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ADDITIONAL NUMERICAL AND GRAPHICAL EVIDENCE TO SUPPORT SOME CONJECTURES ON DISCRETE SCHRÖDINGER OPERATORS WITH A MORE GENERAL LONG RANGE CONDITION

SYLVAIN GOLÉNIA AND MARC-ADRIEN MANDICH

ABSTRACT. This document contains additional numerical and graphical evidence to support some of the conjectures mentioned in [GM3]. We give more evidence for $\kappa = 3, 4$ in dimension 2. As mentioned in that article we still don't quite understand the sets $\mu_\kappa(\Delta)$ and $\Theta_\kappa(\Delta)$ on $(0, 1/2)$ for $\kappa = 3$ in dimension 2. Here we give a bunch more threshold energies for $\kappa = 3$ in dimension 2.

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1. INTRODUCTION

The notation in this document is 100% consistent with that of [GM3]. We start by listing the 2 Conjectures of [GM3] for which the material presented in this document is relevant. The first has to do with the rate of convergence of the thresholds $\mathcal{E}_n \in J_2 = J_2(\kappa) := (2 \cos(\pi/\kappa), 1 + \cos(\pi/\kappa))$.

Conjecture 1.1. *Let $\{\mathcal{E}_n\}$ be the sequence in [GM3, Theorem 1.7]. Then $\mathcal{E}_n - \inf J_2 = c(\kappa)/n^2 + o(1/n^2)$, $\forall \kappa \geq 3$, where $c(\kappa)$ means a constant depending on κ .*

For this conjecture, see section 2. The second conjecture has to do with the existence of a conjugate operator giving a strict Mourre estimate on bands $(\mathcal{E}_n, \mathcal{E}_{n-1}) \subset J_2$.

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Conjecture 1.2. Fix $\kappa \geq 2$. Let $\{\mathcal{E}_n\}$ be the sequence in [GM3, Theorem 1.7]. For each interval $(\mathcal{E}_n, \mathcal{E}_{n-1})$, $n \geq 1$, \exists a conjugate operator $\mathbb{A}(n) = \sum_{q=1}^{N(n)} \rho_{j_q \kappa}(n) A_{j_q \kappa}$, $A_{j_q \kappa} = \sum_{1 \leq i \leq 2} A_i(j_q, \kappa)$, such that the Mourre estimate for Δ holds wrt. $\mathbb{A}(n)$, $\forall E \in (\mathcal{E}_n, \mathcal{E}_{n-1})$. $\mathbb{A}(n)$ is typically not unique. It can be chosen so that $N(n) = 2n$. In particular, $\{\mathcal{E}_n\} = J_2 \cap \Theta_\kappa(\Delta)$, $\forall \kappa \geq 2$.

For this conjecture, see sections 5, 6, 7 and 8. Section 4 lists some thresholds $\in \Theta_{m=1, \kappa=4}(\Delta)$ in dimension 2, and section 9 gives a graphical illustration of some thresholds $\in \Theta_{m, \kappa=3}(\Delta) \cap (0, 1/2)$ in dimension 2, $m \geq 1$.

2. MORE EVIDENCE FOR THE CONJECTURE ON THE RATE OF CONVERGENCE OF \mathcal{E}_n

Figure 1 illustrates solutions $\mathcal{E}_{2n}(\kappa)$ of [GM3, Proposition 7.2] for $\kappa = 5, 6, 8$. In these graphs the slope of the orange trend line is close to -2 , and this is our rationale behind [GM3, Conjecture 1.9].

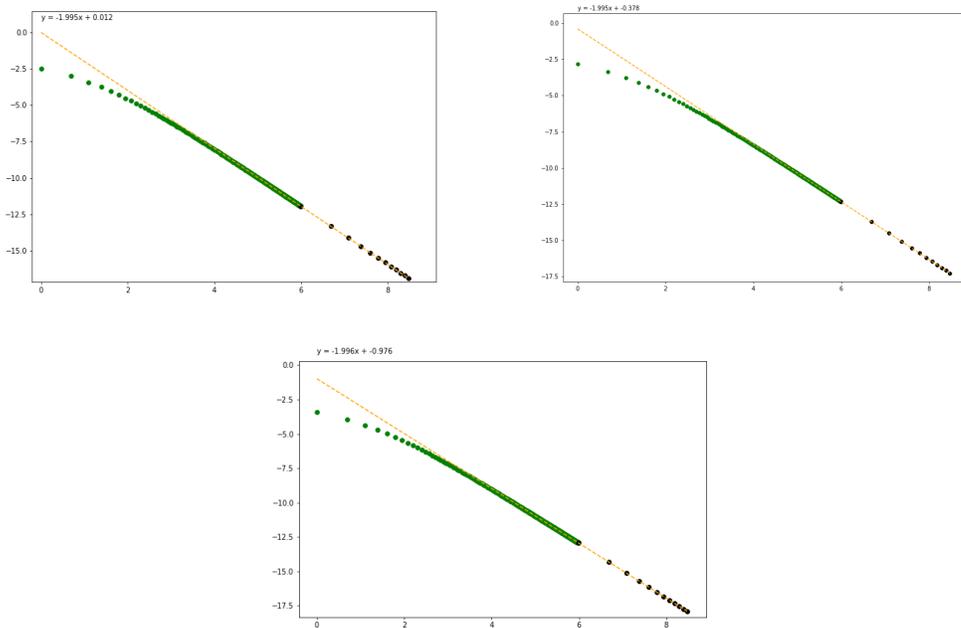


FIGURE 1. Graphs with $\log(n)$ on x -axis and $\log(\mathcal{E}_{2n}(\kappa) - 2 \cos(\pi/\kappa))$ on y -axis. Left : $\kappa = 5$; Middle : $\kappa = 6$, Right : $\kappa = 8$. Green dots are $1 \leq n \leq 400$; black dots are $n = 400, 800, 1200, \dots, 4800$. Orange line is trend line based on linear regression of black dots.

3. ENERGY SOLUTIONS IN $J_2(\kappa) := (2 \cos(\pi/\kappa), 1 + \cos(\pi/\kappa))$

Table 1 below lists the first few energy solutions for $\kappa \in \{2, 3, 4\}$ in [GM3, Theorem 1.7]. In particular we have some exact expressions for $\kappa = 4$.

κ	\mathcal{E}_5	\mathcal{E}_4	\mathcal{E}_3	\mathcal{E}_2	\mathcal{E}_1	\mathcal{E}_0
2	2/7	1/3	2/5	1/2	2/3	1
3	$\simeq 1.112$	$\simeq 1.137$	$\simeq 1.173$	$\frac{9+\sqrt{33}}{12} \simeq 1.228$	$\frac{5+3\sqrt{2}}{7} \simeq 1.320$	3/2
4	(7.4) $\simeq 1.476$	$\simeq 1.491$	(7.3) $\simeq 1.512$	(7.2) $\simeq 1.545$	8/5	$1 + 1/\sqrt{2} \simeq 1.707$

TABLE 1. First values of $\{\mathcal{E}_n\}$ in [GM3, Theorem 1.7]. Δ in dimension 2. $\kappa = 2, 3, 4$.

4. THRESHOLDS IN DIMENSION 2, FOR $\kappa = 4$, $m = 1$ (THE BRUTE FORCE APPROACH)

In [GM3, subsection 4.2], we listed Ansatzes (1) – (6) to find threshold solutions $\in \Theta_{1,\kappa}(\Delta)$, and in [GM3, Lemma 4.2] we listed those solutions for $\kappa = 3$. Table 2 below lists the corresponding solutions for $\kappa = 4$. We recall that these solutions belong to $\Theta_{1,\kappa=4}(\Delta)$, but it is an open question for us if they constitute all of $\Theta_{1,\kappa=4}(\Delta)$.

κ	4
(1)	$E = 1/2 + 1/(2\sqrt{2}) \simeq 0.853, Y_1 = \sqrt{2}/2$ $E = \frac{2+\sqrt{2}+\sqrt{2+4\sqrt{2}}}{4} \simeq 1.545, Y_1 = \sqrt{2}/2$ $E = \frac{2+\sqrt{2}-\sqrt{2+4\sqrt{2}}}{4} \simeq 0.161, Y_1 = \sqrt{2}/2$ $E = 1/2 - 1/(2\sqrt{2}) \simeq 0.146, Y_1 = -\sqrt{2}/2$ $E = 8/5 = 1.6, Y_1 = E/2 = 0.8$
(2)	
(3)	$E = \sqrt{2/5} \simeq 0.632, Y_1 = 3/\sqrt{10} \simeq 0.948$ $E = \sqrt{2}/3 \simeq 0.471, Y_1 = \sqrt{2}/2$
(4)	$E = 2/\sqrt{5} \simeq 0.894, Y_1 = 0, Y_0 = E/2 \simeq 0.447$ $E = 1/\sqrt{5} \simeq 0.447, Y_1 = 0, Y_0 = 2E \simeq 0.894$ $E = (\sqrt{3} - 1)/(2\sqrt{2}) \simeq 0.258, Y_1 = 0, Y_0 = -\sqrt{2}/2$ $E = 1/(2\sqrt{2}) \simeq 0.353, Y_1 = 0, Y_0 = 1/\sqrt{2}$ $E = (\sqrt{2} + \sqrt{6})/4 \simeq 0.965, Y_1 = 0, Y_0 = 1/\sqrt{2}$ $E = 3\sqrt{2}/5 \simeq 0.848, Y_1 = 1/\sqrt{2}, Y_0 = 7/(5\sqrt{2}) \simeq 0.989$ $E = \sqrt{2}/5 \simeq 0.282, Y_1 = -1/\sqrt{2}, Y_0 = E/2 \simeq 0.141$
(5)	
(6)	

TABLE 2. Solutions to (i), $1 \leq i \leq 6$, in [GM3, subsection 4.2] for $\kappa = 4$.

5. POLYNOMIAL INTERPOLATION FOR THE CASE $\kappa = 2$ IN DIMENSION 2, $5 \leq n \leq 9$

In [GM3, section 13] we gave numerical evidence of bands of a.c. spectrum for bands $n = 1, 2, 3, 4$, for $\kappa = 2$ in dimension 2. We briefly mention that :

- For the 5th band, we checked that $\Sigma = [2, 4, 6, 8, 10, 12, 14, 16, \alpha, \beta]$ is also valid for $(\alpha, \beta) = (18, 20), (20, 24), (22, 24), (24, 28), (24, 32), (28, 32)$ whereas it is not valid for $(\alpha, \beta) = (18, 24), (18, 26), (18, 28)$.

- For the 6th band we checked that $\Sigma = [2, 4, 6, 8, 10, 12, 14, 16, 18, 20, \alpha, \beta]$ is valid for $(\alpha, \beta) = (22, 28), (22, 30)$ but not valid for $(\alpha, \beta) = (22, 24), (22, 26)$.
- For the 7th band we checked that $\Sigma = [2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, \alpha, \beta]$ is valid for $(\alpha, \beta) = (26, 28)$ but not valid for $(\alpha, \beta) = (28, 36)$.
- For the 8th band we checked that $\Sigma = [2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, \alpha, \beta]$ is valid for $(\alpha, \beta) = (30, 38), (30, 40)$ but not valid for $(\alpha, \beta) = (30, 32), (30, 36)$.
- For the 9th band we checked $\Sigma = [2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36]$ is valid.

6. POLYNOMIAL INTERPOLATION FOR THE CASE $\kappa = 3$ IN DIMENSION 2, $n = 5$

In [GM3, section 14] we gave numerical evidence of bands of a.c. spectrum for bands $n = 1, 2, 3, 4$, for $\kappa = 3$ in dimension 2. We briefly give the numerical details for $n = 5$, i.e. the 5th band. $X_3 = \mathcal{E}_5/2$ and

$$\begin{cases} T_3(\mathcal{E}_5 - 1) = T_3(\mathcal{E}_5 - X_1) \\ T_3(X_1) = T_3(\mathcal{E}_5 - X_2) \\ T_3(X_2) = T_3(\mathcal{E}_5/2) \end{cases} \Rightarrow \begin{cases} 4[(\mathcal{E}_5 - 1)^2 + (\mathcal{E}_5 - 1)(\mathcal{E}_5 - X_1) + (\mathcal{E}_5 - X_1)^2] = 3 \\ 4[X_1^2 + X_1(\mathcal{E}_5 - X_2) + (\mathcal{E}_5 - X_2)^2] = 3 \\ 4[X_2^2 + X_2(\mathcal{E}_5/2) + (\mathcal{E}_5/2)^2] = 3. \end{cases}$$

Using Python's *fsolve* we get $[\mathcal{E}_5, X_1, X_2] \simeq [1.112, 0.307, 0.441]$. For an analytical solution or perhaps more precise, expand the equations and get rid of the X_1^2 and X_2^2 terms. One ends up with $4(9\mathcal{E}_5^2/4 - 4\mathcal{E}_5X_1 + X_1X_2 - 3\mathcal{E}_5 + 1 + 5\mathcal{E}_5X_2/2 + X_1) = 3$. Then use the fact that

$$X_1 = -\frac{1}{2} + \frac{3\mathcal{E}_5}{2} - \frac{\sqrt{3}}{2}\sqrt{\mathcal{E}_5(2 - \mathcal{E}_5)}, \quad X_2 = -\frac{\mathcal{E}_5}{4} + \frac{\sqrt{3}}{4}\sqrt{4 - \mathcal{E}_5^2}.$$

(signs are chosen based on numerical solution). We get an equation in \mathcal{E}_5 only, which is

$$\begin{aligned} 0 = & -(35\mathcal{E}_5^2)/8 + \left(3\mathcal{E}_5 - \sqrt{3}\sqrt{(2 - \mathcal{E}_5)\mathcal{E}_5} - 1\right) \left((1/8)\sqrt{3}\sqrt{4 - \mathcal{E}_5^2} - \mathcal{E}_5/8\right) \\ & + (5/8)\sqrt{3}\mathcal{E}_5\sqrt{4 - \mathcal{E}_5^2} + 2\sqrt{3}\mathcal{E}_5\sqrt{(2 - \mathcal{E}_5)\mathcal{E}_5} + \mathcal{E}_5/2 - 1/2\sqrt{3}\sqrt{(2 - \mathcal{E}_5)\mathcal{E}_5} - 1/4. \end{aligned}$$

\mathcal{E}_5 is a root of

$$mp(E) = 372775E^8 - 750010E^7 + 536359E^6 - 270784E^5 + 128593E^4 - 36442E^3 + 4333E^2 - 220E + 4.$$

and we suspect it's its minimal polynomial. $\mathcal{E}_5 \simeq 1.11207$. We are not aware of a closed formula for \mathcal{E}_5 . It follows that $X_1 \simeq 0.30753$, $X_2 \simeq 0.44178$, $X_3 \simeq 0.55603$, $X_4 \simeq 0.67028$, $X_5 \simeq 0.80453$.

Next we suppose $\Sigma = [3, 6, 9, 12, 15, 18, 21, 24, 27, 30]$. We fill the matrix M with floats. Python says the solution to $M\rho = 0$ is $[\rho_3, \rho_6, \rho_9, \rho_{12}, \rho_{15}, \rho_{18}, \rho_{21}, \rho_{24}, \rho_{27}, \rho_{30}]^T$ equals

$$\simeq [1, 1.599931, 1.645307, 1.27734, 0.77838, 0.37292, 0.13741, 0.03703, 0.00657, 0.00058]^T.$$

Graphically it seems $x \mapsto G_\kappa^E(x) > 0$ for $E \in (\mathcal{E}_5, \mathcal{E}_4)$, $x \in [E - 1, 1]$. So Σ is valid.

7. POLYNOMIAL INTERPOLATION FOR THE CASE $\kappa = 4$ IN DIMENSION 2, $1 \leq n \leq 6$

This section is the analogue of [GM3, section 13] and [GM3, section 14], but for $\kappa = 4$.

First we note that

$$(7.1) \quad T_4(x) = 8x^4 - 8x^2 + 1 \quad \text{and} \quad T_4(x) = T_4(y) \Leftrightarrow 8(x - y)(x + y)[x^2 + y^2 - 1] = 0.$$

Let \mathcal{E}_n be the energy solutions of [GM3, Proposition 7.1] and [GM3, Proposition 7.2], for $\kappa = 4$. We have : $\mathcal{E}_n \in J_2(\kappa = 4) = (2 \cos(\pi/4), 1 + \cos(\pi/4)) = (\sqrt{2}, 1 + \sqrt{2}/2)$, and

$$\mathcal{E}_n - 1 = X_0 < X_1 < X_2 < \dots < X_n < X_{n+1} := 1.$$

7.1. $n = 1$: **1st band**. On the left, $\mathcal{E}_1 = 8/5$, $X_1 = 4/5$. On the right, $\mathcal{E}_0 = 1 + \cos(\frac{\pi}{4}) = 1 + \frac{\sqrt{2}}{2}$. We choose $\Sigma = [4, 8]$ and get $\rho = [\rho_4, \rho_8]^T = [1, 625/1054]^T$. The function $x \mapsto G_{\kappa}^E(x)$ is strictly positive for $E \in (\mathcal{E}_1, \mathcal{E}_0)$, $x \in [E - 1, 1]$.

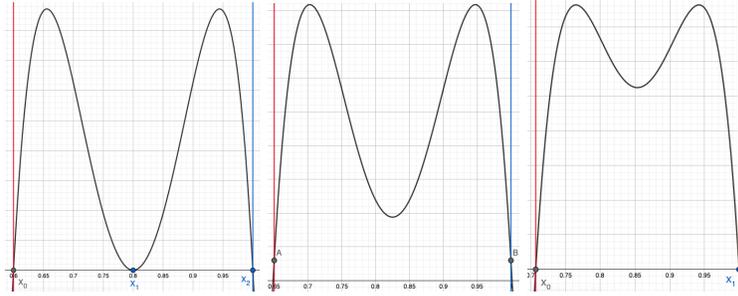


FIGURE 2. $G_{\kappa=4}^E(x)$. $x \in [E - 1, 1]$. From left to right: $E = \mathcal{E}_1$, $E = 1.65$, $E = \mathcal{E}_0$. $G_{\kappa=4}^E(x) > 0$ in the middle picture, but not in the other two.

7.2. $n = 2$: **2nd band**. $X_1 = \sqrt{2}/2$. Then we solve $T_4(\mathcal{E}_2 - 1) = T_4(\mathcal{E}_2 - \sqrt{2}/2)$ which has 2 solutions $\mathcal{E}_2 = (2 + \sqrt{2} \pm \sqrt{2 + 4\sqrt{2}})/4$. Using the context, it must be that

$$(7.2) \quad \mathcal{E}_2 = \frac{2 + \sqrt{2} + \sqrt{2 + 4\sqrt{2}}}{4} \simeq 1.54532.$$

It follows that $X_2 = \mathcal{E}_2 - X_1 = (2 - \sqrt{2} + \sqrt{2 + 4\sqrt{2}})/4$. We suppose $\Sigma = [4, 8, 12, 24]$. The solution to $M\rho = 0$ is $[\rho_4, \rho_8, \rho_{12}, \rho_{24}]^T \simeq [1, 0.81070, 0.21647, -0.06593]^T$. The function $x \mapsto G_{\kappa}^E(x)$ is plotted in Figure 3 for some values $E \in [\mathcal{E}_2, \mathcal{E}_1]$.

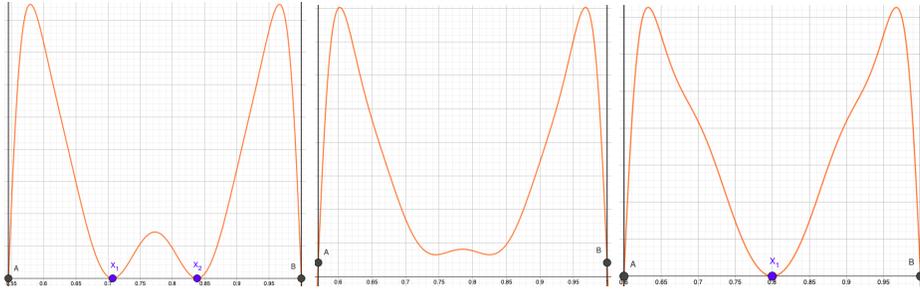


FIGURE 3. $G_{\kappa=4}^E(x)$. $x \in [E - 1, 1]$. From left to right: $E = \mathcal{E}_2$, $E = 1.57$, $E = \mathcal{E}_1$. $G_{\kappa=4}^E(x) > 0$ in the middle picture, but not in the other two.

Moreover it would appear that the combinations $\Sigma = [4, 8, 12, 28], [4, 8, 12, 32], [4, 8, 16, 24]$ are equally valid, whereas $\Sigma = [4, 8, 12, 16], [4, 8, 12, 20], [4, 8, 16, 20]$ are not valid. The linear dependency between rows of M seems to rely (at least partly) on the relations

$$U_{4j-1}(1/\sqrt{2}) = 0, \quad \text{and} \quad U_{4j-1}(\sqrt{2}/\sqrt{3}) = -\sqrt{2}U_{4j-1}(1/\sqrt{3}), \quad j \in \mathbb{N}^*.$$

7.3. $n = 3$: **3rd band**. $X_2 = \mathcal{E}_3/2$ and $T_4(\mathcal{E}_3 - 1) = T_4(\mathcal{E}_3 - X_1)$, $T_4(X_1) = T_4(\mathcal{E}_3/2)$. Taking the context into account and applying (7.1) leads to $(\mathcal{E}_3 - 1)^2 + (\mathcal{E}_3 - X_1)^2 = 1$ and $X_1^2 + \mathcal{E}_3^2/4 = 1$. So

$$(7.3) \quad \mathcal{E}_3 = \frac{28}{65} + \frac{2}{65t} + \frac{1}{2} \sqrt{\frac{4256}{12675} + \frac{368}{195s} - \frac{16}{195}s + \frac{121088t}{4225}} \simeq 1.51271, \quad t := \sqrt{\frac{3}{133 - \frac{1495}{s} + 65s}}$$

and $s := (629 + 48\sqrt{177})^{1/3}$. The minimal polynomial for \mathcal{E}_3 is $mp(E) = 65E^4 - 112E^3 + 56E^2 - 64E + 16$. Also $X_1 \simeq 0.65415$, $X_2 \simeq 0.75635$. We choose the combination $\Sigma = [4, 8, 12, 16, 24, 36]$. The solution to $M\rho = 0$ is

$$[\rho_4, \rho_8, \rho_{12}, \rho_{16}, \rho_{24}, \rho_{36}]^T \simeq [1, 1.18290, 0.68875, 0.18594, -0.00794, -0.00288]^T.$$

The function $G_\kappa^E(x)$ is plotted in Figure 4 for some values $E \in [\mathcal{E}_3, \mathcal{E}_2]$. The linear dependency between rows of M seems to rely (at least partly) on the relation

$$\left[U_{4j-1}(x), U_{4l-1}(\sqrt{1-x^2}) \right] = 0, \quad \forall j, l \in \mathbb{N}^*,$$

where $[\cdot, \cdot]$ is the Bezoutian defined by [GM3, (2.3) of section 2].

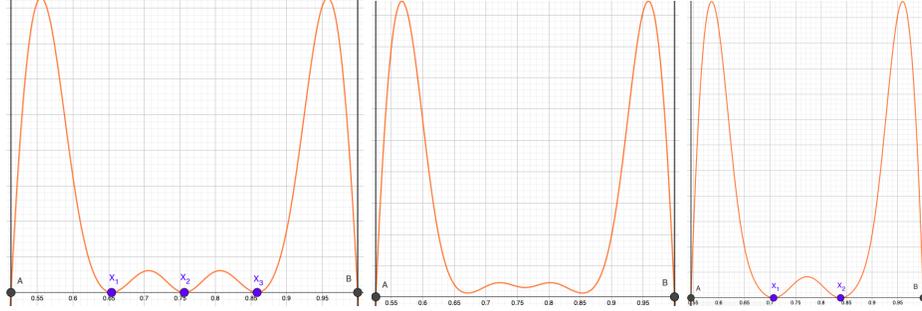


FIGURE 4. $G_{\kappa=4}^E(x)$. $x \in [E - 1, 1]$. From left to right: $E = \mathcal{E}_3$, $E = 1.525$, $E = \mathcal{E}_2$. $G_{\kappa=4}^E(x) > 0$ in the middle picture, but not in the other two.

The combination $\Sigma = [4, 8, 12, 16, 20, 24]$ is equally valid and it gives

$$[\rho_4, \rho_8, \rho_{12}, \rho_{16}, \rho_{20}, \rho_{24}]^T \simeq [1, 1.37002, 1.06973, 0.53992, 0.16964, 0.02655]^T.$$

7.4. $n = 4$: **4th band**. $X_2 = \sqrt{2}/2$. Then we have to solve $(\mathcal{E}_4 - 1)^2 + (\mathcal{E}_4 - X_1)^2 = 1$, $X_1^2 + (\mathcal{E}_4 - \sqrt{2}/2)^2 = 1$. This leads to $1 - (\mathcal{E}_4 - \sqrt{2}/2)^2 = (\mathcal{E}_4 - \sqrt{\mathcal{E}_4(2 - \mathcal{E}_4)})^2$. Thus \mathcal{E}_4 is the root of

$$mp(E) = 5E^4 - (2\sqrt{2} + 4)E^3 + (5 - 4\sqrt{2})E^2 + (\sqrt{2} - 2)E + 1/4 = 0.$$

The closed form formula of \mathcal{E}_4 is horrendous; but $\mathcal{E}_4 \simeq 1.49137$. In turn, $X_1 \simeq 0.62042$.

The simplest valid combination of indices we have found is $\Sigma = [4, 8, 12, 16, 20, 24, 28, 52]$. The solution to $M\rho = 0$ is $\rho = [\rho_4, \rho_8, \rho_{12}, \rho_{16}, \rho_{20}, \rho_{24}, \rho_{28}, \rho_{52}]^T \simeq$

$$[1, 1.46864, 1.29941, 0.80098, 0.34657, 0.09808, 0.01417, 0.000030]^T.$$

Graphically $x \mapsto G_\kappa^E(x)$ is strictly positive for $E \in (\mathcal{E}_4, \mathcal{E}_3)$, $x \in [E - 1, 1]$.

7.5. $n = 5$: **5th band**. We have $X_3 = \mathcal{E}_5/2$, $(\mathcal{E}_5 - 1)^2 + (\mathcal{E}_5 - X_1)^2 = 1$, $X_1^2 + (\mathcal{E}_5 - X_2)^2 = 1$, and $X_2^2 + (\mathcal{E}_5/2)^2 = 1$. This leads to $1 - (\mathcal{E}_5 - (1 - \mathcal{E}_5^2/4)^{1/2})^2 = (\mathcal{E}_5 - \mathcal{E}_5^{1/2}(2 - \mathcal{E}_5)^{1/2})^2$. The solution is

$$(7.4) \quad \mathcal{E}_5 = \frac{16}{1275} \left(42 + \frac{w}{3^{2/3}} - \frac{32533w^{-1}}{3^{1/3}} \right) \simeq 1.47650, \quad w := (13025367 + 208250\sqrt{6294})^{1/3}$$

and its minimal polynomial is $mp(E) = -32768 + 22784E - 6048E^2 + 3825E^3$. In turn $X_1 \simeq 0.59734$, $X_2 \simeq 0.67452$, $X_3 \simeq 0.73825$, $X_4 \simeq 0.80198$ and $X_5 \simeq 0.87916$. We choose $\Sigma = [4, 8, 12, 16, 20, 24, 28, 32, 36, 40]$. $M\rho = 0$ gives $[\rho_4, \rho_8, \rho_{12}, \rho_{16}, \rho_{20}, \rho_{24}, \rho_{28}, \rho_{32}, \rho_{36}, \rho_{40}]^T \simeq$

$$[1, 1.58691, 1.60962, 1.22543, 0.72779, 0.33759, 0.11956, 0.03071, 0.00514, 0.00042]^T.$$

It appears graphically that $x \mapsto G_\kappa^E(x)$ is strictly positive for $E \in (\mathcal{E}_5, \mathcal{E}_4)$, $x \in [E - 1, 1]$.

7.6. $n = 6$: **6th band**. $X_3 = \sqrt{2}/2$, $(\mathcal{E}_6 - 1)^2 + (\mathcal{E}_6 - X_1)^2 = 1$, $X_1^2 + (\mathcal{E}_6 - X_2)^2 = 1$ and $X_2^2 + (\mathcal{E}_6 - \sqrt{2}/2)^2 = 1$. Performing elementary operations shows that $\mathcal{E}_6 \simeq 1.46568$ is a root of the polynomial

$$mp(E) = 384E^6 + (-448 - 224\sqrt{2})E^5 + (200 + 128\sqrt{2})E^4 + (-72 - 52\sqrt{2})E^3 + (16 + 12\sqrt{2})E^2 + (-2 - \sqrt{2})E + 1/8.$$

In turn $X_1 \simeq 0.58072$, $X_2 \simeq 0.65158$, $X_3 \simeq 0.70710$, $X_4 \simeq 0.75857$, $X_5 \simeq 0.81409$, $X_6 \simeq 0.88495$.

8. APPLICATION OF POLYNOMIAL INTERPOLATION FOR THE FIRST BAND ($n = 1$), $2 \leq \kappa \leq 9$

This section is about the first band ($n = 1$) in the interval $J_2(\kappa)$. For the 1st band we suppose only 2 terms in the linear combination [GM3, (1.6) of Introduction] are required. In other words, we suppose $\Sigma = [j_1\kappa, j_2\kappa]$. According to [GM3, section 12] we look to solve the system

$$(8.1) \quad \begin{cases} g_{j_1\kappa}^{\mathcal{E}_1}(x) + \rho_{j_2\kappa} \cdot g_{j_2\kappa}^{\mathcal{E}_1}(x) = 0, & \text{at } x = X_0 = \mathcal{E}_1 - 1, \\ g_{j_1\kappa}^{\mathcal{E}_1}(x) + \rho_{j_2\kappa} \cdot g_{j_2\kappa}^{\mathcal{E}_1}(x) = 0, & \text{at } x = X_1, \\ \frac{d}{dx}g_{j_1\kappa}^{\mathcal{E}_1}(x) + \rho_{j_2\kappa} \cdot \frac{d}{dx}g_{j_2\kappa}^{\mathcal{E}_1}(x) = 0, & \text{at } x = X_1, \\ g_{j_1\kappa}^{\mathcal{E}_0}(x) + \rho_{j_2\kappa} \cdot g_{j_2\kappa}^{\mathcal{E}_0}(x) = 0, & \text{at } \mathcal{E}_0 = 1 + \cos(\pi/\kappa), x = \mathcal{E}_0 - 1. \end{cases}$$

Note we are assuming $\rho_{j_1\kappa} = 1$. By [GM3, Remark 5.2], $X_1 = \mathcal{E}_1/2$. So the 3rd line of (8.1) is trivially true, by [GM3, Lemma 3.4]. The 4th line is also always true, by [GM3, Lemma 1.4]. Assuming $\mathcal{E}_1 \neq 0, \pm 2$, the system (8.1) is equivalent to

$$(8.2) \quad \begin{cases} [U_{j_1\kappa-1}(\mathcal{E}_1 - 1), U_{j_2\kappa-1}(\mathcal{E}_1/2)] = 0, \\ X_1 = \mathcal{E}_1/2, \\ \rho_{j_2\kappa} = -U_{j_1\kappa-1}(\mathcal{E}_1 - 1)/U_{j_2\kappa-1}(\mathcal{E}_1 - 1) = -U_{j_1\kappa-1}(\mathcal{E}_1/2)/U_{j_2\kappa-1}(\mathcal{E}_1/2). \end{cases}$$

Let $X_2 := 1$, $X_0 = \mathcal{E}_1 - X_2 = \mathcal{E}_1 - 1$. From the 3rd line of (8.2) we see that we want $U_{j_1\kappa-1}(X_0) \neq 0$ and $U_{j_2\kappa-1}(X_1) \neq 0$, in particular $U_{\kappa-1}(X_0), U_{\kappa-1}(X_1) \neq 0$. Thus, by [GM3, Corollary 2.3] we see that (8.2) is equivalent to

$$(8.3) \quad \begin{cases} X_2 = 1, \\ X_0 = \mathcal{E}_1 - X_2, \\ X_1 = \mathcal{E}_1/2, \\ T_\kappa(X_0) = T_\kappa(X_1), \\ \rho_{j_2\kappa} = -U_{j_1\kappa-1}(\mathcal{E}_1 - 1)/U_{j_2\kappa-1}(\mathcal{E}_1 - 1) = -U_{j_1\kappa-1}(\mathcal{E}_1/2)/U_{j_2\kappa-1}(\mathcal{E}_1/2). \end{cases}$$

This is in agreement with [GM3, (5.1) of section 5] for $n = 1$. In practice, our assessment is that it is best to simply take $\Sigma = \{j_1\kappa, j_2\kappa\} = \{\kappa, 2\kappa\}$. Table 3 lists the results for $\kappa \in \{2, \dots, 9\}$.

κ	Solution to (8.3)	κ	Solution to (8.3)
2	$\mathcal{E}_1 = \frac{2}{3}$	3	$\mathcal{E}_1 = \frac{5+3\sqrt{2}}{7} \simeq 1.3203$
2	$\rho_4 = \frac{9}{14} \simeq 0.6428$	3	$\rho_6 = \frac{170-81\sqrt{2}}{92} \simeq 0.6027$
4	$\mathcal{E}_1 = \frac{8}{5}$	5	$\mathcal{E}_1 = \frac{49+12\sqrt{10}+\sqrt{5(49+12\sqrt{10})}}{62} \simeq 1.7386$
4	$\rho_8 = \frac{625}{1054} \simeq 0.5929$	5	$\rho_{10} = \frac{-4000073+2667375\sqrt{2}+225\sqrt{5(25786331-6299370\sqrt{2})}}{3122396} \simeq 0.5889$
6	$\mathcal{E}_1 = 1 + \sqrt{\frac{2}{3}} \simeq 1.8164$	7	$\mathcal{E}_1 \simeq 1.8642$ (closed form unknown to us)
6	$\rho_{12} = \frac{27}{46} \simeq 0.5869$	7	$\rho_{14} \simeq 0.5857$
8	$\mathcal{E}_1 = \frac{16+3\sqrt{2}+2\sqrt{26+7\sqrt{2}}}{17}$	9	$\mathcal{E}_1 \simeq 1.9173$ (closed form unknown to us)
8	$\mathcal{E}_1 \simeq 1.8956$		
8	$\rho_{16} \simeq 0.5850$	9	$\rho_{18} \simeq 0.5844$

TABLE 3. Solutions to (8.3). $\mathcal{E}_1 = 1st$ band's left endpoint.9. ENERGY THRESHOLDS IN $(0, 1/2)$ FOR $\kappa = 3$ IN DIMENSION 2

Fix $\kappa = 3$, in dimension 2. We construct graphically a bunch of thresholds in $(0, 1/2)$. Recall that by [GM3, Lemma 5.3], $\mathfrak{T}_{n,\kappa} = -\mathfrak{T}_{n,\kappa}$, or by [GM3, Lemma 3.2], $\Theta_\kappa(\Delta) = -\Theta_\kappa(\Delta)$. So the negative thresholds listed below have a positive counterpart.

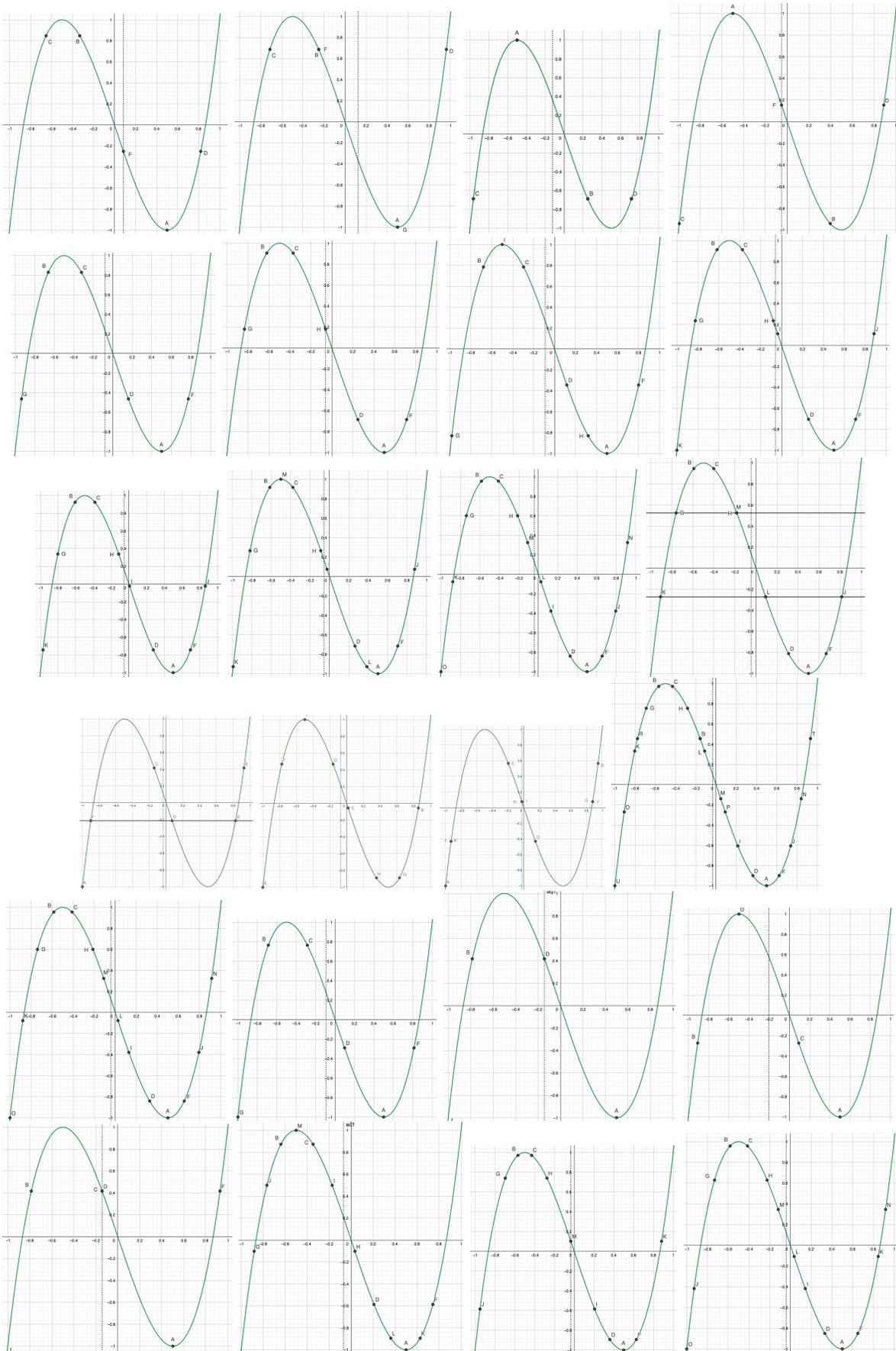


FIGURE 5

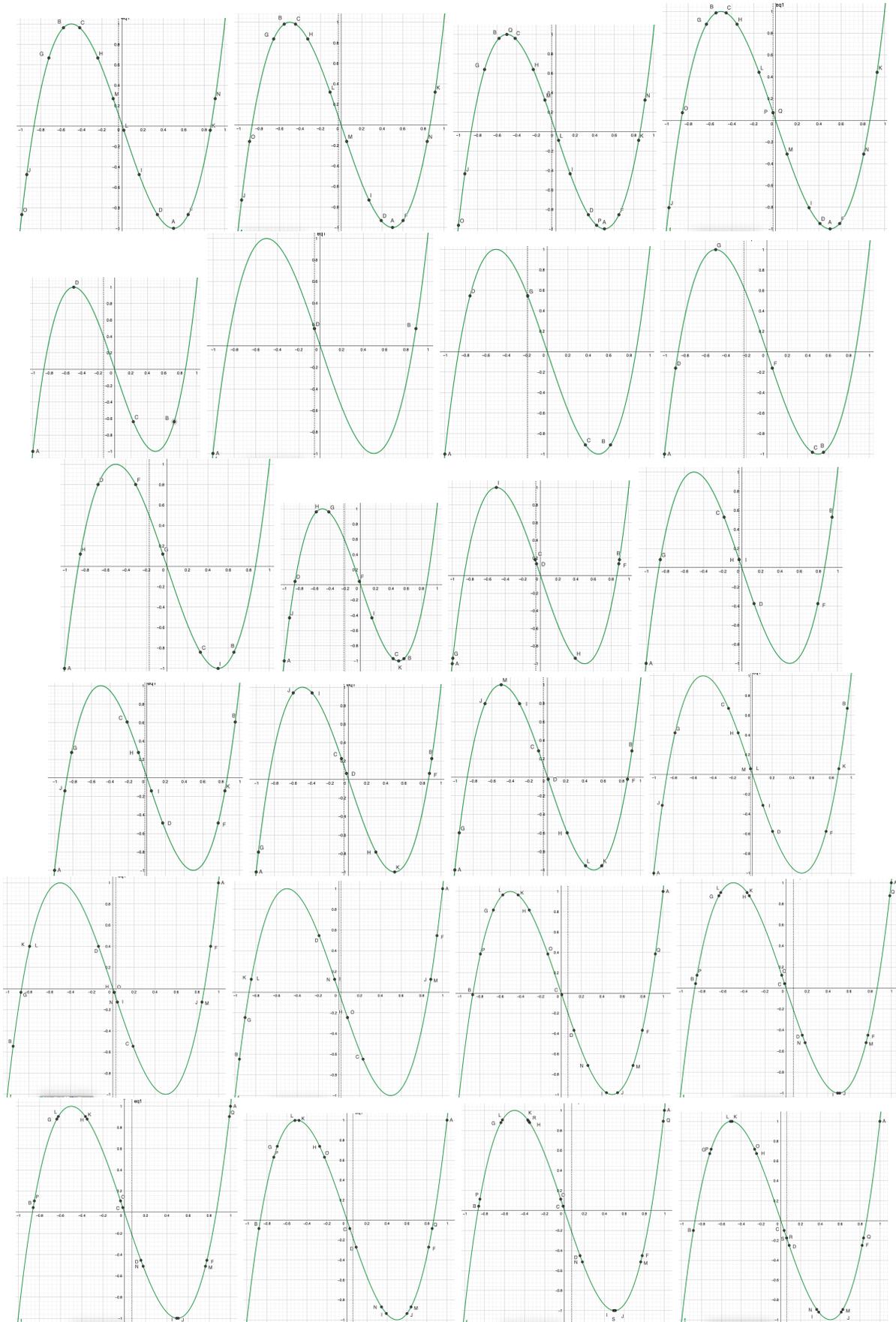


FIGURE 6

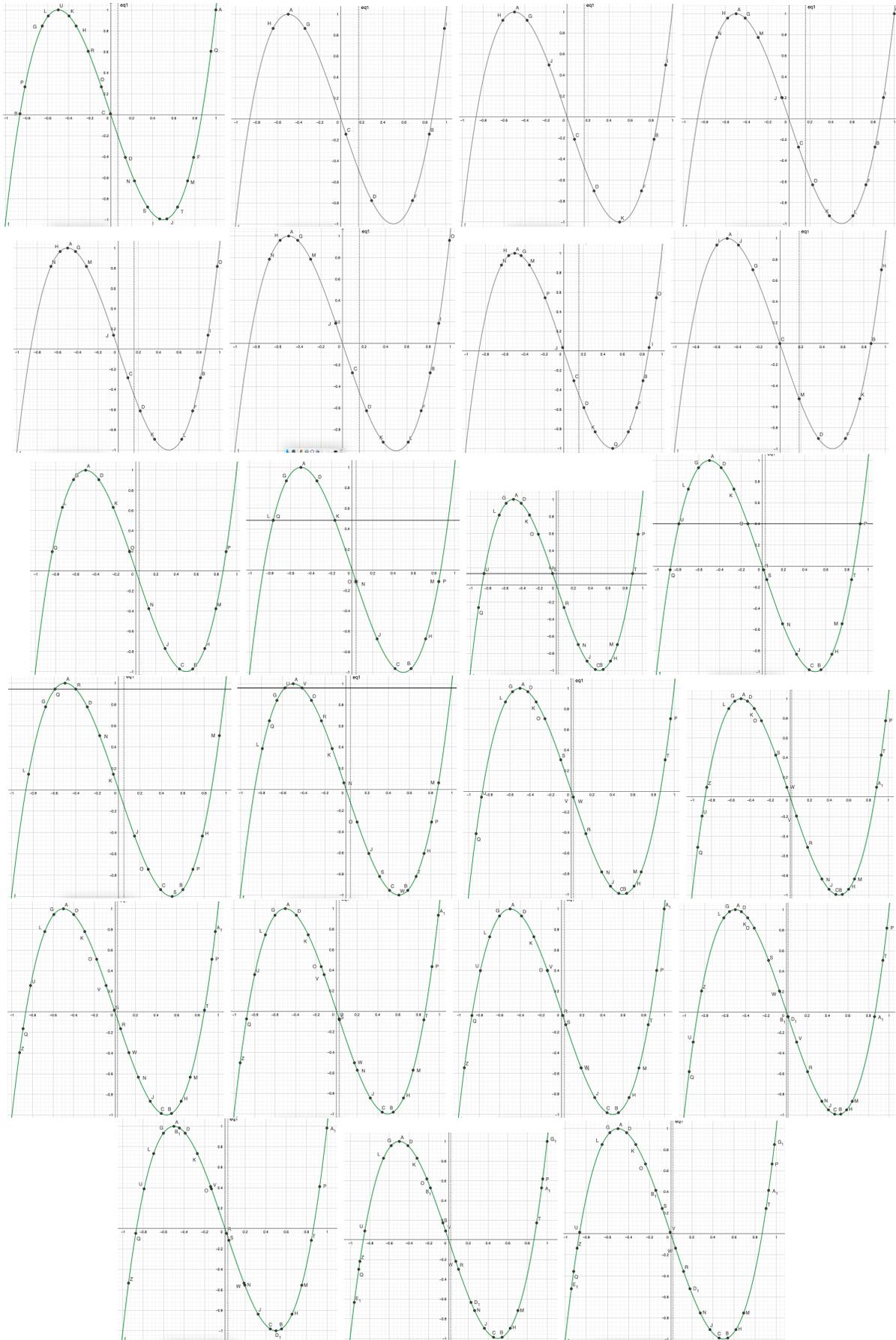


FIGURE 7

- 1) $\mathcal{E} \simeq 0.169$.
- 2) $\mathcal{E} = 0.25$.
- 3) $\mathcal{E} = -0.25$.
- 4) $\mathcal{E} \simeq -0.1028$.
- 5) $\mathcal{E} \simeq -0.16019$.
- 6) $\mathcal{E} \simeq -0.1202$.
- 7) $\mathcal{E} \simeq -0.17911$.
- 8) $\mathcal{E} \simeq -0.11608$.
- 9) $\mathcal{E} \simeq -0.10796$.
- 10) $\mathcal{E} \simeq -0.11385$.
- 11) $\mathcal{E} \simeq -0.08425$.
- 12) $\mathcal{E} \simeq -0.0917$.
- 13) $\mathcal{E} \simeq -0.07143$.
- 14) $\mathcal{E} \simeq -0.14325$.
- 15) $\mathcal{E} \simeq -0.05169$.
- 16) $\mathcal{E} \simeq -0.06615$.
- 17) $\mathcal{E} \simeq -0.08424$.
- 18) $\mathcal{E} \simeq -0.18726$.
- 19) $\mathcal{E} \simeq -0.2857$.
- 20) $\mathcal{E} \simeq -0.40824$.
- 21) $\mathcal{E} \simeq -0.2857$.
- 22) $\mathcal{E} \simeq -0.13911$.
- 23) $\mathcal{E} \simeq -0.06805$.
- 24) $\mathcal{E} \simeq -0.0813$.
- 25) $\mathcal{E} \simeq -0.07704$.
- 26) $\mathcal{E} \simeq -0.05406$.
- 27) $\mathcal{E} \simeq -0.08014$.
- 28) $\mathcal{E} \simeq -0.04594$.
- 29) $\mathcal{E} \simeq -0.27129$.
- 30) $\mathcal{E} \simeq -0.1082$.
- 31) $\mathcal{E} \simeq -0.38229$.
- 32) $\mathcal{E} \simeq -0.4467$.
- 33) $\mathcal{E} \simeq -0.34518$.
- 34) $\mathcal{E} \simeq -0.43085$.
- 35) $\mathcal{E} \simeq -0.105384$.
- 36) $\mathcal{E} \simeq -0.05659$.
- 37) $\mathcal{E} \simeq -0.04657$.
- 38) $\mathcal{E} \simeq -0.09839$.
- 39) $\mathcal{E} \simeq -0.08979$.
- 40) $\mathcal{E} \simeq -0.03862$.
- 41) $\mathcal{E} \simeq +0.05439$.
- 42) $\mathcal{E} \simeq +0.04135$.
- 43) $\mathcal{E} \simeq +0.13104$.
- 44) $\mathcal{E} \simeq +0.14092$.
- 45) $\mathcal{E} \simeq +0.14142$.
- 46) $\mathcal{E} \simeq +0.12009$.
- 47) $\mathcal{E} \simeq +0.14121$.
- 48) $\mathcal{E} \simeq +0.11771$.
- 49) $\mathcal{E} \simeq +0.13562$.

- 50) $\mathcal{E} \simeq +0.34089$.
- 51) $\mathcal{E} \simeq +0.32821$.
- 52) $\mathcal{E} \simeq +0.31674$.
- 53) $\mathcal{E} \simeq +0.31404$.
- 54) $\mathcal{E} \simeq +0.31616$.
- 55) $\mathcal{E} \simeq +0.30948$.
- 56) $\mathcal{E} \simeq +0.36612$.
- 57) $\mathcal{E} \simeq +0.06397$.
- 58) $\mathcal{E} \simeq +0.07628$.
- 59) $\mathcal{E} \simeq +0.04454$.
- 60) $\mathcal{E} \simeq +0.05450$.
- 61) $\mathcal{E} \simeq +0.1001$.
- 62) $\mathcal{E} \simeq +0.08365$.
- 63) $\mathcal{E} \simeq +0.03773$.
- 64) $\mathcal{E} \simeq +0.03277$.
- 65) $\mathcal{E} \simeq +0.04901$.
- 66) $\mathcal{E} \simeq +0.05283$.
- 67) $\mathcal{E} \simeq +0.05445$.
- 68) $\mathcal{E} \simeq +0.02930$.
- 69) $\mathcal{E} \simeq +0.05402$.
- 70) $\mathcal{E} \simeq +0.04300$.
- 71) $\mathcal{E} \simeq +0.04030$.

REFERENCES

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