The discrete harmonic oscillator, Harper's equation, and the discrete fractional Fourier transform

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Abstract. Certain solutions to Harper's equation are discrete analogues of (and approximations to) the Hermite–Gaussian functions. They are the energy eigenfunctions of a discrete algebraic analogue of the harmonic oscillator, and they lead to a definition of a discrete fractional Fourier transform (FT). The discrete fractional FT is essentially the time-evolution operator of the discrete harmonic oscillator.

1. Introduction

The three topics in the title, apparently diverse, are linked by a common theme: they may each be illuminated by focusing attention on certain functions, which we shall call *Harper functions*. These real-valued periodic functions, defined on the integers, are particular solutions to Harper's equation. The Harper functions serve as discrete approximations to the Hermite–Gaussian functions, and furthermore, in an algebraic sense that will be made clear in section 2, they are natural analogues of the Hermite–Gaussian functions. In [6, 8–10], and Ozaktas *et al* [24], the Harper functions were called the *discrete Hermite–Gaussian functions*. We have changed the name in recognition of the many other useful discrete approximations to the Hermite–Gaussians. Nevertheless, we shall give some evidence that the Harper functions deserve a special status among the various such discrete approximations.

In section 2, we give an algebraic treatment of the discrete fractional Fourier transform (FT) that was initiated by Pei and Yeh in [26] (see also [23]), and consolidated in [8, 10]. The discrete FT has diverse applications, of which but one is the numerical calculation of the continuum FT of a given function. The continuum fractional FT has a well-established role in quantum physics and in signal processing; see, for instance, [1, 17, 20, 23, 24, 34]. Any discrete version of the fractional FT surely ought to be of use in numerical calculation: the discrete fractional FT we discuss does indeed perform this service; see [10]. On the other hand, it is desirable that a discrete version of the fractional FT can also perform theoretical

roles analogous to those of the continuum fractional FT. It is this theoretical aspect that is our main concern below.

Atakishiyev and Suslov [2], Atakishiyev and Wolf [3], Grünbaum [13], Namias [21] and many others have interpreted fractional FTs as time-evolution operators of harmonic oscillators. As we shall see in section 3, the algebraic felicity of the discrete fractional FT, as we define it, makes this discrete fractional FT especially amenable to such an interpretation.

The Harper functions have been studied mainly in the context of the Bloch electron problem, also called (sometimes in greater generality) the Azbel–Hofstadter problem. A brief discussion of this connection is given in section 4.

The numerical data in section 5 may be viewed in two ways: it indicates the accuracy of the discrete fractional FT as an approximation to the continuum fractional FT; it indicates the accuracy of the discrete harmonic oscillator as an approximation to the continuum harmonic oscillator.

Wootters [35] suggested the term *discrete quantum system* to refer to a quantum system with a finite-dimensional state space. Such a state space may be regarded as a space of functions whose argument admits only finitely many values. Some discrete quantum systems, such as that of the Bloch electron problem discussed below, or the BI oscillator examined in [4] are not directly related to continuum quantum systems. Nevertheless, discrete quantum mechanics may also be employed as a technique in the study of continuum quantum systems: in [14, 15], phase and action-angle operators on continuum (infinite-dimensional) spaces were constructed as limits of analogous unitary operators on discrete spaces.

We understand the theory of *phase space* as being a general study with applications to physics and signal processing. Such applications have been well established for the continuum theory of phase space; see, for instance, [11, 19, 25, 29, 31, 34]. A satisfactory discrete version of the theory would also be expected to have such applications. In fact, a self-contained, practicable discrete theory would be highly desirable in signal processing and other numerical work—after all, an ensemble of numerical data is actually a discrete entity! Such a discrete theory ought to be an analogue of the continuum theory, and ought to serve as an approximation to the continuum theory in such a way that the continuum theory may be recovered via a limiting process. The question of approximating (or recovering) the continuum theory is not meaningful until a correspondence is established between discrete and continuum systems. One approach to such a correspondence is given in Schwinger [30, ch 7]. Another approach is introduced in [7]. However, a discrete theory encompassing Wigner functions, linear canonical transformations, coherent states, and so forth is, at the time of writing, far from complete. One achievement in this direction, thus far, has been in establishing a satisfactory definition of the discrete fractional FT.

Let us begin by reviewing some properties of the continuum fractional FT. Recall that, given an integer $k \geqslant 0$, then the kth Hermite–Gaussian is defined to be the (real-valued) function $h_k : \mathbb{R} \to \mathbb{C}$ such that

$$h_k(x) = \pi^{-1/4} 2^{-k/2} (k!)^{-1/2} e^{-x^2/2} H_k(x)$$

where H_k denotes the kth Hermite polynomial. The continuum fractional FT of Namias [21] is the unitary operator $\mathcal{F}_\infty^{[t]}$ on $L^2(\mathbb{R})$, defined for all $t \in \mathbb{R}$, such that

$$\mathcal{F}_\infty^{[t]} h_k = e^{2\pi i k t} h_k.$$

It has the property that

$$\mathcal{F}_\infty^{[t+t']} = \mathcal{F}_\infty^{[t]} \mathcal{F}_\infty^{[t']}.$$

The continuum FT, denoted $\mathcal{F}_\infty$, is the special case

$$\mathcal{F}_\infty = \mathcal{F}_\infty^{[1/4]}.$$

Turning now to the discrete scenario, let us consider an integer $n \geqslant 5$. (For the four smallest positive integers, our discussions would still hold, suitably interpreted with attention to some bothersome trivia.) We write $[X]_n$ to denote the modulo n residue class of a (rational) integer X. The set of modulo n residue classes of the integers, denoted $\mathbb{Z}/n = \{[0]_n, [1]_n, \ldots, [n-1]_n\}$, is a cyclic group with additive operation $[X]_n + [Y]_n = [X + Y]_n$. Let $L(n)$ denote the vector space over $\mathbb{C}$ with basis $\mathbb{Z}/n$. We view $L(n)$ as the space of functions $\mathbb{Z}/n \to \mathbb{C}$. Any function $f : \mathbb{Z} \to \mathbb{C}$ with period dividing n may be regarded as an element of $L(n)$, and may be identified with the vector $\sum_{X \in \mathbb{Z}/n} f(X)[X]_n$. We make $L(n)$ become an inner product space such that the set $\mathbb{Z}/n$ is an orthonormal basis.

The discrete FT $\mathcal{F}_n$ with degree n is the unitary linear map $L(n) \to L(n)$, represented, with respect to the orthonormal (ordered) basis $\mathbb{Z}/n = \{[0]_n, \ldots, [n-1]_n\}$ by the matrix with (X, Y)-entry $e^{2\pi i XY/n}$. We shall define the discrete fractional FT to be a continuous function from $\mathbb{R}$ to the group of unitary linear maps $L(n) \to L(n)$. This function, written $t \mapsto \mathcal{F}_n^{[t]}$, will satisfy the group homomorphism property

$$\mathcal{F}_n^{[t]} \mathcal{F}_n^{[t']} = \mathcal{F}_n^{[t+t']}$$

for all $t, t' \in \mathbb{R}$. Our strategy, following Pei and Yeh [26], will be to find an orthonormal basis of $L(n)$ consisting of eigenvectors of $\mathcal{F}_n$, to insist that the discrete fractional FT has the same eigenvectors, and to specify the eigenvalue of $\mathcal{F}_n^{[t]}$ corresponding to each eigenvector. Since $(\mathcal{F}_n)^4 = 1$, the eigenvalues of $\mathcal{F}_n$ are all fourth roots of unity. (The exact multiplicity of each eigenvalue, as a function of n, is given in [18]; the multiplicities always differ from $n/4$ by at most unity.) Evidently, there is considerable freedom for choice of an orthonormal basis diagonalizing F_n. The basis we shall choose consists of vectors which, regarded as functions $\mathbb{Z}/n \to \mathbb{C}$, are solutions to Harper's equation.

Harper's equation is the condition

$$h(X - 1) + 2\cos(2\pi X/n)h(X) + h(X + 1) = \lambda h(X)$$

on a function $h : \mathbb{Z}/n \to \mathbb{C}$ and a real number λ. Letting $\mathcal{G}_n$ be the linear map $L(n) \to L(n)$ such that

$$\mathcal{G}_n[X]_n = [X - 1]_n + 2\cos(2\pi X/n)[X]_n + [X + 1]_n$$

then the solutions h and λ to Harper's equation are precisely the eigenvectors and eigenvalues of $\mathcal{G}_n$. Since $\mathcal{G}_n$ is Hermitian, there are precisely n linearly independent solutions. The eigenvalues of $\mathcal{G}_n$ are not always distinct; Dickinson–Steiglitz [12] conjecture that the eigenvalues are distinct save that, when 4 divides n, the eigenvalue 0 has multiplicity 2. However, as observed in [12], there does exist, uniquely up to a choice of sign, an orthonormal basis of real unit vectors simultaneously diagonalizing $\mathcal{F}_n$ and $\mathcal{G}_n$. These vectors, with signs and an ordering suitably chosen, are precisely the Harper functions.

In section 2 we shall define, for suitable integers k, a function $h_{n,k} : \mathbb{Z}/n \to \mathbb{C}$ (with real values), called the kth Harper function of periodicity n. For given n, the n distinct values allowed for k are such that, if n is odd, then $0 \leqslant k \leqslant n-1$, while if n is even, then $0 \leqslant k \leqslant n-2$ or $k = n$. For an integer X, we shall write $h_{n,k}([X]_n)$ more briefly as $h_{n,k}(X)$, this notation indicating that we sometimes regard $h_{n,k}$ as a function $\mathbb{Z} \to \mathbb{C}$ with period dividing n. The vector $\sum_{X \in \mathbb{Z}/n} h_{n,k}(X)[X]_n$ will also be denoted by the symbol $h_{n,k}$. Thus we also regard $h_{n,k}$ as a vector in $L(n)$.

Proposition 3 below, asserts that, for fixed k and increasing n, the Harper function $h_{n,k}$ converges to the kth Hermite–Gaussian function h_k. The sense of the convergence may be taken either to be in the empirical numerical sense discussed in section 5, or else in the formal sense of [6,7]. In analogy with the definition in Namias [21, equation (2.6)] of the continuum fractional FT, we define, for each $t \in \mathbb{R}$, a unitary linear map $\mathcal{F}_n^{[t]} : L(n) \to L(n)$ such that

$$\mathcal{F}_n^{[t]} h_{n,k} := e^{2\pi i k t} h_{n,k}$$

for each index k. We call $\mathcal{F}_n^{[t]}$ the discrete fractional FT with degree n and exponent t.

We shall also discuss another variant of the discrete fractional FT. This variant, denoted $\mathcal{F}_n^{(t)}$, will be constructed in section 2 using a different analogy with the continuum fractional FT. Although $\mathcal{F}_n^{[t]}$ and $\mathcal{F}_n^{(t)}$ are not the same, we shall see in section 5 that the discrepancy diminishes quickly as $n \to \infty$.

Some rival candidates for the name 'discrete fractional FT' may be constructed in the same way, but with the Harper functions replaced by other discrete versions of the Hermite–Gaussians, for instance, the Kravchuk functions used by Atakishiyev and Suslov [2], Atakishiyev and Wolf [3], or the eigenvectors of $\mathcal{F}_n$ discovered by Grünbaum [13]. Some very accurate discrete versions of the Hermite–Gaussians are given in [8, 27]. Another approach to the discrete fractional FT, with a fast algorithm, appears in [22]. Our concern in this paper, however, is to progress towards a natural and general theory of discrete phase space. An advantage afforded by the Harper functions is that they arise in a simple and natural algebraic way; the connection with the discrete harmonic oscillator underlines this point. At present, a disadvantage of the Harper functions is that no closed formula for their solution is known.

2. Harper functions and the discrete fractional FT

An n-dimensional square matrix A with entries $A_{i,j}$ is said to be tridiagonal provided $A_{i,j} = 0$ whenever $|i - j| \geqslant 2$. Here the indices are *not* interpreted modulo n. Tridiagonal matrices, and matrices that are almost tridiagonal (with the possibility that the top right or bottom left entries may be non-zero) arise from time to time in discrete quantum mechanics; see, for instance, [5]. Before defining the Harper functions, it is worth making some observations about a fairly general class of real symmetric tridiagonal matrices.

Let r be a positive integer. Consider a sequence $\underline{v} = (v_0, \ldots, v_r)$ with each $v_j \in \mathbb{R}$. We say that $\underline{v}$ has a crossing number provided v_0 and v_r are both non-zero, and furthermore, if $v_j = 0$ for some $1 \leqslant j \leqslant r - 1$, then $v_{j-1}v_{j+1} < 0$. When $\underline{v}$ has a crossing number, we define the crossing number of $\underline{v}$ to be the number of integers j with $1 \leqslant j \leqslant r$ such that either $v_j = 0$ or else $v_{j-1}v_j < 0$. The point of these apparently awkward definitions is that if $\underline{v}$ has crossing number t, then t is the minimum number of zeros of a continuous extension $[0, r] \to \mathbb{R}$ of the function $j \mapsto v_j$.

Now let $a_0, \ldots, a_r$ be real numbers, let $b_1, \ldots, b_r$ be strictly positive real numbers, and let A be the tridiagonal $(r + 1) \times (r + 1)$ matrix whose (j, j) entry is a_j for $0 \leqslant j \leqslant r$, and whose $(k - 1, k)$ and $(k, k - 1)$ entries are $A_{k-1,k} = b_k = A_{k,k+1}$ for $1 \leqslant k \leqslant r$. Since A is a real symmetric matrix, it has real eigenvalues and real eigenvectors. By Wilkinson [33, section 5.37], A has no repeated eigenvalues. Let us enumerate an independent set of eigenvectors $\underline{v}_0, \ldots, \underline{v}_r$ such that the corresponding eigenvalues $\lambda_0 > \cdots > \lambda_r$ are monotonically decreasing. The following result, generalizing some arguments in [8] and [10] may be well known: it arises from a fairly direct combination of results in Wilkinson's classic book [33].

Proposition 1. *For the real symmetric tridiagonal matrix A as above, and an integer k with $0 \leqslant k \leqslant r$, the eigenvector $\underline{v}_k$ has crossing number k.*

Proof. Let $\lambda = \lambda_k$ and $\underline{v} = \underline{v}_k$. Write $\underline{v} = (v_0, \ldots, v_r)$. Then

$$(a_0 - \lambda)v_0 + b_1v_1 = 0 = b_rv_{r-1} + (a_r - \lambda)v_r$$

and, for $1 \leqslant j \leqslant r - 1$, we also have

$$b_jv_{j-1} + (a_j - \lambda)v_j + b_{j+1}v_{j+1} = 0.$$

These recurrence relations, together with the condition that $\underline{v} \neq 0$, imply that $\underline{v}$ has a crossing number. We may assume that $v_0 = 1$. For $0 \leqslant k \leqslant r$, let A_k be the leading $(k+1) \times (k+1)$ submatrix of A, and let χ_k be the characteristic polynomial $\chi_k(t) = \det(A_k - t)$. Let χ_{-1} be the constant polynomial $\chi_{-1}(t) = 1$. It is shown in Wilkinson [33, section 5.38] that, for $1 \leqslant k \leqslant r$, the matrices A_{k-1} and A_k have distinct eigenvalues. So if t is not an eigenvalue of the matrix $A = A_r$, then the sequence $(\chi_{-1}(t), \chi_0(t), \ldots, \chi_r(t))$ has a crossing number $c(t)$ It is also shown in [33] that, for such t, the number of eigenvalues of A strictly greater than t is $r + 1 - c(t)$. Since $\chi_r(\lambda) = 0$, we have $c(\lambda + \epsilon) = 1 + c(\lambda - \epsilon)$ for small $\epsilon > 0$, we deduce that the sequence $(\chi_{-1}(\lambda), \chi_0(\lambda), \ldots, \chi_{r-1}(\lambda))$ has a crossing number $c(\lambda - \epsilon)$, and furthermore, $k = r + 1 - c(\lambda + \epsilon) = r - c(\lambda - \epsilon)$. By [33, section 5.38]

$$v_k = (-1)^k \chi_{k-1}(\lambda)/b_1 \ldots b_k$$

with the interpretation that $v_0 = \chi_{-1}(\lambda)$. The assertion follows because the numbers $b_1, \ldots, b_r$ are strictly positive. $\qquad\square$

Let us return to the discrete FT $\mathcal{F}_n : L(n) \to L(n)$. For brevity, we shall often drop the subscript n. An easy calculation shows that $\mathcal{F}^2[X] = [-X]$ for all integers X. Let E_+ and E_- denote the eigenspaces of $\mathcal{F}^2$ corresponding to the eigenvalues 1 and -1, respectively. For each integer X in the (open) interval $0 \leqslant X \leqslant n/2$, let $e_+(X) := [X] + [-X]$. For each integer X in the (closed) interval $0 < X < n/2$, let $e_-(X) := [X] - [-X]$. Then E_+ has an orthogonal basis consisting of the vectors $e_+(X)$, while E_- has an orthogonal basis consisting of the vectors $e_-(X)$. Note that E_+ has dimension either $n/2 + 1$ or $(n+1)/2$ (whichever is an integer), while E_- has dimension either $n/2 - 1$ or $(n-1)/2$.

The linear map $\mathcal{G}$ (defined in section 1) stabilizes the complementary subspaces E_+ and E_- of $L(n)$. Let $\mathcal{G}_+$ and $\mathcal{G}_-$ denote the restrictions of $\mathcal{G}$ to E_+ and E_-, respectively. With respect to the bases of E_+ and E_- mentioned above, $\mathcal{G}_+$ and $\mathcal{G}_-$ are represented by real symmetric tridiagonal matrices satisfying the hypothesis of proposition 1. Up to a non-zero real factor, we define $h_{n,0}, h_{n,2}, h_{n,4}, \ldots$ by insisting they be independent real eigenvectors of $\mathcal{G}_+$ such that the corresponding sequence of eigenvectors $\lambda_{n,0}, \lambda_{n,2}, \lambda_{n,4}, \ldots$ is strictly monotonically decreasing. By proposition 1, each $h_{n,2j}[0] \neq 0$. We uniquely determine the vectors $h_{n,2j}$ by insisting they be of unit modulus, and $h_{n,2j}[0] > 0$. Similarly, we define $h_{n,1}, h_{n,3}, h_{n,5}, \ldots$ to be the independent real eigenvectors of $\mathcal{G}_-$ such that the corresponding sequence of eigenvectors $\lambda_{n,1}, \lambda_{n,3}, \lambda_{n,5}, \ldots$ is strictly monotonically decreasing; moreover, each $h_{n,2j+1}$ is of unit modulus, and $h_{n,2j+1}[1] > 0$. We have thus completed the definition of the Harper functions $h_{n,k}$, where the integer index k satisfies $0 \leqslant k \leqslant n$, and is subject only to the further conditions that, if n is even then $k \neq n - 1$, while if n is odd then $k \neq n$. The Harper functions form an orthonormal basis of solutions to Harper's equation:

$$h_{n,k}(X - 1) + 2\cos(2\pi X/n)h_{n,k}(X) + h_{n,k}(X + 1) = \lambda_{n,k}h_{n,k}(X).$$

We mention that our construction of the Harper functions, in effect, reduces Harper's equation to two independent systems of equations, each of which is the eigenvector problem for a real symmetric tridiagonal matrix. As indicated in the proof of proposition 1, the eigenvectors of such a matrix may easily be calculated by a recursive formula once the eigenvalues are known; furthermore, Wilkinson [33, section 5.38] describes a straightforward process for obtaining the characteristic polynomial. However, due to ill-conditioning, this is not an effective method for calculating the Harper functions numerically.

Proposition 2. *Up to multiplication by real factors, the vectors $h_{n,k}$ comprise the unique basis of $L(n)$ simultaneously diagonalizing $\mathcal{F}^2$ and $\mathcal{G}$. With respect to the basis E_+, the coordinates of $h_{n,2j}$ have crossing number j. With respect to the basis E_-, the coordinates of $h_{n,2j+1}$ have crossing number j. If $\lambda_{n,k} = \lambda_{n,k'}$, then either $k = k'$ or else k and k' have opposite parity.*

Proof. Any basis B diagonalizing $\mathcal{G}$ must be contained in $E_+ \cup E_-$. By considering, separately, the actions of $\mathcal{G}$ on E_+ and E_-, the assertion follows from proposition 1. $\qquad\square$

To discuss the matter of convergence to functions on the continuum, let us consider a square-integrable function $\psi_\infty : \mathbb{R} \to \mathbb{C}$, and a sequence of functions $\psi_n : \mathbb{C}(\mathbb{Z}/n) \to \mathbb{C}$ defined for infinitely many (but not necessarily all) positive integers n. Let

$$\nu(n) := (n/2\pi)^{1/4}.$$

Roughly speaking, we say that the sequence $(\psi_n)_n$ converges to ψ provided, given an integer X, then for sufficiently large n we have an approximate equality

$$\psi_n(X) \approx \nu(n)^{-1} \psi(\nu(n)^{-2} X).$$

For a real number x, let $x(n)$ denote the largest integer not exceeding $\nu(n)^2 x$. The condition that $(\psi_n)_n$ converges to ψ may be rewritten as

$$\psi(x) \approx \nu(n) \psi_n(x(n)).$$

(Greater care over the definition of convergence is needed to ensure certain desirable properties, for instance, the property that $\|\psi\|_2 = \lim_{n\to\infty} \|\psi_n\|_2$. If the approximate equality symbol $\approx$ were interpreted as indicating a limit as $n \to \infty$, then propositions 3, 5, 8 would still hold, but propositions 4, 6, 7, 9 would be false. See [6] or [7] for a formal definition of convergence.)

The discrete Hermite–Gaussian functions $h_{n,k}$ converge to the Hermite–Gaussian functions in the following sense, from [6, theorem 2.5].

Proposition 3. *Consider an integer $k \geqslant 0$. For suitable infinite sequences of positive integers n, the sequence $(h_{n,k})_n$ converges to h_k.*

Numerical evidence in [8, 10], Pei and Yeh [26], and below in section 5, indicates that the word 'suitable' may be omitted from proposition 3. A further indication in support of this conjecture is provided by the crossing number characterization of the Harper functions, together with the fact that h_k has precisely k zeros.

A sense in which the discrete fractional FT $\mathcal{F}_n^{[t]}$ converges to the continuum fractional FT $\mathcal{F}_\infty^{[t]}$ may already be gleaned from proposition 3. We can make this more precise by introducing a notion of convergence of operators. Consider an operator $\mathcal{A}_\infty$ on the space $L^2(\mathbb{R})$ of square-integrable functions. Consider also an infinite sequence $(\mathcal{A}_n)_n$, where each $\mathcal{A}_n$ is a linear map $L(n) \to L(n)$. We say that the sequence $(\mathcal{A}_n)_n$ converges to $\mathcal{A}_\infty$ provided the sequence $(\mathcal{A}_n \psi_n)_n$ converges to $\mathcal{A}_\infty \psi_\infty$, where ψ_∞ is any function in the domain of $\mathcal{A}_\infty$, and $(\psi_n)_n$ is any sequence with $\psi_n \in L(n)$ such that $(\psi_n)_n$ converges to ψ_∞. (Note that our definition of convergence is precise, but it is in terms of the definition in [6,7] of convergence of vectors.) The result is as follows [6, theorems 2.7, 2.8].

Proposition 4. *For suitable infinite sequences of positive integers n, the discrete fractional FT $\mathcal{F}_n^{[t]}$ converges to the continuum fractional FT $\mathcal{F}_\infty^{[t]}$. Furthermore, the discrete FT $\mathcal{F}_n$ converges to the continuum FT $\mathcal{F}_\infty$.*

Proposition 4 tells us that $\mathcal{F}_n^{[1/4]}$ is approximately equal to $\mathcal{F}_n$ for large n. It is an unresolved question as to whether or not $\mathcal{F}_n^{[1/4]} = \mathcal{F}_n$. The question is equivalent to asking whether or not $h_{n,k}$, as an eigenvalue of $\mathcal{F}_n$, always has eigenvalue i^k. We conjecture an affirmative answer.

Another version of a discrete fractional FT, denoted $\mathcal{F}_n^{(t)}$, is very similar to $\mathcal{F}_n^{[t]}$: the two operators have the same eigenvectors but slightly different eigenvalues. Before defining $\mathcal{F}_n^{(t)}$, it is convenient to record the following easy consequence of proposition 4.

Proposition 5. *Given an integer $k \geqslant 0$, and writing $\mu(n, k)$ for the $k + 1$th largest eigenvalue of $\mathcal{G}_n$, then for suitable infinite sequences of positive integers n, we have $\mu(n, k)_n = 4 - 2\pi(2j + 1)/n + \mathrm{o}(1/n)$.*

Let $\eta(n, k)$ be the $k + 1$th smallest eigenvector of the linear map

$$\mathcal{K}_n := \frac{n}{2\pi}(2 - \mathcal{G}_n/2) - \tfrac{1}{2}$$

By proposition 5, $\eta(n, k) = n(2 - \mu(n, k)/2)/2\pi - 1/2 = k + \mathrm{o}(1)$. Defining the linear map $\mathcal{F}_n^{(t)} : L(n) \to L(n)$ by

$$\mathcal{F}_n^{(t)} h_{n,k} = \mathrm{e}^{2\pi \mathrm{i} \eta(n,k)t} h_{n,k}$$

then $\mathcal{F}_n^{(t)}$ may also be expressed by the formula

$$\mathcal{F}_n^{(t)} := \mathrm{e}^{2\pi \mathrm{i} \mathcal{K}_n t}.$$

Thus, the Harper functions $h_{n,k}$ are the eigenvectors of $\mathcal{F}_n^{(t)}$ and $\mathcal{F}_n^{[t]}$; the corresponding eigenvalues are the same up to $\mathrm{o}(1/n)$. The following result is immediate from propositions 4 and 5.

Proposition 6. *For suitable infinite sequences of positive integers n, the operator $\mathcal{F}_n^{(t)}$ converges to the continuum fractional FT $\mathcal{F}_\infty^{[t]}$.*

3. The discrete harmonic oscillator

Let us begin with some general comments about discrete realizations of continuum quantum systems. We examine only single-particle quantum systems with a time-invariant Hamiltonian. In the case where the state space is a Hilbert space of countably infinite dimension, we say that the quantum system is a continuum quantum system. In the case where the state space is a finite-dimensional Hilbert space (a finite-dimensional inner product space), we say that the system is discrete.

Consider a Hermitian operator $\mathcal{H}$ on a Hilbert space V (such that the domain of $\mathcal{H}$ is dense in V). We interpret $\mathcal{H}$ as the Hamiltonian of a quantum system. By a state vector ψ of the system, we mean a differentiable function $\mathbb{R} \to V$ satisfying the Schrödinger equation:

$$\mathcal{H}\psi(t) = \mathrm{i}\frac{\mathrm{d}\psi(t)}{\mathrm{d}t}.$$

We insist that the initial state $\psi(0)$ has norm $\|\psi(0)\|_2 = 1$, whereupon, of course, $\|\psi(t)\|_2 = 1$ for all $t \in \mathbb{R}$. Let $U(V)$ denote the group of unitary operators on V (understood to have domain and co-domain V). The time evolution $\mathcal{S}$ of the system is defined to be the group homomorphism $\mathbb{R} \to U(V)$ given by

$$\mathcal{S}(t) := \mathrm{e}^{-\mathrm{i}\mathcal{H}t}.$$

(The right-hand expression extends uniquely to the domain V.) The Schrödinger equation may be rewritten as

$$\psi(t) = \mathcal{S}(t)\psi(0).$$

Consider now a Hermitian operator $\mathcal{H}_\infty$ on $L^2(\mathbb{R})$ (with a dense domain). Consider also, for infinitely many positive integers n, Hermitian operators $\mathcal{H}_n$ on $L(n)$ (with domain $L(n)$). Let $\psi_\infty = \psi_\infty(t)$ be a state vector of a quantum system with Hamiltonian $\mathcal{H}_\infty$. For each n, let $\psi_n = \psi_n(t)$ be a state vector of a quantum system with Hamiltonian $\mathcal{H}_n$. Our concern is with the condition that, for all $t \in \mathbb{R}$, the sequence $(\psi_n(t))_n$ (the sequence of $\psi_n(t)$ indexed by n) converges to $\psi_\infty(t)$. The following observation is immediate from the definition of convergence of operators.

Proposition 7. *Let us fix a sequence of positive integers n. Then the following two conditions are equivalent:*

(a) *The time evolutions $S_n(t)$ converge to the time evolution $S_\infty(t)$ for all t.*
(b) *Given any initial states $\phi_n(0)$ converging to an initial state $\phi_\infty(0)$, then $\phi_n(t)$ converges to $\phi_\infty(t)$ for all t.*

Note that, when the equivalent conditions (a) and (b) hold, it does not follow that the Hamiltonians $\mathcal{H}_n$ converge to the Hamiltonian $\mathcal{H}_\infty$. (The theory simply does not work with the Hamiltonians in place of the time evolutions.) To indicate the applicability of proposition 7 in general, we record the following special case of a result in [7].

Proposition 8. *Consider any infinite sequence of positive integers n. Let $\mathcal{H}_\infty$ be any Hermitian operator (with a dense domain) on $L^2(\mathbb{R})$. Then there exist Hermitian operators $\mathcal{H}_n$ on $L(n)$ such that the equivalent conditions (a) and (b) in proposition 7 hold.*

To illustrate propositions 7 and 8, let us now turn to the harmonic oscillator. A (single-particle conservative) discrete quantum system is said to be a discrete harmonic oscillator provided the Hamiltonian is of the form

$$\mathcal{H} = 4(A + B) - \frac{A}{2}(\mathcal{U} + \mathcal{U}^{-1}) - \frac{B}{2}(\mathcal{V} + \mathcal{V}^{-1})$$

where A and B are positive real numbers, and $\mathcal{U}$, $\mathcal{V}$ are unitary operators such that

$$\mathcal{V}\mathcal{U} = \zeta\mathcal{U}\mathcal{V}$$

for some complex number ζ of unit modulus.

As a special case, let $\mathcal{U}$ and $\mathcal{V}$ be, respectively, the unitary operators $\mathcal{U}_n$ and $\mathcal{V}_n$ on $L(n)$ given by

$$\mathcal{U}_n[X] = [X - 1] \qquad \text{and} \qquad \mathcal{V}_n[X] = e^{2\pi iX/n}[X]$$

for $X \in \mathbb{Z}$. Thus $\mathcal{U}_n\mathcal{V}_n = \zeta_n\mathcal{V}_n\mathcal{U}_n$ where $\zeta_n = e^{2\pi i/n}$. Putting $A = B = v(n)^4 = n/2\pi$, then our Hamiltonian $\mathcal{H} = \mathcal{H}_n$ is the Hermitian operator on $L(n)$ given by

$$\mathcal{H}_n = \frac{n}{2\pi}(4 - \mathcal{U}_n - \mathcal{U}_n^{-1} - \mathcal{V}_n - \mathcal{V}_n^{-1}) = \frac{n}{2\pi}(4 - \mathcal{G}_n) = 2\mathcal{K}_n + 1.$$

More explicitly,

$$\mathcal{H}_n[X] = \frac{n}{2\pi}(-[X - 1] + (4 - 2\cos(2\pi iX/n))[X] - [X + 1]).$$

The quantum system with Hamiltonian $\mathcal{H}_n$ is called a standard discrete harmonic oscillator. The time evolution of this quantum system is

$$S_n(t) = e^{-i\mathcal{H}_n t} = e^{-i(2\mathcal{K}_n+1)t} = e^{-it}\mathcal{F}_n^{(-t/\pi)}.$$

On the other hand, the standard continuum harmonic oscillator is defined to be the quantum system whose Hamiltonian is

$$\mathcal{H}_\infty := -\frac{d^2}{d\xi^2} + \xi^2$$

as a Hermitian operator on functions in $L^2(\mathbb{R})$ with argument $\xi \in \mathbb{R}$. Heuristically, one might regard the operators $n(2 - \mathcal{U}_n - \mathcal{U}_n^{-1})/2\pi$ and $n(2 - \mathcal{V}_n - \mathcal{V}_n^{-1})/2\pi$ as approximations to the operators $-d^2/d\xi^2$ and ξ^2, respectively. Thence, one might regard $\mathcal{H}_n$ as an approximation to $\mathcal{H}_\infty$. Common sense might lead us to imagine that $\mathcal{H}_n$ converges to $\mathcal{H}_\infty$. Alas, common sense is, on this occasion, deceptive. The operators $\mathcal{H}_n$ do not converge to $\mathcal{H}_\infty$. We must shift our attention from the Hamiltonians to the time evolutions.

It is well known that the solutions to the Schrödinger equation of the standard continuum harmonic oscillator are

$$\mathcal{H}_\infty h_k = (2k+1)h_k.$$

Therefore, the time evolution for this quantum system is

$$\mathcal{S}_\infty(t) = \mathrm{e}^{\mathrm{i}\mathcal{H}_\infty t} = \mathrm{e}^{-\mathrm{i}t}\mathcal{F}_\infty^{[-t/\pi]}.$$

Our comments on the time evolutions of standard harmonic oscillators, together with proposition 6, imply the following result.

Proposition 9. *The Hamiltonians $\mathcal{H}_n$ and $\mathcal{H}$ of the standard harmonic oscillators are such that, for suitable infinite sequences of positive integers n, the time evolution $\mathcal{S}_n(t)$ corresponding to $\mathcal{H}_n$ converges to the time evolution $\mathcal{S}_\infty(t)$ corresponding to $\mathcal{H}_\infty$.*

4. Connections with the Bloch electron problem

The Bloch electron problem models the behaviour of a charged particle constrained to a two-dimensional square lattice and subject to a transverse time-invariant magnetic field. Let us write the state function as a function $\psi : \mathbb{Z} \times \mathbb{Z} \to \mathbb{C}$. As explained in Harper [16], we can impose a particular gauge, called the Landau gauge, such that the Hamiltonian $\mathcal{H}$ is given by

$$(\mathcal{H}\psi)(X,Y) = \psi(X-1,Y) + \psi(X+1,Y) + \mathrm{e}^{-2\pi\mathrm{i}\omega X}\psi(X,Y-1) + \mathrm{e}^{2\pi\mathrm{i}\omega X}\psi(X,Y+1)$$

where ω is a real constant proportional to the magnetic flux. See also Rammal–Bellissard [28]. Assuming that ω is rational, let us write write $\omega = m/n$ where m is an integer, and n is a positive integer coprime to m. The energy eigenstates ψ with energy eigenvalue E are given by

$$\psi(X,Y) = \mathrm{e}^{2\pi\mathrm{i}kY/n}\phi(X)$$

where k is an integer, and ϕ is a solution to

$$\phi(X-1) + \phi(X+1) + 2\cos(2\pi(mX+k)/n)\phi(X) = E\phi(X).$$

Replacing X with a variable W such that $mX + k = mW$, then replacing ϕ with its image θ under a Galois automorphism such that $\mathrm{e}^{2\pi\mathrm{i}m/n} \mapsto \mathrm{e}^{2\pi\mathrm{i}/n}$, we recover Harper's equation

$$\theta(W-1) + \theta(W+1) + 2\cos(2\pi W/n)\theta(W) = E\theta(W).$$

Although no closed formula for the solution to Harper's equation is known, Wiegmann and Zabrodin [32] have obtained some deep algebraic properties of the solutions. We ask whether the algebraic study of difference equations relating to the Bloch electron problem throws any light on the discrete fractional FT. We also ask whether material in this paper throws any light on the Bloch electron problem.

5. Comparison of the Harper functions and the Hermite–Gaussians

The techniques used in the arguments above appear to provide no information on the accuracy of the Harper functions as approximations to the Hermite–Gaussians. In this last section, we give some numerical information on the speed at which the Harper functions converge to the Hermite–Gaussians.

In figure 1, with $n = 16$, the first six Harper functions $h_{16,0}, \ldots, h_{16,5}$ (indicated by circles) are compared with the first six Hermite–Gaussians (indicated by the curves). The period $n = 16$ is usually too small for useful calculation; the point is that, for this small value of n, and for $k \leqslant 3$, the convergence already looks fairly good.
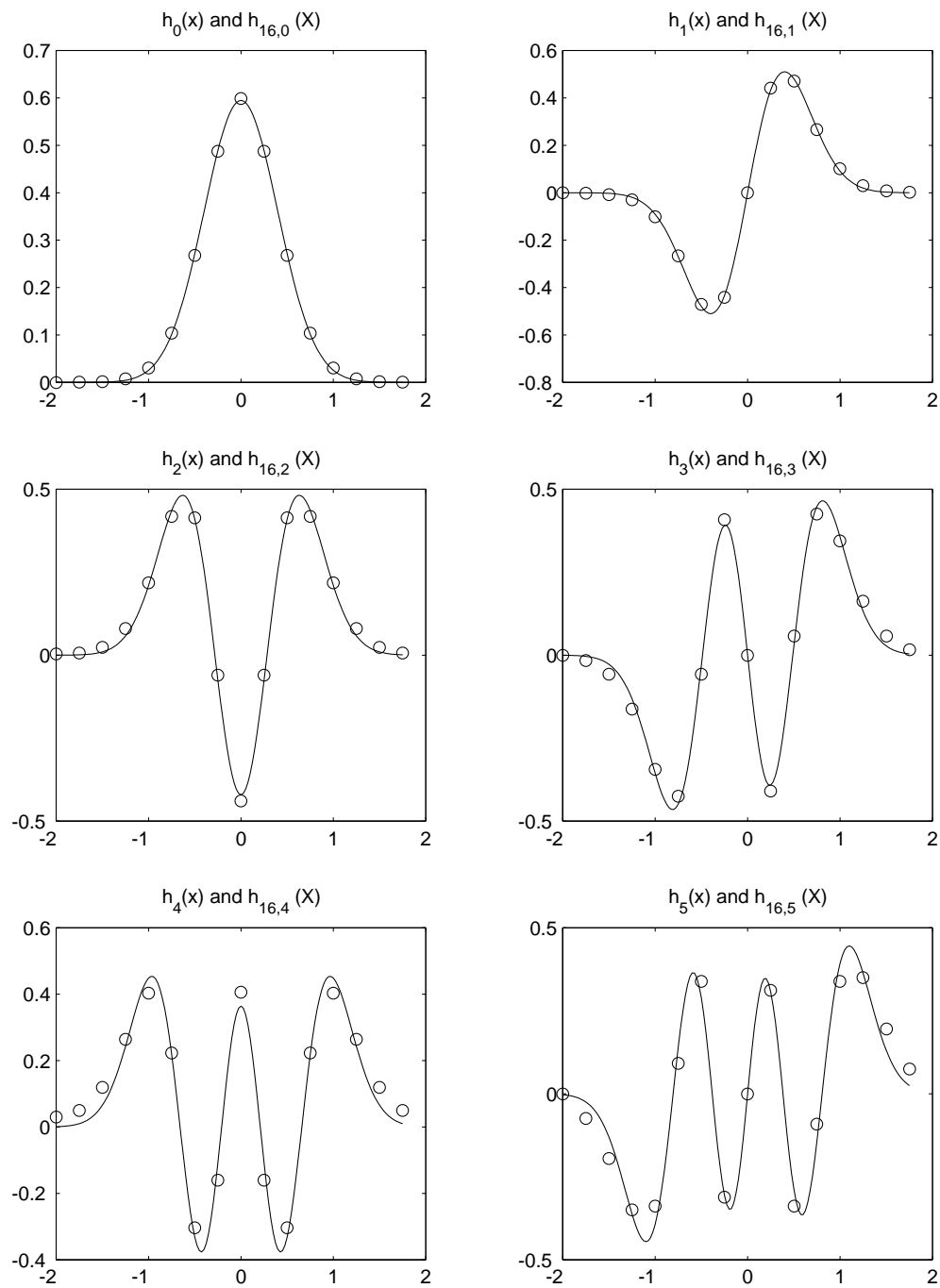
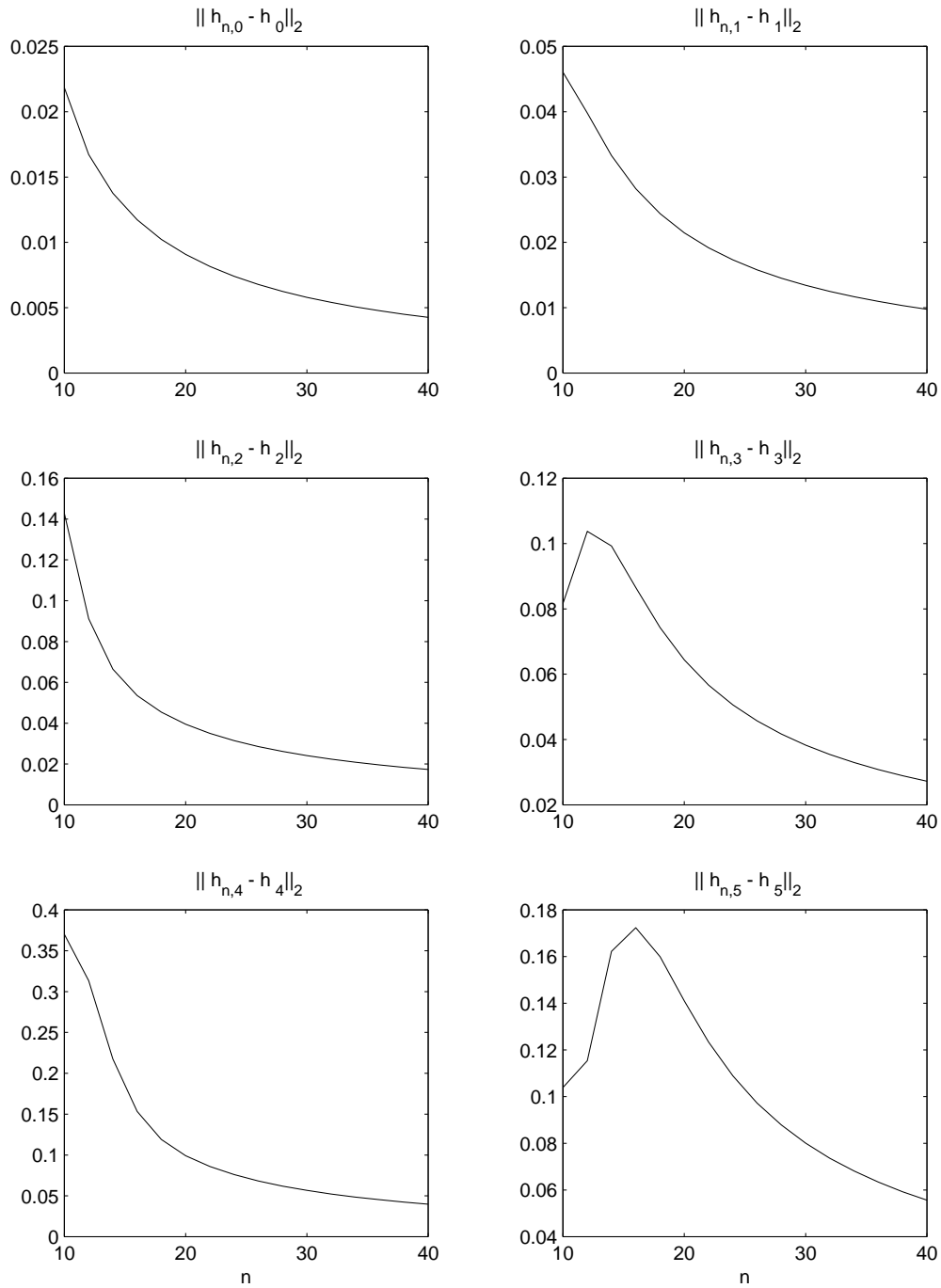**Figure 1.** Harper functions $h_{16,k}$ compared with Hermite–Gaussians h_k.

Figure 2. L^2-difference between Harper functions $h_{n,k}$ and Hermite–Gaussians h_k.
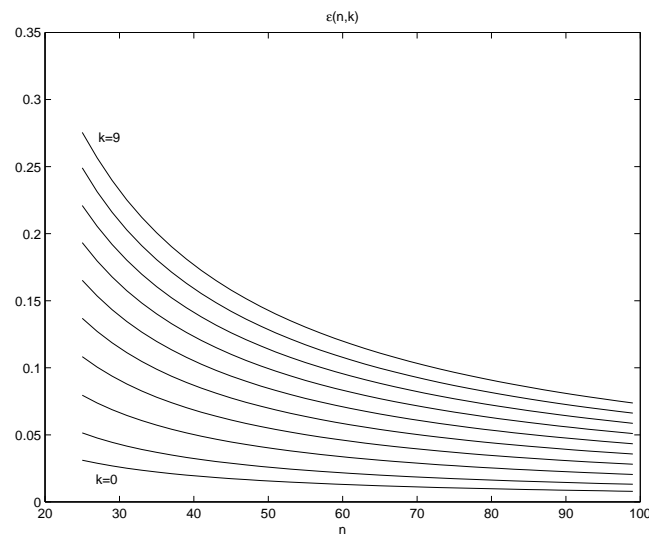
Figure 3. Weighted difference $\epsilon(n, k)$ between eigenvalues.

Figure 2 shows, for $10 \leqslant n \leqslant 40$ and $0 \leqslant k \leqslant 5$, the L^2-norm $\|h_{n,k} - h_k\|_2$ of the difference between the Harper function $h_{n,k}$ and the Hermite–Gaussian h_k. The difference was calculated by evaluating h_n at the sample points, normalizing, and comparing with the vector $h_{n,k}$. Again, the convergence looks fairly good.

In section 3, we found it convenient to replace $\mathcal{F}_n^{[t]}$ with the slightly different version $\mathcal{F}_n^{(t)}$ of the fractional FT. The former is a little easier to calculate with, and has the desirable property that $\mathcal{F}_n^{[1]} = 1$. The latter was defined quite algebraically as the exponential of an imaginary multiple of a Hermitian operator. We take the view that, for many purposes (numerical or theoretical) it matters little which version one chooses; they have the same convergence properties because, for fixed k, the eigenvalues of $\mathcal{F}_n^{[t]}$ and $\mathcal{F}_n^{(t)}$ associated with their common eigenvector $h_{n,k}$ are $e^{2\pi ikt}$ and $e^{2\pi i\eta(n,k)t}$, respectively. We saw, in proposition 5, that $\lim_{n\to\infty} \eta(n, k) = k$ (at least, this is proven for suitable sequences of integers n). Empirical confirmation that $\eta(n, k)$ converges to k is given by the graphs, in figure 3, of

$$\epsilon(n, k) := 1 - \eta(n, k)/k$$

against n, where $25 \leqslant n \leqslant 100$ and $0 \leqslant k \leqslant 9$.

For any square-integrable function $f : \mathbb{R} \to \mathbb{C}$, we can write

$$f(x) = \sum_{k=0}^{\infty} c_k h_k(x)$$

where the complex coefficients c_k satisfy $\sum_{k=0}^{\infty} |c_k|^2 < \infty$. Let us assume that f is reasonably well behaved (as it will be if, for instance, it is infinitely differentiable). Let f_n denote the vector in $L(n)$ whose coordinates are the sample values of f. For fixed f, if n is chosen large enough to ensure that, for each k, at least one of $|c_k|$ or $\|h_{n,k} - h_k\|_2$ is negligible, then $\mathcal{F}_n^{[t]} f_n$ and $\mathcal{F}_n^{(t)}$ will be approximately equal to the vector of sample values of $\mathcal{F}_\infty^{[t]} f$. Thus the discrete fractional FT, as an approximation, is good for those functions whose coefficients c_k converge quickly to zero as k increases.

In conclusion, we have given evidence that the discrete fractional FT is a good numerical approximation to the continuum fractional FT. This may be interpreted as saying that the

discrete fractional FT provides a good numerical approximation to the time evolution of the continuum harmonic oscillator. At least as importantly, the discrete fractional FT is also an algebraic analogue of the continuum fractional FT, and provides an algebraic analogue of the continuum harmonic oscillator. Furthermore, the continuum constructions are realized as limits of the discrete constructions. These observations support the proposal that, from a general theoretical point of view, the discrete fractional FT (as defined above) and the Harper functions have particular merit as discrete versions of the continuum fractional FT and the continuum Hermite–Gaussians.

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