mu - q(x)]z(x) = 0, & 0 \leqslant x \leqslant 1, \\ z'(0) = 0, & z'(1) = 0. \end{cases}$$

Although it is known that $\sigma_{ND}(q)$ and $\sigma_N(q)$ determine $q(x)$ uniquely, it is difficult to detect all eigenvalues of these spectrum in fact. How many eigenvalues of $\sigma_{ND}(q)$ and $\sigma_N(q)$ can be ignored when determining $q(x)$ became a new interesting topic for researchers of inverse Sturm-Liouville eigenvalues problem. In [12], Levinson mentioned that if (i) $\sigma_{ND}(q) = \sigma_{ND}(\tilde{q})$, (ii) $\sigma_N(q) \setminus \{\nu_1(q)\} = \sigma_N(\tilde{q}) \setminus \{\nu_1(\tilde{q})\}$, where

$\nu_1(q)$ ($\nu_1(\tilde{q})$) is the first eigenvalue in $\sigma_N(q)$ ($\sigma_N(\tilde{q})$), then $q \equiv \tilde{q}$. Levinson's assertion was proven by Hochstadt (see [11]). In this section, we prove some analogous theorems for discrete Schrödinger operators. First, we prove the following lemma:

Lemma 3.2. *Let $J = \mathcal{J}[a_1, \ldots, a_n; b_1, \ldots, b_{n-1}]$ be an $n \times n$ irreducible Jacobi matrix. Suppose λ_1 (λ_n) is the smallest (the largest) eigenvalue of J. Then $\lambda_1 < a_i$ ($a_i < \lambda_n$) for all $1 \leqslant i \leqslant n$.*

Proof. By using the variational principle, we have

$$\lambda_1 = \min_{\|\vec{v}\|=1} \langle J\vec{v},\ \vec{v}\,\rangle.$$

Let $\vec{e}_i$ denote the elementary vector of $\mathbb{R}^n$ with the ith component equal to 1 and 0 elsewhere. Then

$$\lambda_1 \leqslant \langle J\vec{e}_i, \vec{e}_i\rangle = a_i. \tag{3.1}$$

For $\lambda \in \sigma(J)$, if $J\vec{e}_i^{\top} = \lambda\vec{e}_i^{\top}$, we obtain $b_{i-1} = b_i = 0$, which contradicts the notion that J is irreducible. Hence, $\vec{e}_i$ cannot be the eigenvector of J, and (3.1) implies $\lambda_1 < a_i$ for all $1 \leqslant i \leqslant n$.

However,

$$\lambda_n = \max_{\|\vec{v}\|=1} \langle J\vec{v}, \vec{v}\rangle.$$

By using the same argument, we can prove $a_i < \lambda_n$ for all $1 \leqslant i \leqslant n$. Thus, the assertion is proven. □

Let $S_{k,l} = \mathcal{J}(a_k, \ldots, a_l)$ be an $(l-k+1)\times(l-k+1)$ discrete Schrödinger operator, and denote the characteristic polynomial of $S_{k,l}$ by $\mathcal{P}_{k,l}(x)$. We have the following theorem:

Theorem 3.3. *Let $S_{1,n}$ and $\widetilde{S}_{1,n}$ be two $n \times n$ discrete Schrödinger operators. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ (or $\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_n$) be the eigenvalues of $S_{1,n}$ (or $\widetilde{S}_{1,n}$), and let $\nu_1, \nu_2, \ldots, \nu_{n-1}$ (or $\widetilde{\nu}_1, \widetilde{\nu}_2, \ldots, \widetilde{\nu}_{n-1}$) be the eigenvalues of $S_{2,n}$ (or $\widetilde{S}_{2,n}$). Suppose the conditions*

(i) $\sigma(S_{1,n}) \setminus \{\lambda_1\} = \sigma(\widetilde{S}_{1,n}) \setminus \{\tilde{\lambda}_1\}$,

(ii) $\sigma(S_{2,n}) = \sigma(\widetilde{S}_{2,n})$,

are satisfied. Then $S_{1,n} = \widetilde{S}_{1,n}$.

P r o o f. We can express $\mathcal{P}_{1,n}(x)$ and $\widetilde{\mathcal{P}}_{1,n}(x)$ as

$$\mathcal{P}_{1,n}(x) = (x - a_1)\mathcal{P}_{2,n}(x) - \mathcal{P}_{3,n}(x), \tag{3.2}$$

and

$$\widetilde{\mathcal{P}}_{1,n}(x) = (x - \tilde{a}_1)\widetilde{\mathcal{P}}_{2,n}(x) - \widetilde{\mathcal{P}}_{3,n}(x). \tag{3.3}$$

By (ii),

$$\mathcal{P}_{2,n}(x) = \widetilde{\mathcal{P}}_{2,n}(x),$$

therefore (3.2) and (3.3) imply

$$(x - \tilde{a}_1)\mathcal{P}_{1,n}(x) - (x - a_1)\widetilde{\mathcal{P}}_{1,n}(x) = (x - a_1)\widetilde{\mathcal{P}}_{3,n}(x) - (x - \tilde{a}_1)\mathcal{P}_{3,n}(x). \tag{3.4}$$

Furthermore, because $\mathcal{P}_{3,n}(x)$ and $\widetilde{\mathcal{P}}_{3,n}(x)$ are monic, the degree of the polynomial

$$(x - a_1)\widetilde{\mathcal{P}}_{3,n}(x) - (x - \tilde{a}_1)\mathcal{P}_{3,n}(x)$$

is at most $n - 2$. However, because condition (i) and (3.4) imply

$$(\lambda_i - a_1)\widetilde{\mathcal{P}}_{3,n}(\lambda_i) - (\lambda_i - \tilde{a}_1)\mathcal{P}_{3,n}(\lambda_i) = 0, \quad 2 \leqslant i \leqslant n,$$

the polynomial $(x-a_1)\widetilde{\mathcal{P}}_{3,n}(x)-(x-\tilde{a}_1)\mathcal{P}_{3,n}(x)$ must be the zero polynomial. Hence, (3.4) becomes

$$(x - \tilde{a}_1)\mathcal{P}_{1,n}(x) - (x - a_1)\widetilde{\mathcal{P}}_{1,n}(x) = 0. \tag{3.5}$$

Because $\lambda_i = \tilde{\lambda}_i$ for $2 \leqslant i \leqslant n$, we can write

$$\mathcal{P}_{1,n}(x) = (x - \lambda_1)\prod_{i=2}^{n}(x - \lambda_i) \tag{3.6}$$

and

$$\widetilde{\mathcal{P}}_{1,n}(x) = (x - \tilde{\lambda}_1)\prod_{i=2}^{n}(x - \lambda_i). \tag{3.7}$$

By using (3.5), (3.6), and (3.7), we obtain

$$[(x - \tilde{a}_1)(x - \lambda_1) - (x - a_1)(x - \tilde{\lambda}_1)]\prod_{i=2}^{n}(x - \lambda_i) = 0. \tag{3.8}$$

Because (3.8) is true for real x,

$$(x-\tilde{a}_1)(x-\lambda_1)=(x-a_1)(x-\tilde{\lambda}_1).$$

Hence,

$$\tilde{a}_1\lambda_1=a_1\tilde{\lambda}_1 \tag{3.9}$$

and

$$\tilde{a}_1+\lambda_1=a_1+\tilde{\lambda}_1. \tag{3.10}$$

If $\tilde{a}_1=0$, then by Lemma 3.2, $\tilde{\lambda}_1<\tilde{a}_1=0$. By using (3.9) and (3.10), we determine that $a_1=\tilde{a}_1=0$ and $\lambda_1=\tilde{\lambda}_1$. In this case, we have $\mathcal{P}_{1,n}(x)=\widetilde{\mathcal{P}}_{1,n}(x)$. If $\tilde{a}_1\neq 0$, then (3.9) implies

$$\lambda_1=\frac{a_1\tilde{\lambda}_1}{\tilde{a}_1}. \tag{3.11}$$

Combining (3.10) and (3.11), we obtain

$$\tilde{a}_1+\frac{a_1\tilde{\lambda}_1}{\tilde{a}_1}=a_1+\tilde{\lambda}_1,$$

which implies

$$(\tilde{a}_1-a_1)(\tilde{a}_1-\tilde{\lambda}_1)=0. \tag{3.12}$$

Because $\tilde{\lambda}_1$ is the smallest eigenvalue of $\widetilde{\mathcal{S}}_{1,n}$ and $\tilde{a}_1$ is a diagonal element of $\widetilde{\mathcal{S}}_{1,n}$, Lemma 3.2 implies $\tilde{\lambda}_1<\tilde{a}_1$. Thus (3.12) leads to $a_1=\tilde{a}_1$. Then by (3.11), $\lambda_1=\tilde{\lambda}_1$, which implies $\mathcal{P}_{1,n}(x)=\widetilde{\mathcal{P}}_{1,n}(x)$.

From the previous argument, we have $\mathcal{P}_{1,n}(x)=\widetilde{\mathcal{P}}_{1,n}(x)$ and $\mathcal{P}_{2,n}(x)=\widetilde{\mathcal{P}}_{2,n}(x)$ under conditions (i) and (ii). According to Theorem 2.2, $\mathcal{S}_{1,n}=\widetilde{\mathcal{S}}_{1,n}$. □

A more interesting question, however, is what the case would be when ν_1 and $\widetilde{\nu}_1$ are missing.

Corollary 3.4. *Suppose $n\geqslant 3$. Let $\mathcal{S}_{1,n}$, $\widetilde{\mathcal{S}}_{1,n}$, $\{\lambda_i\}_{i=1}^n$, $\{\tilde{\lambda}_i\}_{i=1}^n$, $\{\nu_j\}_{j=1}^{n-1}$, and $\{\widetilde{\nu}_j\}_{j=1}^{n-1}$ be as defined in Theorem 3.3. If*

(i) $\sigma(\mathcal{S}_{1,n})=\sigma(\widetilde{\mathcal{S}}_{1,n})$,

(ii) $\sigma(\mathcal{S}_{2,n})\setminus\{\nu_1\}=\sigma(\widetilde{\mathcal{S}}_{2,n})\setminus\{\widetilde{\nu}_1\}$,

then $\mathcal{S}_{1,n}=\widetilde{\mathcal{S}}_{1,n}$.

P r o o f. Because $\mathcal{P}_{1,n}(x)$ and $\widetilde{\mathcal{P}}_{1,n}(x)$ are monic, the assumption (i) implies

$$\mathcal{P}_{1,n}(x) = \widetilde{\mathcal{P}}_{1,n}(x). \tag{3.13}$$

According to assumption (ii), we can write

$$\mathcal{P}_{2,n}(x) = (x - \nu_1) \prod_{j=2}^{n-1} (x - \nu_j) \tag{3.14}$$

and

$$\widetilde{\mathcal{P}}_{2,n}(x) = (x - \widetilde{\nu}_1) \prod_{j=2}^{n-1} (x - \nu_j). \tag{3.15}$$

It follows from (3.2), (3.3), (3.13), (3.14), and (3.15) that

$$[(x - a_1)(x - \nu_1) - (x - \tilde{a}_1)(x - \widetilde{\nu}_1)] \prod_{j=2}^{n-1} (x - \nu_j) = \widetilde{\mathcal{P}}_{3,n}(x) - \mathcal{P}_{3,n}(x). \tag{3.16}$$

Because $\mathcal{P}_{3,n}(x)$ and $\widetilde{\mathcal{P}}_{3,n}(x)$ are monic and have the degree $n-2$, the polynomial $\widetilde{\mathcal{P}}_{3,n}(x) - \mathcal{P}_{3,n}(x)$ has a degree that is at most $n-3$. However, according to (3.16), we know that

$$\widetilde{\mathcal{P}}_{3,n}(\nu_j) - \mathcal{P}_{3,n}(\nu_j) = 0, \quad 2 \leqslant j \leqslant n-1.$$

Thus,

$$\mathcal{P}_{3,n}(x) \equiv \widetilde{\mathcal{P}}_{3,n}(x). \tag{3.17}$$

With (3.17) and assumption (ii), Theorem 3.3 implies $\mathcal{S}_{2,n} = \widetilde{\mathcal{S}}_{2,n}$; therefore $\mathcal{P}_{2,n}(x) \equiv \widetilde{\mathcal{P}}_{2,n}(x)$. Now we have $\mathcal{P}_{1,n}(x) \equiv \widetilde{\mathcal{P}}_{1,n}(x)$ and $\mathcal{P}_{2,n}(x) \equiv \widetilde{\mathcal{P}}_{2,n}(x)$. Hence, $\mathcal{S}_{1,n} = \widetilde{\mathcal{S}}_{1,n}$. □

R e m a r k s.

(1) Theorem 3.3 (or Corollary 3.4) is also valid when λ_1 (or ν_1) is replaced by λ_n (or ν_{n-1}).

(2) We cannot apply the method used in Theorem 3.3 for general Jacobi matrices, because the off-diagonal elements are unknown. However, if the two Jacobi matrices have the same off-diagonal elements and conditions (i) and (ii) of Theorem 3.3 (or Corollary 3.4) are satisfied, then our method can be used to prove that these two Jacobi matrices are the same.

(3) Corollary 3.4 is not valid for $n = 2$. As a counterexample, if $S = \begin{bmatrix} a & 1 \\ 1 & b \end{bmatrix}$ and $\widetilde{S} = \begin{bmatrix} b & 1 \\ 1 & a \end{bmatrix}$, then S and $\widetilde{S}$ have the same λ_1 and λ_2 but possess distinct ν_1 values if $a \neq b$.

4. Two extremal eigenvalue problems of discrete Schrödinger operators

Consider the equation

$$(J_n + Q)\vec{v} = \lambda \vec{v}, \tag{4.1}$$

where $J_n = \mathcal{J}(0, \dots, 0)$, $Q = \mathcal{J}[q_1, \dots, q_n; 0, \dots, 0]$, and $q_i \in \mathbb{R}$, $1 \leqslant i \leqslant n$. Let $\lambda_1 < \lambda_2 < \dots < \lambda_n$ be the eigenvalues of $J_n + Q$ and $\vec{w}_i = (a_{i1}, a_{i2}, \dots, a_{in})^\top$ be the eigenvectors corresponding to λ_i, $1 \leqslant i \leqslant n$. It is clear that λ_i depends on $q_1, q_2, \dots,$ and q_n. Therefore λ_i can be regarded as a function of $q_1, q_2, \dots,$ and q_n. Identifying an explicit formula for $d_Q \lambda_i$ is useful. We may and shall assume that $a_{i1} = 1$ to make $\vec{w}_i$ a differentiable function of $q_1, q_2, \dots,$ and q_n.

Because we know that λ_i maps $\mathbb{R}^n$ into $\mathbb{R}$, $d_Q \lambda_i$ must be a $1 \times n$ matrix. By taking the derivative on both sides of (4.1) and replacing λ with λ_i, we have

$$d_Q[(J_n + Q)\vec{w}_i] = d_Q[\lambda_i \vec{w}_i]. \tag{4.2}$$

Note that

$$d_Q[(J_n + Q)\vec{w}_i] = d_Q[J_n \vec{w}_i + Q\vec{w}_i] = J_n d_Q \vec{w}_i + d_Q(Q\vec{w}_i) \tag{4.3}$$

and $Q\vec{w}_i = [q_1 a_{i1} \quad q_2 a_{i2} \quad \dots \quad q_n a_{in}]^\top$; therefore we have

$$\begin{aligned} d_Q(Q\vec{w}_i) &= \begin{bmatrix} \frac{\partial(q_1 a_{i1})}{\partial q_1} & \frac{\partial(q_1 a_{i1})}{\partial q_2} & \cdots & \frac{\partial(q_1 a_{i1})}{\partial q_n} \\ \frac{\partial(q_2 a_{i2})}{\partial q_1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial(q_n a_{in})}{\partial q_1} & \cdots & \cdots & \frac{\partial(q_n a_{in})}{\partial q_n} \end{bmatrix} \\ &= \begin{bmatrix} a_{i1} + q_1 \frac{\partial a_{i1}}{\partial q_1} & q_1 \frac{\partial a_{i1}}{\partial q_2} & \cdots & q_1 \frac{\partial a_{i1}}{\partial q_n} \\ q_2 \frac{\partial a_{i2}}{\partial q_1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ q_n \frac{\partial a_{in}}{\partial q_1} & \cdots & \cdots & a_{in} + q_n \frac{\partial a_{in}}{\partial q_n} \end{bmatrix} \\ &= \mathcal{W} + Q d_Q \vec{w}_i, \end{aligned} \tag{4.4}$$

where

$$\mathcal{W} = \begin{bmatrix} a_{i1} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & a_{in} \end{bmatrix}, \quad Qd_Q\vec{w}_i = \begin{bmatrix} q_1\frac{\partial a_{i1}}{\partial q_1} & q_1\frac{\partial a_{i1}}{\partial q_2} & \dots & q_1\frac{\partial a_{i1}}{\partial q_n} \\ q_2\frac{\partial a_{i2}}{\partial q_1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ q_n\frac{\partial a_{in}}{\partial q_1} & \dots & \dots & q_n\frac{\partial a_{in}}{\partial q_n} \end{bmatrix}.$$

However,

$$\begin{aligned}
d_Q[\lambda_i\vec{w}_i] &= \begin{bmatrix} \frac{\partial(\lambda_i a_{i1})}{\partial q_1} & \frac{\partial(\lambda_i a_{i1})}{\partial q_2} & \dots & \frac{\partial(\lambda_i a_{i1})}{\partial q_n} \\ \frac{\partial(\lambda_i a_{i2})}{\partial q_1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial(\lambda_i a_{in})}{\partial q_1} & \dots & \dots & \frac{\partial(\lambda_i a_{in})}{\partial q_n} \end{bmatrix} \\
&= \begin{bmatrix} a_{i1}\frac{\partial\lambda_i}{\partial q_1} + \lambda_i\frac{\partial a_{i1}}{\partial q_1} & \dots & a_{i1}\frac{\partial\lambda_i}{\partial q_n} + \lambda_i\frac{\partial a_{i1}}{\partial q_n} \\ \vdots & \ddots & \vdots \\ a_{in}\frac{\partial\lambda_i}{\partial q_1} + \lambda_i\frac{\partial a_{in}}{\partial q_1} & \dots & a_{in}\frac{\partial\lambda_i}{\partial q_n} + \lambda_i\frac{\partial a_{in}}{\partial q_n} \end{bmatrix} \\
&= \begin{bmatrix} a_{i1}\frac{\partial\lambda_i}{\partial q_1} & \dots & a_{i1}\frac{\partial\lambda_i}{\partial q_n} \\ \vdots & \ddots & \vdots \\ a_{in}\frac{\partial\lambda_i}{\partial q_1} & \dots & a_{in}\frac{\partial\lambda_i}{\partial q_n} \end{bmatrix} + \begin{bmatrix} \lambda_i\frac{\partial a_{i1}}{\partial q_1} & \dots & \lambda_i\frac{\partial a_{i1}}{\partial q_n} \\ \vdots & \ddots & \vdots \\ \lambda_i\frac{\partial a_{in}}{\partial q_1} & \dots & \lambda_i\frac{\partial a_{in}}{\partial q_n} \end{bmatrix} \\
&= \vec{w}_i d_Q\lambda_i + \lambda_i d_Q\vec{w}_i.
\end{aligned} \tag{4.5}$$

By using (4.3), (4.4) and (4.5), we see that (4.2) becomes

$$\mathcal{W} + (J_n + Q)d_Q\vec{w}_i = \vec{w}_i d_Q\lambda_i + \lambda_i d_Q\vec{w}_i. \tag{4.6}$$

In (4.1), by replacing λ by λ_i, we obtain

$$(J_n + Q)\vec{w}_i = \lambda_i\vec{w}_i,$$

which can be rewritten as

$$\vec{w}_i^\top(J_n + Q) = \lambda_i\vec{w}_i^\top. \tag{4.7}$$

(4.6) and (4.7) imply that

$$\vec{w}_i^\top\mathcal{W} = \vec{w}_i^\top\vec{w}_i d_Q\lambda_i.$$

Hence,

$$[\,a_{i1}^2 \quad a_{i2}^2 \quad \dots \quad a_{in}^2\,] = \|\vec{w}_i\|^2 d_Q\lambda_i.$$

Definition 4.1. Let $\vec{v}^\top = (v_1, v_2, \dots, v_n)$. We use the notation $(\vec{v}^\top)^p$ to denote the vector $(v_1^p, v_2^p, \dots, v_n^p)$.

From previous discussion, we obtain the following result:

Theorem 4.2. *Suppose λ_i is the ith eigenvalue of $J_n + Q$ and $\vec{w}_i$ is the eigenvector corresponding to λ_i whose first component is* 1. *Then*

$$d_Q\lambda_i = \frac{(\vec{w}_i^\top)^2}{\|\vec{w}_i\|^2}.$$

Next, we investigate the extremum problem for λ_1 and λ_n with the constraint $q_1^2 + q_2^2 + \dots + q_n^2 \leqslant 1$. For this purpose, the *Lagrange multiplier* method is used. Let $(a_{k1}, a_{k2}, \dots, a_{kn})^\top$ be the normalized eigenvector corresponding to λ_k of $J_n + Q$, $a_{k1} > 0$, $k = 1, n$. The eigenvector of $J_n + Q$ corresponding to λ_j can be described explicitly as follows:

Lemma 4.3. *Let $J = \mathcal{J}[a_1, \dots, a_n; b_1, \dots, b_{n-1}]$ be an irreducible Jacobi matrix and denote*

$$\vec{v}_j = \Big(1, \frac{P_{1,1}(\lambda_j)}{b_1}, \frac{P_{1,2}(\lambda_j)}{b_1 b_2}, \dots, \frac{P_{1,n-1}(\lambda_j)}{b_1 \dots b_{n-1}}\Big)^\top.$$

Thus, $J\vec{v}_j = \lambda_j \vec{v}_j$, $1 \leqslant j \leqslant n$.

Proof. Because $b_i \neq 0$ for all $1 \leqslant i \leqslant n-1$, denote

$$\frac{P_{1,r}(x)}{b_1 \dots b_r} = \widehat{P}_r(x),$$

where $P_{1,r}(x)$ is the characteristic polynomial of $J_{1,r}$, $1 \leqslant r \leqslant n$, and let $P_{1,-1}(x) = \widehat{P}_{-1}(x) = 0$, $P_{1,0}(x) = \widehat{P}_0(x) = 1$, $b_0 = b_n = 1$. Note that the following recurrence relations hold:

$$P_{1,r}(x) = (x - a_r)P_{1,r-1}(x) - b_{r-1}^2 P_{1,r-2}(x), \quad 1 \leqslant r \leqslant n.$$

Hence, it is clear that

$$b_{r-1}^2 P_{1,r-2}(x) + a_r P_{1,r-1}(x) + P_{1,r}(x) = xP_{1,r-1}(x), \quad 1 \leqslant r \leqslant n. \tag{4.8}$$

For $r \geqslant 2$, by dividing (4.8) by $b_1 \dots b_{r-1}$ and using the notation presented, (4.8) can be rewritten as

$$b_{r-1}\widehat{P}_{r-2}(x) + a_r\widehat{P}_{r-1}(x) + b_r\widehat{P}_r(x) = x\widehat{P}_{r-1}(x), \quad 2 \leqslant r \leqslant n. \tag{4.9}$$

Easily, we can see (4.9) is true for $r = 1$. Thus,

$$J_{1,n} \begin{bmatrix} \widehat{P}_0(x) \\ \vdots \\ \widehat{P}_{n-2}(x) \\ \widehat{P}_{n-1}(x) \end{bmatrix} = x \begin{bmatrix} \widehat{P}_0(x) \\ \vdots \\ \widehat{P}_{n-2}(x) \\ \widehat{P}_{n-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \widehat{P}_n(x) \end{bmatrix}. \tag{4.10}$$

Because

$$\widehat{P}_n(\lambda_j) = \frac{P_{1,n}(\lambda_j)}{b_1 \dots b_{n-1}} = 0$$

when λ_j is an eigenvalue of $J_{1,n}$, the proof is complete. □

Denote by $\lambda_k(q_1, \dots, q_n)$ the kth eigenvalue of $\mathcal{J}(q_1, \dots, q_n)$.

Lemma 4.4. *Restricting $\lambda_k(q_1, \dots, q_n)$ on the ball $\sum\limits_{i=1}^{n} q_i^2 \leqslant 1$, the extremum of $\lambda_k(q_1, \dots, q_n)$ is attained on the boundary $\sum\limits_{i=1}^{n} q_i^2 = 1$, where $k = 1, n$.*

P r o o f. Let $(\tilde{q}_1, \dots, \tilde{q}_n)$ be an extremum point of $\lambda_k(q_1, \dots, q_n)$ in $\sum\limits_{i=1}^{n} q_i^2 \leqslant 1$. For the maximum case, suppose that $\sum\limits_{i=1}^{n} \tilde{q}_i^2 = c < 1$; we can then find a constant $c_1 > 0$ such that $\sum\limits_{i=1}^{n} (\tilde{q}_i + c_1)^2 \leqslant (\sqrt{c} + c_1\sqrt{n})^2 \leqslant 1$. However, when $\vec{v}$ is the normalized eigenvector corresponding to $\lambda_k(\tilde{q}_1, \dots, \tilde{q}_n)$,

$$\langle (J_n + Q + c_1 I_n)\vec{v}, \vec{v} \rangle = \lambda_k(\tilde{q}_1 + c_1, \dots, \tilde{q}_n + c_1) = \lambda_k(\tilde{q}_1, \dots, \tilde{q}_n) + c_1 > \lambda_k(\tilde{q}_1, \dots, \tilde{q}_n).$$

This contradicts the notion that $\lambda_k(\tilde{q}_1, \dots, \tilde{q}_n)$ is the maximum. Hence, the maximum must be attained by $\sum\limits_{i=1}^{n} q_i^2 = 1$. Similarly, we can prove the assertion for the minimum case. □

According to Theorem 4.2 and Lemma 4.4, it is clear that if λ_k attains its extremum at $(q_1, \dots, q_n)$, then we have the following system of equations:

$$\begin{cases} a_{k1}^2 = 2Lq_1, \\ a_{k2}^2 = 2Lq_2, \\ \vdots \\ a_{kn}^2 = 2Lq_n, \\ q_1^2 + \dots + q_n^2 = 1. \end{cases} \tag{4.11}$$

Lemma 4.5. *Let $\vec{\mathbf{q}} = (q_1, \dots, q_n)$ be the unit vector for which $\lambda_k(q_1, \dots, q_n)$ attains its extremum, where $k = 1, n$. Then $q_i > 0$ (or < 0) for all $1 \leqslant i \leqslant n$ when $\lambda_k(q_1, \dots, q_n)$ attains its maximum (or minimum), $k = 1, n$.*

P r o o f. We only prove the assertion for λ_n here because the assertion for λ_1 follows from the same argument. Using Theorem 2.2, we can easily see that λ_n (λ_1) is at the right (left) side of all zeros of $P_{1,r}(x)$, $r = 1, \ldots, n$. Therefore, according to Lemma 4.3, the components of the eigenvector corresponding to the largest and smallest eigenvalue are nonzero. Thus, (4.11) implies that q_i values are neither all negative nor all positive when λ_n attains its extremum.

Suppose all q_i values are negative when λ_n attains its maximum. Then

$$\max_{\|\vec{v}\|=1} \langle (J_n + Q)\vec{v}, \vec{v}\rangle - \max_{\|\vec{v}\|=1} \langle (J_n - Q)\vec{v}, \vec{v}\rangle \leqslant \max_{\|\vec{v}\|=1} \langle (2Q)\vec{v}, \vec{v}\rangle < 0,$$

because $2Q$ is negative-definite. However, this contradicts the notion that λ_n attains a maximum. Thus, the assertion for the maximum case is proven. Similarly, we can prove the assertion for the minimum case. This completes the proof. □

First, we observe the case $n = 2$,

$$\begin{cases} a_{k1}^2 = 2Lq_1, \\ a_{k2}^2 = 2Lq_2, \\ q_1^2 + q_2^2 = 1. \end{cases} \tag{4.12}$$

Note that we also have

$$\begin{cases} q_1 a_{k1} + a_{k2} = \lambda_k a_{k1}, \\ a_{k1} + q_2 a_{k2} = \lambda_k a_{k2}, \\ a_{k1}^2 + a_{k2}^2 = 1. \end{cases} \tag{4.13}$$

Because $a_{ij} \neq 0$, $1 \leqslant i, j \leqslant 2$, we know that $L \neq 0$. If we replace q_1 and q_2 with $\frac{1}{2}a_{k1}^2/L$ and $\frac{1}{2}a_{k2}^2/L$ in the first and second equation of (4.13), then

$$\begin{cases} \dfrac{a_{k1}^3}{2L} + a_{k2} = \lambda_k a_{k1}, \\[2ex] a_{k1} + \dfrac{a_{k2}^3}{2L} = \lambda_k a_{k2}. \end{cases} \tag{4.14}$$

By multiplying the first equation of (4.14) by a_{k2}^3, the second equation of (4.14) by $-a_{k1}^3$ and adding them together, the result is

$$a_{k2}^4 - a_{k1}^4 = \lambda_k a_{k1} a_{k2} (a_{k2}^2 - a_{k1}^2). \tag{4.15}$$

According to (4.13), we know $a_{k1}^2 + a_{k2}^2 = 1$; hence, equation (4.15) becomes

$$(1 - \lambda_k a_{k1} a_{k2})(a_{k2}^2 - a_{k1}^2) = 0. \tag{4.16}$$

By multiplying the first equation of (4.13) by a_{k2}, the second equation of (4.13) by a_{k1}, and adding them together, we find

$$(q_1 + q_2) a_{k1} a_{k2} + a_{k1}^2 + a_{k2}^2 = 2\lambda_k a_{k1} a_{k2}. \tag{4.17}$$

We wish to show that in (4.16), $\lambda_k a_{k1} a_{k2} \neq 1$. Suppose that on the contrary, $\lambda_k a_{k1} a_{k2} = 1$. Because $a_{k1}^2 + a_{k2}^2 = 1$, equation (4.17) becomes

$$(q_1 + q_2) a_{k1} a_{k2} = 1.$$

Because a_{k1}, $a_{k2} \neq 0$, and we assume that $\lambda_k a_{k1} a_{k2} = 1$, we find that $q_1 + q_2 = \lambda_k$. By replacing λ_k in (4.13) with $q_1 + q_2$, we obtain

$$q_1 q_2 = 1.$$

However, this is absurd because $q_1^2 + q_2^2 = 1$. Because $\lambda_k a_{k1} a_{k2} \neq 1$, $k = 1, 2$, equation (4.16) implies $a_{k1}^2 = a_{k2}^2$. By returning to (4.12), we find that $q_1 = q_2$. We conclude with the following result:

Theorem 4.6. *Let $\mathcal{S}$ be a 2×2 discrete Schrödinger operator in which the square sum of the diagonal elements equals one. Thus, the eigenvalues of $\mathcal{S}$ attain their extremum when $\mathcal{S}$ is persymmetric. Moreover, they attain the maximum when $q_1 = q_2 = 1/\sqrt{2}$ and attain the minimum when $q_1 = q_2 = -1/\sqrt{2}$.*

By using Theorem 4.6, we may guess that among all $n \times n$ discrete Schrödinger operators for which the square sum of the diagonal elements equals one, λ_n (or λ_1) attains its extremum when the discrete Schrödinger operator is *persymmetric*.

For a general n, denote $(a_{k1}, a_{k2}, \ldots, a_{kn})^\top$ by $\vec{u}_k$, $k = 1, n$. For $k = 1, n$, because $\vec{u}_k$ is the normalized eigenvector corresponding to λ_k of $J_n + Q$, we have

$$\langle (J_n + Q)(\mathcal{S}_n \vec{u}_n), \mathcal{S}_n \vec{u}_n \rangle \leqslant \langle (J_n + Q)\vec{u}_n, \vec{u}_n \rangle \tag{4.18}$$

and

$$\langle (J_n + Q)(\mathcal{S}_n \vec{u}_1), \mathcal{S}_n \vec{u}_1 \rangle \geqslant \langle (J_n + Q)\vec{u}_1, \vec{u}_1 \rangle, \tag{4.19}$$

where $\mathcal{S}_n$ is as defined in Section 2.

Suppose that λ_k attains the extremum at $(q_1, \ldots, q_n)$, $k = 1, n$. Consequently, according to (4.11), we have $q_j = \frac{1}{2} a_{kj}^2 / L$, $k = 1, n$. By applying (4.18) and (4.19), we obtain

$$\frac{1}{2L}\left(\sum_{i=1}^{n} a_{ni}^2 a_{n,n+1-i}^2\right) \leqslant \frac{1}{2L}\left(\sum_{j=1}^{n} a_{nj}^4\right) \tag{4.20}$$

and

$$\frac{1}{2L}\left(\sum_{i=1}^{n} a_{1i}^2 a_{1,n+1-i}^2\right) \geqslant \frac{1}{2L}\left(\sum_{j=1}^{n} a_{1j}^4\right). \tag{4.21}$$

In order to obtain more information from (4.20) and (4.21), we need the following lemma:

Lemma 4.7 (Hardy-Littlewood-Pólya inequality)**.** *Suppose*

$$a_1 \leqslant a_2 \leqslant \ldots \leqslant a_n, b_1 \leqslant b_2 \leqslant \ldots \leqslant b_n$$

and $(j_1, j_2, \ldots, j_n)$ *is a rearrangement of* $(1, 2, \ldots, n)$*. Then*

$$\sum_{i=1}^{n} a_i b_i \geqslant \sum_{i=1}^{n} a_i b_{j_i} \geqslant \sum_{i=1}^{n} a_i b_{n+1-i}.$$

Proof. See [9].

□

According to Lemma 4.7, it is clear that

$$\sum_{i=1}^{n} a_{ki}^2 a_{k,n+1-i}^2 \leqslant \sum_{j=1}^{n} a_{kj}^4, k = 1, n. \tag{4.22}$$

From Lemma 4.5, for $k = 1, n$, we have $L > 0$ (or < 0) when λ_k attains the maximum (or minimum). If λ_n attains the minimum, then (4.20) becomes

$$\sum_{i=1}^{n} a_{ni}^2 a_{n,n+1-i}^2 \geqslant \sum_{j=1}^{n} a_{nj}^4. \tag{4.23}$$

By using (4.22) and (4.23), we obtain

$$\sum_{i=1}^{n} a_{ni}^2 a_{n,n+1-i}^2 = \sum_{j=1}^{n} a_{nj}^4. \tag{4.24}$$

This equation leads to

$$\sum_{i=1}^{[n/2]} (a_{ni}^4 - 2a_{ni}^2 a_{n,n+1-i}^2 + a_{n,n+1-i}^4) = 0, \tag{4.25}$$

which can be rewritten as $a_{ni} = a_{n,n+1-i}$ for $1 \leqslant i \leqslant n$. By applying the same argument, we can obtain the result of the case when λ_1 attains the maximum. In summary of the preceding discussion, we can conclude the following:

Theorem 4.8. *For $n \times n$ discrete Schrödinger operators for which the square sum of diagonal elements equals one, the largest (the smallest) eigenvalue attains the minimum (maximum) when the discrete Schrödinger operator is persymmetric.*

Theorem 4.8 shows that one of extremal values of the largest (the smallest) eigenvalue of the discrete Schrödinger operator occurs when the potential function is even. However, the question of when the largest (smallest) eigenvalue attains its maximum (minimum) remains unanswered.

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