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NORM ESTIMATES OF DISCRETE SCHRÖDINGER OPERATORS

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Harper's operator is defined on $\ell^2(\mathbb{Z})$ by

$$H_\theta\xi(n) = \xi(n+1) + \xi(n-1) + 2\cos n\theta\, \xi(n),$$

where $\theta \in [0,\pi]$. We show that the norm of $\|H_\theta\|$ is less than or equal to $2\sqrt{2}$ for $\pi/2 \le \theta \le \pi$. This solves a conjecture stated in [1]. A general formula for estimating the norm of self-adjoint tridiagonal infinite matrices is also derived.

1. Introduction. This paper is an appendix to [1]. The authors considered there a random walk on the discrete Heisenberg group. They reduced the problem of determining the spectrum of the corresponding transition operator to estimating the norm of the Harper operator, well known in mathematical physics (see the references in [1]). This is a discrete Schrödinger operator which acts on square summable doubly infinite sequences $\{\xi(n)\}_{n=-\infty}^{\infty}$ according to the rule

$$H_\theta\xi(n) = \xi(n+1) + \xi(n-1) + 2\cos n\theta\, \xi(n), \tag{1}$$

where θ is a fixed angle from the interval $[0,\pi]$. The authors of [1] were satisfied with the estimate

$$\|H_\theta\| \le 2(1+\sqrt{2}+\cos\theta). \tag{2}$$

This estimate is interesting only in the interval $[\pi/2,\pi]$ because elsewhere the obvious bound by 4 is sharper. The authors conjectured, supported by numerical evidence, that in $[\pi/2,\pi]$ the estimate $2\sqrt{2}$ holds. In this note we prove this conjecture by introducing a method of estimating the norms of tridiagonal operators, which originates in the theory of orthogonal polynomials.

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2. Norm estimates. We start with a general method of estimating the norms of self-adjoint tridiagonal operators. The method goes back to the theory of orthogonal polynomials, where it is used to localize the supports of orthogonality measures (see [2, Theorem I.9.2]).

Let J be a linear operator defined on $\ell^2(\mathbb{Z})$ by

$$J\xi(n) = \lambda_{n+1}\xi(n+1) + \beta_n\xi(n) + \lambda_n\xi(n-1), \tag{3}$$

where $\beta_n \in \mathbb{R}$ and $\lambda_n > 0$ are fixed bounded sequences.

PROPOSITION 1. *Let* $M > \max \beta_n$ *and* $m < \min \beta_n$. *Assume also that there exist sequences* $0 < g_n < 1$ *and* $0 < h_n < 1$ *such that*

$$\frac{\lambda_n^2}{(M-\beta_{n-1})(M-\beta_n)} \le g_n(1-g_{n-1}), \tag{4}$$

$$\frac{\lambda_n^2}{(m-\beta_{n-1})(m-\beta_n)} \le h_n(1-h_{n-1}). \tag{5}$$

Then $mI \le J \le MI$, *i.e. the spectrum of* J *is contained in* $[m, M]$.

Proof. Let $\xi(0) = 1$ and define $\xi(n)$ recursively for $n \ne 0$ by

$$\frac{\lambda_n\xi(n-1)}{(M-\beta_n)\xi(n)} = g_n.$$

Then $\xi(n) > 0$. By (3) and (4) we get

$$J\xi(n) \le M\xi(n).$$

Let $\beta = -\min \beta_n$. Then $\beta + \beta_n \ge 0$ for each n. We have

$$(J + \beta I)\xi(n) \le (M + \beta)\xi(n).$$

The matrix $J+\beta I$ has nonnegative entries and the sequence $\xi(n)$ is positive. Thus by Schur's test (see [3, Theorem 5.2]) we obtain

$$\|J + \beta I\| \le M + \beta.$$

In particular, $J + \beta I \le (M + \beta)I$. This shows the upper estimate of the spectrum of J.

The lower estimate can be obtained from the upper estimate of the matrix $-J$. But this matrix has negative entries on the upper and lower diagonals. So instead of $-J$ we consider the unitarily equivalent matrix $J' = -UJU^{-1}$, where $U\xi(n) = (-1)^n\xi(n)$. The operator J' acts as follows:

$$J'\xi(n) = \lambda_{n+1}\xi(n+1) - \beta_n\xi(n) + \lambda_n\xi(n-1).$$

Observe that assumption (4) of Proposition 1 is satisfied for J' with $M = -m$. Hence by the first part of the proof we get $J' \le -mI$. Since J is similar to $-J'$ we get $J \ge mI$. ∎

The converse of Proposition 1 also holds. In fact, we have the following.

PROPOSITION 2. *Assume that the operator J in* (3) *satisfies $mI \le J \le MI$. Then $M > \max \beta_n$ and $m < \min \beta_n$ and there exist sequences $0 < g_n < 1$ and $0 < h_n < 1$ such that* (4) *and* (5) *hold.*

Proof. We focus on showing (4), since (5) can be proved analogously by considering the operator J' introduced in the proof of Proposition 1. Let e_n denote the sequence whose terms are all zero except the nth term which is 1. From $J \le MI$ we get

$$\beta_n = (Je_n, e_n) \le M(e_n, e_n) = M. \tag{6}$$

We claim that the inequality in (6) is strict for each n. Otherwise we would have $Je_n = Me_n$. This is impossible, because $Je_n(n+1) = \lambda_{n+1} \neq 0$. Thus we have proved the first part of Proposition 2.

In the remaining part we will make use of the following lemma, whose origins lie in the Frobenius–Perron method in the theory of finite stochastic matrices (see [4, Lemma 9.2.2]).

LEMMA 1. *Le $A = \{a(i,j)\}$ be an $N \times N$ symmetric matrix with nonnegative entries such that $a(i, i+1) > 0$ and $a(i+1, i) > 0$ for $i = 1, \ldots, N-1$. Let $M \ge \|A\|$, where $\|A\|$ denotes the operator norm with respect to the ℓ^2-norm on $\mathbb{R}^N$. There exists a nonzero vector $\xi \in \mathbb{R}^N$ with positive coordinates such that*

$$A\xi(n) \le M\xi(n), \qquad 1 \le n \le N.$$

Proof. Assume $M = \|A\|$. Then M or $-M$ is an eigenvalue of A. Thus there is $\xi \neq 0$ such that

$$A\xi = \pm M\xi.$$

Taking absolute values of both sides gives

$$A|\xi| \ge M|\xi|. \tag{7}$$

We claim that equality holds in (7). If not, we would have

$$M(|\xi|, |\xi|) \ge (A|\xi|, |\xi|) > M(|\xi|, |\xi|),$$

a contradiction. Thus

$$A|\xi| = M|\xi|.$$

We will show that the coordinates $\xi(n)$ are all nonzero. Assume that $\xi(n) = 0$. Then

$$a(n-1, n)|\xi(n-1)| + a(n+1, n)|\xi(n+1)| \le M|\xi(n)| = 0.$$

Hence $\xi(n \pm 1) = 0$. Repeating this reasoning we finally get $\xi(m) = 0$ for all $m = 1, \ldots, N$, which contradicts $\xi \neq 0$. This completes the proof of Lemma 1. ■

Let us return to the proof of Proposition 2. Let $\beta = -\min \beta_n$. Then the matrix $A = J + \beta I$ has nonnegative entries and $A \le (M + \beta)I$. Let

P_N denote the projection onto a $(2N+1)$-dimensional subspace of $\ell^2(\mathbb{Z})$, defined by

$$P_N\xi = \sum_{n=-N}^{N} \xi(n)e_n.$$

Let A_N denote the truncated matrix P_NAP_N. It is clear that

$$A_N \le A \le (M+\beta)I.$$

By Lemma 1 there exist sequences $\xi_N \in \mathbb{R}^{2N+1}$ with positive entries such that

$$A_N\xi_N(n) \le (M+\beta)\xi_N(n), \quad -N \le n \le N. \tag{8}$$

Since the entries of ξ_N are positive we may assume, by multiplying by a positive constant if necessary, that $\xi_N(0) = 1$. We may also assume that (8) holds for all $n \in \mathbb{Z}$ upon extending ξ_N by 0 for $|n| > N$.

We show by induction that for any fixed $n \in \mathbb{Z}$ the sequence of values $N \mapsto \xi_N(n)$ is bounded. For $n = 0$ it is constantly 1. Let $n = \pm 1$. Then by (8) we have

$$A_N\xi_N(0) = \lambda_1\xi_N(1) + (\beta_0+\beta)\xi_N(0) + \lambda_0\xi_N(-1) \le M\xi_N(0).$$

Since $\beta_1 + \beta \ge 0$ we get

$$\lambda_1\xi_N(1) + \lambda_0\xi_N(-1) \le M.$$

Since $\lambda_{\pm 1} \ne 0$, we conclude that $\xi_N(\pm 1)$ are bounded. Similarly the induction step follows from the inequalities

$$\lambda_{n+1}\xi_N(n+1) \le M\xi_N(n), \quad \lambda_n\xi_N(n-1) \le M\xi_N(n).$$

Now, using Helly's selection principle we can choose a subsequence N_k of N's for which all sequences $k \mapsto \xi_{N_k}(n)$ are convergent. Let

$$\xi(n) = \lim_k \xi_{N_k}(n).$$

By (8) we get

$$A\xi(n) = (J+\beta I)\xi(n) \le (M+\beta)\xi(n).$$

We have $\xi(n) \ge 0$ and $\xi(0) = 1$. As in the proof of Lemma 1 we can derive that $\xi(n) > 0$ because the matrix $J + \beta I$ has nonnegative entries. Hence we have constructed a positive sequence $\xi(n)$ such that

$$J\xi(n) \le M\xi(n), \quad n \in \mathbb{Z}.$$

Now by taking

$$g_n = \frac{\lambda_n\xi(n-1)}{(M-\beta_n)\xi(n)}$$

we get (4). ∎

Let us turn to the Harper operator H_θ, i.e. $\lambda_n \equiv 1$ and $\beta_n = 2\cos n\theta$. We will focus on the upper estimate M. It will follow from the proof that the lower estimate is $-M$ in this case. This also follows from the fact that the spectrum of H_θ is symmetric about the origin (see [1, comments before (2)]).

Let $M > 2$ be the smallest number such that

$$\frac{1}{(M - 2\cos(n-1)\theta)(M - 2\cos n\theta)} \le \frac{1}{4} = \frac{1}{2}\left(1 - \frac{1}{2}\right). \tag{9}$$

By Proposition 1 we get $H_\theta \le MI$. The condition (9) gives the same estimate as in Proposition 4 of [1]. To get the sharper estimate $2\sqrt{2}$ we need a better choice of g_n.

Theorem 1. *Let* $\pi/2 \le \theta \le \pi$. *Then* $\|H_\theta\| \le 2\sqrt{2}$.

Proof. We have to find an appropriate g_n in order to satisfy (4) with $M = 2\sqrt{2}$. First we look for g_n in the form

$$g_n = \frac{1}{2} - \frac{\alpha_n}{2\sqrt{2} - 2\cos n\theta}.$$

Now assumption (4) can be transformed into

$$(\sqrt{2} - \cos n\theta - \alpha_n)(\sqrt{2} - \cos(n-1)\theta + \alpha_{n-1}) \ge 1. \tag{10}$$

So the problem reduces to finding α_n such that (10) is satisfied and both the factors are positive. We first look for α_n in the form

$$\alpha_n = \gamma_n - \sin n\theta \cot\frac{\theta}{2}. \tag{11}$$

Then

$$\alpha_n + \cos n\theta = \gamma_n - \frac{\sin(2n-1)\frac{\theta}{2}}{\sin\frac{\theta}{2}},$$

$$\alpha_{n-1} - \cos(n-1)\theta = \gamma_{n-1} + \frac{\sin(2n-1)\frac{\theta}{2}}{\sin\frac{\theta}{2}}.$$

Let $\theta = \pi - 2\varphi$. Then $0 \le \varphi \le \pi/4$. Moreover,

$$\alpha_n + \cos n\theta = \gamma_n + s_n,$$

$$\alpha_n - \cos(n-1)\theta = \gamma_{n-1} - s_n,$$

where

$$s_n = (-1)^{n+1}\frac{\cos(2n-1)\varphi}{\cos\varphi}. \tag{12}$$

Now (10) takes the form

$$(\sqrt{2} - s_n - \gamma_n)(\sqrt{2} + s_n + \gamma_{n-1}) \ge 1. \tag{13}$$

The following fact, which follows obviously from (12), will be essential.

Fact 1. *If* $|s_n| > 1$ *then* $|s_{n\pm1}| < 1$ *for* $0 \le \varphi \le \pi/4$.

Now we are going to define the sequence γ_n. First we take care of those n for which $|s_n|>1$ or $|s_{n+1}|>1$. If $s_n>1$ we put

$$\gamma_n=\frac{1-s_n^2}{\sqrt{2}+s_n}.$$

If $s_{n+1}<-1$ we put

$$\gamma_n=\frac{1-s_{n+1}^2}{\sqrt{2}-s_{n+1}}.$$

By Fact 1 we do not run into contradiction, because the indices with $|s_n|>1$ must be at least at distance 2 from one another if $0\le\varphi\le\pi/4$. Next we put $\gamma_n=0$ for all n for which γ_n has not been defined yet. Now we have to check if (13) is satisfied. In doing this we will use another obvious fact.

FACT 2. *Let $|x|<1<y$ and $x^2+y^2\le 2$. Then*

$$\frac{y^2-1}{\sqrt{2}+y}\le\frac{1-x^2}{\sqrt{2}+x}.$$

LEMMA 2. $s_n^2+s_{n+1}^2\le 2$.

Proof. We have

$$\begin{aligned}s_n^2+s_{n+1}^2&=\frac{\cos^2(2n-1)\varphi}{\cos^2\varphi}+\frac{\cos^2(2n+1)\varphi}{\cos^2\varphi}\\&=\frac{2+\cos{(2n-1)2\varphi}+\cos{(2n+1)2\varphi}}{2\cos^2\varphi}=\frac{1+\cos 2\varphi\cos 4n\varphi}{\cos^2\varphi}\\&\le\frac{1+\cos 2\varphi}{\cos^2\varphi}=2.\ \blacksquare\end{aligned}$$

We return to the proof of (13). We consider four cases.

(i) $\gamma_{n-1}=\gamma_n=0$. Then $|s_n|\le 1$. Therefore

$$(\sqrt{2}-s_n-\gamma_n)(\sqrt{2}+s_n+\gamma_{n-1})=2-s_n^2\ge 1.$$

(ii) $\gamma_{n-1}=0$, $\gamma_n\ne 0$. This has two subcases.

(a) $s_n>1$. Then

$$(\sqrt{2}-s_n-\gamma_n)(\sqrt{2}+s_n+\gamma_{n-1})=\left(\sqrt{2}-s_n-\frac{1-s_n^2}{\sqrt{2}+s_n}\right)(\sqrt{2}+s_n)=1.$$

(b) $s_{n+1}<-1$. By Fact 1 we have $|s_n|<1$. Therefore

$$\begin{aligned}(\sqrt{2}-s_n-\gamma_n)(\sqrt{2}+s_n+\gamma_{n-1})&=\left(\sqrt{2}-s_n-\frac{1-s_{n+1}^2}{\sqrt{2}-s_{n+1}}\right)(\sqrt{2}+s_n)\\&\ge(\sqrt{2}-s_n)(\sqrt{2}+s_n)=2-s_n^2\ge 1.\end{aligned}$$

(iii) $\gamma_{n-1}\ne 0$, $\gamma_n=0$. This also splits in two subcases.

(a) $s_{n-1} > 1$. Then $|s_n| < 1$ and

$$(\sqrt{2} - s_n - \gamma_n)(\sqrt{2} + s_n + \gamma_{n-1}) = (\sqrt{2} - s_n)\left(\sqrt{2} + s_n + \frac{1 - s_{n-1}^2}{\sqrt{2} + s_{n-1}}\right).$$

This is greater than 1 if

$$\frac{s_{n-1}^2 - 1}{\sqrt{2} + s_{n-1}} \le \frac{1 - s_n^2}{\sqrt{2} - s_n}.$$

The last inequality follows from Fact 2 and Lemma 1.

(b) $s_n < -1$. Then

$$(\sqrt{2} - s_n - \gamma_n)(\sqrt{2} + s_n + \gamma_{n-1}) = (\sqrt{2} - s_n)\left(\sqrt{2} + s_n + \frac{1 - s_n^2}{\sqrt{2} - s_n}\right) = 1.$$

(iv) $\gamma_{n-1} \ne 0$, $\gamma_n \ne 0$. By Fact 1 this is possible only when $s_{n-1} > 1$, $|s_n| < 1$ and $s_{n+1} < -1$. By Fact 2 and Lemma 1 we have

$$\frac{s_{n-1}^2 - 1}{\sqrt{2} + s_{n-1}} \le \frac{1 - s_n^2}{\sqrt{2} - s_n}.$$

Hence

$$\begin{aligned}
&(\sqrt{2} - s_n - \gamma_n)(\sqrt{2} + s_n + \gamma_{n-1}) \\
&\quad = \left(\sqrt{2} - s_n + \frac{s_{n+1}^2 - 1}{\sqrt{2} - s_{n+1}}\right)\left(\sqrt{2} + s_n + \frac{1 - s_{n-1}^2}{\sqrt{2} + s_{n-1}}\right) \\
&\quad \ge \left(\sqrt{2} - s_n + \frac{s_{n+1}^2 - 1}{\sqrt{2} - s_{n+1}}\right)\left(\sqrt{2} + s_n - \frac{1 - s_n^2}{\sqrt{2} - s_n}\right) \\
&\quad = 1 + \frac{s_{n+1}^2 - 1}{(\sqrt{2} - s_n)(\sqrt{2} - s_{n+1})} \ge 1. \quad \blacksquare
\end{aligned}$$

REMARK 1. Taking $\gamma_n \equiv 0$ in (13) gives

$$\|H_\theta\| \le 2\sqrt{1 + \sin^{-2}\frac{\theta}{2}}.$$

Let us try to determine the smallest positive M such that (9) holds. By solving the quadratic inequality generated by (9) we see that

$$M \ge 2\cos\frac{\theta}{2}\cos{(2n+1)}\frac{\theta}{2} + 2\sqrt{1 + \sin^2\frac{\theta}{2}\sin^2(2n+1)\frac{\theta}{2}}.$$

Let $a = \sin^2\frac{\theta}{2}$ and $x = \sin^2(2n+1)\frac{\theta}{2}$. Then it suffices that

$$M = 2\max\{\sqrt{1-a}\sqrt{1-x} + \sqrt{1+ax} \mid 0 \le x \le 1\}.$$

By easy calculus the maximum is attained at $x = 0$ or at $x = a - a^{-1} + 1$ according to whether $a \le (\sqrt{5} - 1)/2$ or $a > (\sqrt{5} - 1)/2$. Summarizing we get

$$\|H_\theta\| \le M = \begin{cases} 2+2\cos\frac{\theta}{2} & \text{if } \sin^2\frac{\theta}{2} \le (\sqrt{5}-1)/2, \\ 2\sqrt{1+\sin^{-2}\frac{\theta}{2}} & \text{if } \sin^2\frac{\theta}{2} \ge (\sqrt{5}-1)/2. \end{cases} \tag{14}$$

Now, combining this with Theorem 1 and the fact that $\theta = \pi/2$ falls into the first case of formula (14), gives

$$\|H_\theta\| \le \begin{cases} 2+2\cos\frac{\theta}{2} & \text{if } 0 \le \theta \le \pi/2, \\ 2\sqrt{2} & \text{if } \pi/2 \le \theta \le \pi. \end{cases}$$

REMARK 2. Proposition 2 can be used to show that the estimate $2\sqrt{2}$ is sharp for the endpoint π, which has also been proved in [1] by different methods. Indeed, assume that $\|H_\pi\| \le M$. Then there exist $0 < g_n < 1$ such that

$$\frac{1}{(M-2)(M+2)} \le g_n(1-g_{n-1}).$$

Assume for contradiction that $M^2 < 8$. Then

$$\frac{1}{4} < \frac{1}{(M-2)(M+2)} \le g_n(1-g_{n-1}).$$

One can easily check that the sequence g_n is increasing. Let g denote its limit. Then

$$\frac{1}{4} < \frac{1}{(M-2)(M+2)} \le g(1-g) \le \frac{1}{4}.$$

This is a contradiction. Hence $M \ge 2\sqrt{2}$.

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