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REFLECTIONS ON THE ALMOST MATHIEU OPERATOR

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An explicit derivation of a tridiagonal matrix form for the almost Mathieu operator (Harper's equation) is obtained via conjugation with a reflection operator, valid for all rational values of the rotation parameter. The difference between even and odd values of the denominator is highlighted. This tridiagonal form is useful for numerical eigenvalue computations; some Matlab code is included.

1. INTRODUCTION

The almost Mathieu operator is given by the difference equation

$$\phi_{n+1} + [\lambda \cos 2\pi(n\theta - \beta)]\phi_n + \phi_{n-1} = E\phi(n),$$

where θ, β, λ are real constants and $\{\phi_n\}_{n=-\infty}^{\infty}$ is a square summable sequence indexed by the integers. This operator is interesting both physically and mathematically and has been studied by a number of authors [1–8,10–18]. Several questions about this operator focus on the structure of its spectrum; previous works have investigated for instance, its measure and Hausdorff dimension, its Cantor-like set properties, and its fractal behaviour as suggested in Figure 1 (a reproduction of the the figure calculated first in [8]). Many of these spectral questions can be investigated to a certain extent by numerical methods, as pursued in [1,2,15–18] and others, so there is interest in finding fast, accurate methods of extracting numerical information about the spectral data for this infinite dimensional operator.

In this paper, we consider the case where the rotation parameter θ is a rational number $\theta = p/q$, and give an explicit reduction of the spectral problem to the computation of eigenvalues for a certain tridiagonal matrices of size about $q/2$ by $q/2$. From

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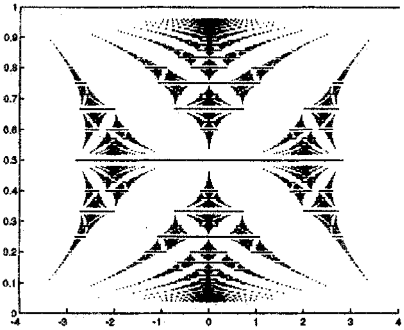

FIGURE 1: MATHIEU LINE SPECTRA

this derivation, one can immediately apply any one of a number of well-known numerical methods for diagonalizing a tridiagonal matrix to obtain the eigenvalues in order q^2 steps (see [9,19]); some Matlab code is presented in the appendix to do just that.

It is worthwhile to point out what is new in this derivation. The reduction of the spectral calculation to finding eigenvalues of a finite matrix is well-known, and this process is recapped in Section 2. However, the $q \times q$ matrix so obtained is not quite tridiagonal. A tridiagonal form has been obtained previously by Thouless as described in [15] (see also [16–18]), but he omits the derivation and only presents the explicit form for odd values of the denominator q. The derivation presented in Section 3 of the current work is valid for both odd and even values of q, and makes an interesting use of reflection operators to provide the orthogonal transformation carrying the $q \times q$ matrix of Section 2 into a tridiagonal. This derivation also provides insight into how the even q case is trickier than the odd case, as we see in Section 4 that a careful choice of reflection matrices must be made to find one that successfully tridiagonalizes. The tridiagonal form also has its own interesting symmetries, and Section 5 gives the explicit form of the tridiagonal in all cases.

Arveson [1,2] has used the tridiagonal form in a somewhat different context, by taking θ irrational, truncating the infinite matrix of the corresponding almost Mathieu operator, to obtain a finite tridiagonal matrix from which an approximation to the spectrum may be computed.

Order q^2 methods for finding the rational spectrum have been obtained before. For instance, a cofactor expansion for the determinant of the almost tridiagonal $q \times q$ matrix of Section 2 computes the characteristic polynomial for the matrix, roots of which give the eigenvalues in about q^2 steps, and appears to be the numerical method used in [8,10–13]. We prefer tridiagonal form, since there is a large literature on how to extract eigenvalues quickly and accurately for such matrices.

I thank Bill Arveson for introducing me to this "ten martini" problem.

2. Reduction to finite dimensions

In this section, we reduce the spectral problem for the rational almost Mathieu operator to a finite dimensional calculation. This reduction is well-known (see in particular [6]), but we include a summary of the ideas for completeness.

Considering $E = E_{\theta,\beta,\lambda}$ as a bounded operator on the Hilbert space of square-summable functions ϕ, it is known that the spectrum of E is independent of β for irrational θ; more generally, taking the union of spectra for all β in $[0,1]$ gives a compact set

$$S(\theta,\lambda) = \bigcup_{\beta} \mathrm{Sp}\ E_{\theta,\beta,\lambda}$$

depending only on θ and λ. The set $S(\theta,\lambda)$ depends continuously on the parameters θ,λ and is simply the spectrum of the self-adjoint operator $h = h_{\theta,\lambda} = u + u^* + (\lambda/2)(v + v^*)$ in the C^*-algebra A_θ generated by two universal unitaries u, v satisfying $vu = e^{2\pi i\theta}uv$.

When θ is rational, one computes the spectrum as follows. Letting $\theta = p/q$ with p, q integers in reduced form, the irreducible representations of A_θ are all q-dimensional and parameterized by two complex coefficients z_1, z_2 of modulus one. The corresponding irreducible representation maps u to a $q \times q$ matrix z_1U, and v to a matrix z_2V, where U is the cyclic permutation matrix and V is the diagonal matrix with entries $\{e^{2\pi i\theta}, e^{4\pi i\theta}\ldots, e^{2q\pi i\theta}\}$. Thus $S(\theta,\lambda)$ is the union over z_1, z_2 of the eigenvalues of the $q \times q$ matrices

$$H = z_1U + \overline{z}_1U^* + \frac{\lambda}{2}(z_2V + \overline{z}_2V^*).$$

Since the characteristic polynomials for such H are independent of z_1, z_2 except in the constant term $c = c(z_1, z_2, \lambda)$, the set $S(\theta,\lambda)$ will be a union of intervals whose endpoints are the roots of the two polynomials with constant terms equal to the maximum and minimum values for $c(z_1, z_2, \lambda)$. This constant term in the polynomial is just a fixed constant (independent of z_1 and z_2) plus or minus the value $z_1^q + z_1^{-q} + (\lambda/2)^q(z_2^q + z_2^{-q})$, so these extreme values occur at parameter values z_1, z_2 with $z_1^q = z_2^q = 1$ or $z_1^q = z_2^q = -1$. Consequently, it suffices to compute the eigenvalues of just two $q \times q$ matrices, then join endpoints to obtain $S(\theta,\lambda)$. Observe that these square matrices are almost tridiagonal, except for the $z_1, \overline{z}_1$ entries in the off-diagonal corners. The form is also basically a diagonal plus a permutation matrix (and its transpose), so to tridiagonalize we must tridiagonalize the permutation matrix, without moving the diagonal part too much. Section 3 builds the matrix that does just that; Section 4 uses the freedom we have in selecting z_1 and z_2 to find a diagonal with appropriate symmetry properties.

3. Some reflection operators

We begin with some terminology. Recall the main diagonal of a matrix is formed by those entries stretching from the top-left corner to the bottom-right corner; call the antidiagonal those entries stretching from the top-right corner to the bottom-left corner. The transpose of a matrix is the usual operation of exchanging rows for columns; call the operation of transposing across the antidiagonal the flip transpose. A matrix is symmetric if it equals its transpose; it is flip symmetric if it equals its own flip transpose. We will need (for the even q case) matrices which are rank-one extensions of flip symmetric matrices; that is, a matrix of the form

$$A = \begin{bmatrix} a & 0 \\ 0 & F \end{bmatrix},$$

where a is 1 by 1 and F is flip symmetric. We say the matrix A is flip-plus-one symmetric.

The results in this section depend on the choice of a sign parameter ϵ; for physical reasons, it is traditional to call $\epsilon = 1$ the periodic case and $\epsilon = -1$ the antiperiodic case. Throughout the following, the rational p/q is assumed to be in reduced form, with q positive, and p, q with no common factors. To avoid certain degenerate cases, it is useful to assume q is greater than 3.

Let I denote the $n \times n$ identity matrix (ones on the diagonal), J the $n \times n$ anti-identity matrix (ones on the antidiagonal), and $\epsilon = \pm 1$ a sign parameter. For any even integer $q = 2n$, we define a $q \times q$ matrix R_ϵ in block form as

$$R_\epsilon = \frac{1}{\sqrt{2}} \begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix};$$

for odd $q = 2n + 1$ we insert one row and column and define the matrix as

$$R_\epsilon = \frac{1}{\sqrt{2}} \begin{bmatrix} \epsilon I & 0 & J \\ 0 & \sqrt{2} & 0 \\ J & 0 & -\epsilon I \end{bmatrix}.$$

Clearly R_ϵ is symmetric, and a quick calculation shows R_ϵ is orthogonal: in the even case,

$$R_\epsilon R_\epsilon^t = R_\epsilon^2 = \frac{1}{2} \begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix} \begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix} = \frac{1}{2} \begin{bmatrix} I^2 + J^2 & \epsilon(IJ - JI) \\ \epsilon(JI - IJ) & J^2 + I^2 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}.$$

The odd case is similar. Thus R_ϵ is a reflection operator.

We also define the rank one extension of R_ϵ as the matrix S_ϵ given in block form as

$$S_\epsilon = \begin{bmatrix} 1 & 0 \\ 0 & R_\epsilon \end{bmatrix}.$$

Clearly S_ϵ is also a reflection operator.

Since conjugating by the submatrix J just reverses rows and columns, it is apparent that a matrix which commutes with R_ϵ or S_ϵ must have some symmetry properties. We make this precise for diagonal matrices in the following:

PROPOSITION 1. *Suppose D is a diagonal matrix. Then $R_\epsilon D R_\epsilon$ is diagonal if and only if D is flip symmetric, in which case $R_\epsilon D R_\epsilon = D$. Similarly, $S_\epsilon D S_\epsilon$ is diagonal if and only if D is flip-plus-one symmetric, in which case $S_\epsilon D S_\epsilon = D$.*

PROOF. When q is even, decompose D into a direct sum of diagonal matrices D_1 plus D_2, so

$$\begin{aligned} R_\epsilon D R_\epsilon &= \frac{1}{2}\begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix}\begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}\begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} \epsilon D_1 & JD_2 \\ JD_1 & -\epsilon D_2 \end{bmatrix}\begin{bmatrix} I & J \\ J & -I \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} D_1 + JD_2J & \epsilon(D_1J - JD_2) \\ \epsilon(JD_1 - D_2J) & JD_1J + D_2 \end{bmatrix}, \end{aligned}$$

which is diagonal only when $JD_1 - D_2J = 0$; equivalently the flip transpose of D_1 is D_2, so the matrix D is flip symmetric. In this case, $D_1 + JD_2J = 2D_1$ and $JD_1J + D_2 = 2D_2$ so by the calculation above, $R_\epsilon D R_\epsilon = D$. The proof for q odd is similar, and the result for commuting with S_ϵ follows immediately. ∎

These reflection matrices R_ϵ and S_ϵ are the ones needed to tridiagonalize the permutation matrices. Let C_ϵ be the $q \times q$ matrix which cyclically permutes the standard basis vectors, with a sign change ϵ at the boundary. That is, $C_\epsilon e_k = e_{k+1}$ for $k = 1, \ldots q-1$ and $C_\epsilon e_q = \epsilon \cdot e_1$. We call C_1 the periodic permutation matrix and C_{-1} the antiperiodic permutation matrix. The symmetric matrix $C_\epsilon + C_\epsilon^t$ is almost tridiagonal, except that for the nonzero entry ϵ in the off-diagonal corners. A straightforward calculation gives the following:

PROPOSITION 2. *The matrices $R_\epsilon(C_\epsilon + C_\epsilon^t)R_\epsilon$ and $S_\epsilon(C_\epsilon + C_\epsilon^t)S_\epsilon$ are tridiagonal.*

PROOF. It is convenient to define M to be the tridiagonal matrix with ones on the super- and sub-diagonal only, P the diagonal matrix with a single one in the bottom-right corner, and k a column vector with a single one in the last entry. Observe $JMJ = M$, JPJ is a diagonal matrix with a single one in the top-left corner, and Jk is a column vector with a one in the first entry.

When the matrix C_ϵ has even dimension, write

$$C_\epsilon + C_\epsilon^t = \begin{bmatrix} M & PJ+\epsilon JP \\ JP+\epsilon PJ & M \end{bmatrix},$$

and compute:

$$\begin{aligned} R_\epsilon(C_\epsilon + C_\epsilon^t)R_\epsilon &= \frac{1}{2}\begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix}\begin{bmatrix} M & PJ+\epsilon JP \\ JP+\epsilon PJ & M \end{bmatrix}\begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} \epsilon M + P + \epsilon JPJ & \epsilon PJ + JP + JM \\ JM - \epsilon JP - PJ & JPJ + \epsilon P - \epsilon M \end{bmatrix}\begin{bmatrix} \epsilon I & J \\ J & -\epsilon I \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} M + 2\epsilon P + 2JPJ + JMJ & \epsilon MJ - \epsilon JM \\ \epsilon JM - \epsilon MJ & JMJ - 2\epsilon JPJ - 2P + M \end{bmatrix} \\ &= \begin{bmatrix} M + \epsilon P + JPJ & 0 \\ 0 & M - \epsilon JPJ - P \end{bmatrix}, \end{aligned}$$

where the last simplification results from the flip symmetry of M, so $JM - MJ = 0$ and $M + JMJ = 2M$. This last matrix is tridiagonal since the submatrices P and JPJ are diagonal while M is tridiagonal.

When C_ϵ has odd dimension, it is somewhat easier to do the $\epsilon = \pm 1$ cases separately. Proceeding as above, one verifies that for $\epsilon = 1$,

$$C_1 + C_1^t = \begin{bmatrix} M & k & JP \\ k^t & 0 & k^tJ \\ PJ & Jk & M \end{bmatrix}, \qquad R_1(C_1 + C_1^t)R_1 = \begin{bmatrix} M+JPJ & \sqrt{2}k & 0 \\ \sqrt{2}k^t & 0 & 0 \\ 0 & 0 & M-P \end{bmatrix};$$

while for $\epsilon = -1$, the matrices are

$$C_{-1}+C_{-1}^t = \begin{bmatrix} M & k & -JP \\ k^t & 0 & k^tJ \\ -PJ & Jk & M \end{bmatrix}, \; R_{-1}(C_{-1}+C_{-1}^t)R_{-1} = \begin{bmatrix} M+JPJ & 0 & 0 \\ 0 & 0 & \sqrt{2}k^tJ \\ 0 & \sqrt{2}Jk & M-P \end{bmatrix}.$$

In both cases, the matrices $R_\epsilon(C_\epsilon + C_\epsilon^t)R_\epsilon$ are also tridiagonal.

For the conjugation by S_ϵ, one can verify similar calculations, and obtain for odd sized matrices,

$$(C_\epsilon + C_\epsilon^t) = \begin{bmatrix} 0 & k^tJ & \epsilon k^t \\ Jk & M & PJ \\ \epsilon k & JP & M \end{bmatrix}, \quad S_\epsilon(C_\epsilon + C_\epsilon^t)S_\epsilon = \begin{bmatrix} 0 & \epsilon\sqrt{2}k^tJ & 0 \\ \epsilon\sqrt{2}Jk & M+\epsilon P & 0 \\ 0 & 0 & M - \epsilon JPJ \end{bmatrix}.$$

For even-sized matrices, the two cases of ϵ split: for $\epsilon = 1$,

$$(C_1 + C_1^t) = \begin{bmatrix} 0 & k^tJ & 0 & k^t \\ Jk & M & k & 0 \\ 0 & k^t & 0 & k^tJ \\ k & 0 & Jk & M \end{bmatrix}, \; S_1(C_1 + C_1^t)S_1 = \begin{bmatrix} 0 & \sqrt{2}k^tJ & 0 & 0 \\ \sqrt{2}Jk & M & \sqrt{2}k & 0 \\ 0 & \sqrt{2}k^t & 0 & 0 \\ 0 & 0 & 0 & M \end{bmatrix};$$

while with $\epsilon = -1$,

$$(C_{-1} + C_{-1}^t) = \begin{bmatrix} 0 & k^t J & 0 & -k^t \\ Jk & M & k & 0 \\ 0 & k^t & 0 & k^t J \\ -k & 0 & Jk & M \end{bmatrix},$$

and

$$S_{-1}(C_{-1} + C_{-1}^t)S_{-1} = \begin{bmatrix} 0 & -\sqrt{2}k^t J & 0 & 0 \\ -\sqrt{2}Jk & M & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2}k^t J \\ 0 & 0 & \sqrt{2}Jk & M \end{bmatrix}.$$

A quick inspection confirms the matrix $S_\epsilon(C_\epsilon + C_\epsilon^t)S_\epsilon$ is tridiagonal in all cases. ∎

When a matrix is given in the form $H_\epsilon = C_\epsilon + C_\epsilon^t + D$, where C_ϵ is the signed permutation matrix and D is diagonal, combining the above results gives the following:

PROPOSITION 3. *The matrix $H_\epsilon = C_\epsilon + C_\epsilon^t + D$ is tridiagonalized by R_ϵ when the diagonal is flip symmetric and is tridiagonalized by S_ϵ when the diagonal is flip-plus-one symmetric.*

REMARK. Although the calculations above use the same sign ϵ for C_ϵ with R_ϵ, and for C_ϵ with S_ϵ, it turns out this doesn't matter for the R_ϵ, although it does matter for the S_ϵ. We will see in the next section that in the even q case, we are forced to use the S_ϵ form to tridiagonalize, so it is important to get the signs correct. It is worth noting that in Proposition 3, the tridiagonalized matrix is the direct sum of two tridiagonal blocks, consequently the eigenvalues for each block can be computed independently. More specifically, the tridiagonal form is a direct sum of two smaller matrices M of sizes about $q/2$, plus four other non-zero entries.

4. FORCING SYMMETRY OF THE ALMOST MATHIEU OPERATOR

In the rational case, computing the spectrum of the operator $h = u + u^* + (\lambda/2)(v + v^*)$ is equivalent to computing the eigenvalues of two extreme matrices of the form $H = z_1 U + \bar{z}_1 U^* + (\lambda/2)(z_2 V + \bar{z}_2 V^*)$ where z_1, z_2 are unit complex numbers with $z_1^q = z_2^q = \pm 1$, U is the (unsigned) $q \times q$ cyclic permutation matrix and V the diagonal matrix with consecutive powers of $e^{2\pi i p/q}$ for entries. We will choose z_1, z_2 so that Proposition 3 applies; that is, making H look like a sum $C_\epsilon + C_\epsilon^t + D$, with appropriate symmetry on the diagonal.

Choosing $z_1 = 1$ gives one extreme value for z_1; the operator $z_1 U$ is just the periodic permutation matrix C_1 of the last section. The other extreme value is obtained by

$z_1 = e^{\pi i/q}$; conjugating with the diagonal unitary $W = \text{diag}(z_1, z_1^2, \ldots, z_1^q)$ turns $z_1 U$ into the antiperiodic permutation matrix C_{-1}. Since the diagonal matrix W commutes with V, in both cases the matrix H_ϵ is unitarily equivalent to $C_\epsilon + C_\epsilon^t + (\lambda/2)(z_2 V + \overline{z}_2 V^*)$. By Proposition 3, this matrix can be tridiagonalized by reflection matrices R_ϵ or S_ϵ provided z_2 can be chosen so that the diagonal matrix $(\lambda/2)(z_2 V + \overline{z}_2 V^*)$ is either flip symmetric or flip-plus-one symmetric.

In the case $\epsilon = +1$, the matrix H_{+1} is obtained with $z_1^q = z_2^q = 1$; since z_1 was fixed above, the general solution is given by $z_2 = e^{2\pi i r/q}$ where r is any integer. The diagonal entries of H_{+1} are given by $d_k = \lambda \cos 2\pi(pk + r)/q$, for $k = 1 \ldots q$. To force flip symmetry requires $d_k = d_{q+1-k}$ for all k; since cos is even and 2π-periodic, this occurs if there exists an integer r with

$$pk + r \equiv -(p(q + 1 - k) + r) \bmod q;$$

equivalently,

$$2r \equiv -p \bmod q.$$

To force flip-plus-one symmetry requires $d_k = d_{q+2-k}$; this occurs for an integer r with

$$pk + r \equiv -(p(q + 2 - k) + r) \bmod q;$$

equivalently,

$$2r \equiv -2p \bmod q.$$

In the $\epsilon = -1$ case, the extreme matrix H_{-1} is given by $z_1^q = z_2^q = -1$. Again, as z_1 was fixed above, the general solution is $z_2 = e^{\pi i(2r+1)/q}$ where r is any integer. The diagonal entries of H_{-1} are given by $d'_k = \lambda \cos \pi(2pk + 2r + 1)/q$; solving for flip symmetry gives the equation

$$2r + 1 \equiv -p \bmod q.$$

For flip-plus-one symmetry, the required equation is

$$2r + 1 \equiv -2p \bmod q.$$

Solving these equations for r just involves a division by 2; depending on the parity of p and q, one adjusts mod q to obtain an integer solution for r, when the solution exists. The following table provides the integer solutions for r which yield the required symmetries in all cases:

	$\epsilon = +1$	(periodic)	$\epsilon = -1$	(antiperiodic)
Parity	Flip symmetric	Flip-plus-one	Flip symmetric	Flip-plus-one
p, q odd	$r = (q-p)/2$	$r = -p$	$r = -(p+1)/2$	$r = (q-2p-1)/2$
p even, q odd	$r = -p/2$	$r = -p$	$r = (q-p-1)/2$	$r = (q-2p-1)/2$
p odd, q even	no sol'n	$r = -p$	$r = -(p+1)/2$	no sol'n

Thus for any choice of p, q the extreme matrices H_{+1} and H_{-1} can be tridiagonalized by first making a good choice for z_1, z_2, conjugating with the diagonal unitary W, then conjugating with either R_ϵ or S_ϵ.

Curiously, for q odd, the chart gives two ways to tridiagonalize H_ϵ, via either flip symmetry or flip-plus-one symmetry (a choice of R_ϵ or S_ϵ); moreover, as mentioned in the last section, when using R_ϵ to tridiagonalize, the sign ϵ for R_ϵ need not correspond with the sign for C_ϵ. In these cases, it turns out the final results are identical up to a flip. Even more curious is the observation that in the q even case, it is impossible to find a flip symmetric solution for $\epsilon = +1$ (periodic case), thus the flip-plus-one symmetry is essential. In the q even, antiperiodic case, flip-plus-one symmetry is impossible, so flip symmetry is forced. The odd q case is much more flexible in symmetrizing than the even case.

5. Explicit tridiagonal forms

Combining the results of the last two sections gives an explicit tridiagonal form for the extreme matrices H_1 and H_{-1} via a good choice of parameters z_1 and z_2 and conjugation by reflections R_ϵ or S_ϵ. The tridiagonalized matrix can be written as a sum $D + T$, where D is the diagonal, and T is the tridiagonal matrix given as either $R_\epsilon(C_\epsilon + C_\epsilon^t)R_\epsilon$ or $S_\epsilon(C_\epsilon + C_\epsilon^t)S_\epsilon$.

The diagonal entries for D can be obtained explicitly by substituting the appropriate values of r from the chart in Section 4 into the formulas $d_k = \lambda \cos 2\pi(pk + r)/q$ and $d_k' = \lambda \cos \pi(2pk + 2r + 1)/q$. After simplification, the resulting diagonal entries are given by the following table:

	$\epsilon = +1$	(periodic)	$\epsilon = -1$	(antiperiodic)
Parity	Flip symmetric	Flip-plus-one	Flip symmetric	Flip-plus-one
p, q odd	$-\lambda \cos \pi(2k-1)p/q$	$\lambda \cos 2\pi(k-1)p/q$	$+\lambda \cos \pi(2k-1)p/q$	$-\lambda \cos 2\pi(k-1)p/q$
p even, q odd	$+\lambda \cos \pi(2k-1)p/q$	$\lambda \cos 2\pi(k-1)p/q$	$-\lambda \cos \pi(2k-1)p/q$	$-\lambda \cos 2\pi(k-1)p/q$
p odd, q even	no sol'n	$\lambda \cos 2\pi(k-1)p/q$	$+\lambda \cos \pi(2k-1)p/q$	no sol'n

It is useful to write out the tridiagonalized matrices fully. For q even, the chart shows only one way to tridiagonalize, so in fact this is the place where some care in needed in forcing symmetry. In the case $\epsilon = +1$, one must force flip-plus-one symmetry so $C_1 + C_1^t$ is tridiagonalized as

$$S_1(C_1 + C_1^t)S_1 = \begin{bmatrix} 0 & \sqrt{2}k^tJ & 0 & 0 \\ \sqrt{2}Jk & M & \sqrt{2}k & 0 \\ 0 & \sqrt{2}k^t & 0 & 0 \\ 0 & 0 & 0 & M \end{bmatrix}.$$

Observing the symmetries of the diagonal entries $d_k = \lambda \cos 2\pi(k-1)p/q$ and the block diagonal form of the above, one obtains

$$q \text{ even}: \quad H_{+1} \cong \begin{bmatrix} d_1 & \sqrt{2} & & & \\ \sqrt{2} & d_2 & 1 & & \\ & 1 & d_3 & \ddots & \\ & & \ddots & \ddots & \sqrt{2} \\ & & & \sqrt{2} & d_{q^*+1} \end{bmatrix} \oplus \begin{bmatrix} d_2 & 1 & & & \\ 1 & d_3 & 1 & & \\ & 1 & d_4 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d_{q^*} \end{bmatrix},$$

where $q^* = q/2$. In the antiperiodic case, one must force flip symmetry so

$$R_{-1}(C_{-1} + C_{-1}^t)R_{-1} = \begin{bmatrix} M + P + JPJ & 0 \\ 0 & M - JPJ - P \end{bmatrix}.$$

Thus with diagonal entries $d'_k = \lambda \cos \pi(2k-1)p/q$, the other extreme matrix is tridiagonalized as

$$q \text{ even}: \quad H_{-1} \cong \begin{bmatrix} d'_1+1 & 1 & & & \\ 1 & d'_2 & 1 & & \\ & 1 & d'_3 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d'_{q^*}-1 \end{bmatrix} \oplus \begin{bmatrix} d'_1-1 & 1 & & & \\ 1 & d'_2 & 1 & & \\ & 1 & d'_3 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d'_{q^*}+1 \end{bmatrix}.$$

For q odd, the chart indicates some choice in how to tridiagonalize; flip symmetry confirms directly the result in [15], so we choose the other possibility for completeness. In the $\epsilon = +1$ case, we force flip-plus-one symmetry so $C_1 + C_1^t$ is tridiagonalized as

$$S_1(C_1 + C_1^t)S_1 = \begin{bmatrix} 0 & \sqrt{2}k^tJ & 0 \\ \sqrt{2}Jk & M+P & 0 \\ 0 & 0 & M - JPJ \end{bmatrix}.$$

Thus with diagonal entries $d_k = \lambda \cos 2\pi(k-1)p/q$, one obtains

$$q \text{ odd}: \quad H_{+1} \cong \begin{bmatrix} d_1 & \sqrt{2} & & & \\ \sqrt{2} & d_2 & 1 & & \\ & 1 & d_3 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d_{q^*}+1 \end{bmatrix} \oplus \begin{bmatrix} d_2 & 1 & & & \\ 1 & d_3 & 1 & & \\ & 1 & d_4 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d_{q^*}-1 \end{bmatrix},$$

where $q^* = (q+1)/2$. In the $\epsilon = -1$ case, forcing flip-plus-one symmetry gives

$$S_{-1}(C_{-1}+C_{-1}^t)S_{-1} = \begin{bmatrix} 0 & -\sqrt{2}k^tJ & 0 \\ -\sqrt{2}Jk & M-P & 0 \\ 0 & 0 & M+JPJ \end{bmatrix}.$$

Thus with diagonal entries $d'_k = -\lambda\cos 2\pi(k-1)p/q$, one obtains

$$q \text{ odd}: \quad H_{-1} \cong \begin{bmatrix} d'_1 & -\sqrt{2} & & & \\ -\sqrt{2} & d'_2 & 1 & & \\ & 1 & d'_3 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d'_{q^*}-1 \end{bmatrix} \oplus \begin{bmatrix} d'_2 & 1 & & & \\ 1 & d'_3 & 1 & & \\ & 1 & d'_4 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & d'_{q^*}+1 \end{bmatrix}.$$

One can verify that forcing flip symmetry instead of flip-plus-one symmetry in the q odd case results in tridiagonal matrices which are the flip transpose of the above tridiagonalizations, thus we obtain nothing new in these alternatives.

REMARK. In numerical calculations, it helps to take any speedups one can find. Thus, since finding the eigenvalues of a $q \times q$ tridiagonal matrix is an order q^2 operation, we can observe that as H_ϵ is made up of two tridiagonal blocks of size about $q/2$ by $q/2$, it is faster (by a factor of two) to compute the eigenvalues of the smaller blocks separately. Moreover, in the case of q odd, the eigenvalues of H_{-1} are just the negatives of H_{+1}, thus it suffices to compute the eigenvalues of just one of the H's. (This can be seen by noting the diagonal coefficients for the two matrices satisfy $d'_k = -d_k$, thus conjugating by a diagonal matrix with alternating $+1, -1$ entries shows H_{-1} is equivalent to the negative of H_{+1}.) In the case of q even, we are not so lucky, as the eigenvalues of H_{+1} and H_{-1} are not directly related. It is true that the eigenvalues of each are symmetric about zero; indeed this is also true of the tridiagonal subblocks. Thus one can see that if μ is an eigenvalue of one block, with eigenvector $(x_1, x_2, \dots, x_n)$, then $-\mu$ is also an eigenvalue, with eigenvector $(-x_n, +x_{n-1}, \dots ; (-1)^n x_1)$. However, it is not known how this information might yield a numerical speedup.

Also important for the numerical calculations is to begin with matrix coefficients that are very accurate. The coefficients 1 and $\sqrt{2}$ are not a problem; however there is a wrong way and a right way to compute the coefficients such as $d_k = \lambda\cos 2\pi(k-1)p/q$. The wrong way is to set $\theta = p/q$, and then compute the number as $d_k = \lambda\cos 2\pi(k-1)\theta$; the problem is that any truncation error in the floating point number θ is amplified by multiplying by $(k-1)$, where k may be a large integer. The right way is to compute an integer $s \equiv (k-1)p \bmod q$ with $0 \le s < q$, which can be done in exact integer arithmetic;

then let $d_k = \lambda \cos(2\pi s/q)$, which can be computed to machine accuracy. It is interesting to contrast this approach with the case of irrational θ, as in [1], where there is no obvious way out of the floating point truncation problem.

These numerical considerations are incorporated into the Matlab code in the appendix, which was written to produce the spectral picture shown in Figure 1. These lines represents a range of line spectra of the almost Mathieu operator, for values of p/q running between 0 and 1, where the denominator is bounded by 25. Matlab is sophisticated enough to automatically use a fast (order q^2) algorithm in finding the eigenvalues of our tridiagonal matrices. The main routine is `PlotAll`, which plots the range of line spectra via calls to the routine `PlotOne`. The routine `PlotOne` plots a single line spectrum for a given value of p/q by computing eigenvalues, sorting them, and drawing lines between the corresponding endpoints/eigenvalues. The routines `Hper` and `Hanti` compute the tridiagonal matrices as two block matrices of size $q/2$ using the results of Section 5, and `gcd` is a useful utility routine. This code is also available at the author's web site.

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Appendix: Matlab code

```
function PlotAll()
% Plots a range of spectra for the almost Mathieu operators,
% theta = p/q ranging between 0 and 1, lambda = 2.

for q = 1:25
    for p = 1:q
        if gcd(p,q) == 1
            PlotOne(p,q,2)
        end
    end
end
```

```
function PlotOne(p,q,lambda)
% Plots the line spectra for one Mathieu operator at theta = p/q
% Variables Xper, Xanti are the sorted eigenvalues of Hper, Hanti.
% In the odd q case, takes a shortcut.

[H1 H2] = Hper(p,q,lambda); Xper = sort([eig(H1);eig(H2)]);
if rem(q,2) = 1
    Xanti = -Xper(q:-1:1);
else
    [H1 H2] = Hanti(p,q,lambda); Xanti = sort([eig(H1);eig(H2)]);
end
line([Xper';Xanti'], [p/q p/q],'Color','w')
```

```
function [H1,H2] = Hper(p,q,lambda)
% Computes two tridiagonal summands for the tridiagonal
% form of the Mathieu operator, periodic case.

if q == 1
    H1 = [2 + lambda]; H2 = [];
elseif q == 2
    H1 = [-lambda 2; 2 lambda]; H2 = [];
elseif rem(q,2) == 0
    q2 = q/2;
    np = rem(0:p:p*q2,q);
    D = lambda*cos(2*pi*np/q);
    C = [sqrt(2) ones(1,q2-2) sqrt(2)];
    H1 =spdiags([ [C 0]' D' [0 C]' ], -1:1, q2+1,q2+1);
    H2 = H1(2:q2,2:q2);
else
    q2 = (q+1)/2;
    np = rem(0:p:p*(q2-1),q);
    D = lambda*cos(2*pi*np/q);
    C = [sqrt(2) ones(1,q2-2)];
    H1 = spdiags([ [C 0]' D' [0 C]' ], -1:1, q2,q2);
    H2 = H1(2:q2,2:q2);
    H1(q2,q2) = H1(q2,q2) + 1;
    H2(q2-1,q2-1) = H2(q2-1,q2-1) -1;
end
```

```
function [H1,H2] = Hanti(p,q,lambda)
% Computes two tridiagonal summands for the tridiagonal
% form of the Mathieu operator, antiperiodic case.

if q == 1
    H1 = [-lambda-2]; H2 = [];
elseif q == 2
    H1 = [0]; H2 = [0];
elseif rem(q,2) == 0
    q2 = q/2;
    np = rem(p:2*p:p*(q-1),2*q);
    D = lambda*cos(pi*np/q);
    C = ones(1,q2);
    H1 = spdiags([ C' D' C' ], -1:1, q2,q2);
    H2 = H1;
    H1(1,1) = H1(1,1) + 1; H1(q2,q2) = H1(q2,q2) - 1;
    H2(1,1) = H2(1,1) - 1; H2(q2,q2) = H2(q2,q2) + 1;
else
    q2 = (q+1)/2;
    np = rem(0:p:p*(q2-1),q);
    D = -lambda*cos(2*pi*np/q);
    C = [-sqrt(2) ones(1,q2-2)];
    H1 = spdiags([ [C 0]' D' [0 C]' ], -1:1, q2,q2);
    H2 = H1(2:q2,2:q2);
    H1(q2,q2) = H1(q2,q2) - 1;
    H2(q2-1,q2-1) = H2(q2-1,q2-1) + 1;
end
```

```
function c = gcd(a,b)
% Greatest Common Divisor of two integers

if (min(a,b) <= 0)
    c = 0;
else
    c = b; r = rem(a,c);
    while (r ~= 0)
        a = c; c = r; r = rem(a,c);
    end
end
```