DISCRETE QUANTUM HARMONIC OSCILLATOR AND KRAVCHUK TRANSFORM

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Abstract. We consider a particular discretization of the harmonic oscillator which admits an orthogonal basis of eigenfunctions called Kravchuk functions possessing appealing properties from the numerical point of view. We analytically prove the almost second-order convergence of these discrete functions towards Hermite functions, uniformly for large numbers of modes. We then describe an efficient way to simulate these eigenfunctions and the corresponding transformation. We finally show some numerical experiments corroborating our different results.

1. Introduction

Let us consider the harmonic oscillator operator, for $x \in \mathbb{R}^d$,

$$H = -\Delta + |x|^2. \tag{1}$$

We are interested in discretizing this operator on a uniform grid $h\mathbb{Z}^d$ where $h > 0$ denotes the stepsize of the grid. The harmonic oscillator appears in a lot of natural contexts, in particular as a fundamental model in quantum mechanics, and its well-known spectral properties in the whole space $\mathbb{R}^d$ make it a primary example of unbounded operators on Hilbert spaces.

Hermite functions are eigenfunctions of the operator H. They are given by the expressions, for $d = 1$,

$$\psi_n(x) := \frac{1}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} e^{-\frac{x^2}{2}} H_n(x), \quad n \geq 0, \tag{2}$$

where $H_n(x)$ are the Hermite polynomials defined by the relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad H_0 = 1, \tag{3}$$

with $H_n = 0$ for $n < 0$. The set $\{\psi_n\}_{n\in\mathbb{N}}$ forms a basis of $L^2(\mathbb{R})$ satisfying the relation

$$\forall\, n, m \in \mathbb{N}, \quad \int_{\mathbb{R}} \psi_n(x)\psi_m(x)dx = \delta_{n,m},$$

where $\delta_{n,m}$ denotes the Kronecker symbol, and

$$H\psi_n = (2n+1)\psi_n.$$

Any function of $L^2(\mathbb{R})$ can thus be written

$$f = \sum_{n \geq 0} c_n(f)\psi_n, \quad c_n(f) = \int_{\mathbb{R}} f(x)\psi_n(x)\mathrm{d}x, \tag{4}$$

and we can generalize these properties to any dimension d by tensorization. The Hermite functions can also be expressed using the raising an lowering operators

$$L = \partial_x + x, \quad \text{and} \quad R = -\partial_x + x$$

for which we have $(Lf, g)_{L^2(\mathbb{R})} = (f, Rg)_{L^2(\mathbb{R})}$ for any functions f ang g, and

$$H = \frac{1}{2}(RL + LR), \quad L\psi_n = \sqrt{2n}\,\psi_{n-1}, \quad \text{and} \quad R\psi_n = \sqrt{2n+2}\,\psi_{n+1}.$$

The discretization of the operator H poses the question of the transfer of the previous properties to discrete operators in a global perspective of geometric numerical integration or for robustness and stability arguments. For example the use of discrete Fourier transform will induce naturally a truncation on a large grid which has in general serious drawbacks. The same phenomenon appears in the classical discretization by finite differences. Also, the eigenvalues of the operator will be distorted in ways that are difficult to estimate, see for instance [14, 4]. It is also not clear at all if the natural hierarchy given by the operators L and R is preserved by space discretization.

Another option would be to use spectral methods and Gauss-Hermite quadrature, but the computations of the roots of Hermite polynomials as well as the associated quadrature weights appears to be quite computationally expensive in practice [6, 12], and moreover, the solution is not evaluated on a standard regular grid $h\mathbb{Z}$ making delicate the possible combination with other type of operator discretization.

The goal of this paper is to revitalize, amongst all possible discretizations by finite differences, the operator and functions associated with the Kravchuk polynomials, named after the Ukrainian mathematician Mikhailo Pylypovych Kravchuk[1]. These polynomials are well documented in the existing literature, see in particular [11], and they appear in discrete quantum mechanics [9], digital signal processing [13], and coding theory [8], or probability in the context of multinomial distribution [5]. However, to the best of the authors knowledge, none of these properties has yet been exploited in the context of numerical analysis of quantum systems, while several important features make them *a priori* very appealing and worth deserving more elaborate studies. Let us summarize the main advantage of the Kravchuk functions denotes by $\varphi_{n,h}$ and defined on a regular grid $h\mathbb{Z}$ for $h > 0$:

[1]Note that a writing difference subsists in the literature between "Kravchuk" or "Krawtchouk" polynomials, which both refer to the same mathematical object. We adopt in this paper the transcription "Kravchuk" as commonly employed in most physical contexts, contrary to the transliteration "Krawtchouk" he may have used when writing in french, which seems to be mostly adopted in the combinatorics and probabilistic literature.

- They diagonalize on a regular grid a discrete tridiagonal operator H_h similar to the classical order 2 finite difference scheme.
- The eigenvalue associated with the Kravchuk functions are *exactly* the one of the Harmonic oscillator: $H_h\varphi_{n,h} = (2n+1)\varphi_{n,h}$. This isospectral diagonalization, which is usually a feature reserved to spectral methods, is very promising in particular in the numerical approximation of nonlinear evolution equations of Schrödinger form where discrete resonances are essential.
- The Kravchuk functions form an orthonormal set defined on a discrete finite grid for the standard discrete scalar product.
- They uniformly approximate the Hermite functions when $h \to 0$, and thus the Hermite coefficients.
- Finally, the computation of the Kravchuk coefficients corresponding to the Hermite coefficients (the *Kravchuk transform*) can be reduced to the multiplication by the exponential of a skew hermitian tridiagonal matrix.

Each of these point would deserve complete numerical and analytical study, but we believe that the use of these polynomials could be particularly appealing in nonlinear situations, for ground states computing, or for equations coupled with operators naturally defined on regular grid. As a very first example of result, we consider in Section 6 the discretization of the time dependent Schrödinger equation

$$i\partial_t\psi = H\psi$$

by the Kravchuk operator, and we obtain a global convergence in time as an immediate consequence of the isospectral nature of the discretization and our uniform bounds. In Theorem 4 we show that if f is a given smooth function, and $\psi(t,x) = e^{-itH}f$, then we can construct a solution $\psi_h(t)$ to the equation

$$i\partial\psi_h = H_h\psi_h \tag{5}$$

such that

$$\|\pi_h\psi(t,\cdot) - \psi_h(t,\cdot)\|_{\ell^2(h\mathbb{Z})} \leq \epsilon(h)$$

where $\epsilon(h) \to 0$ in a way depending on the smoothness of f, but where this estimate holds uniformly in time. We also note that the solution of (5) can be obtained by the computation of the exponential of a skew-hermitian tridiagonal matrix, which can be easily done by using Padé approximations, see for instance [10].

2. Main results

Let $N \in \mathbb{N}^*$ be an even integer and $h = \sqrt{2}N^{-\frac{1}{2}}$. We define the scaled Kravchuk polynomials by the relation

$$k_{n+1,h}(x) = 2xk_{n,h}(x) - 2n\left(1 - h^2\Big(\frac{n-1}{2}\Big)\right)k_{n-1,h}(x), \quad k_{0,h} = 1, \tag{6}$$

with the convention $k_{n,h} = 0$ for $n < 0$ (we will moreover prove that $k_{n,h} = 0$ for $n > N$). We denote the finite set

$$A_h := h\mathbb{Z} \cap \left[-\frac{1}{h}, \frac{1}{h}\right], \tag{7}$$

and we consider the discrete Hilbert space $\ell^2(h\mathbb{Z})$ defined through the norm

$$\|u\|^2_{\ell^2(h\mathbb{Z})} = h \sum_{a \in h\mathbb{Z}} |u(a)|^2$$

induced by the scalar product

$$\langle u, v \rangle_{\ell^2(h\mathbb{Z})} = h \sum_{a \in h\mathbb{Z}} u(a)\overline{v}(a)$$

for u, $v : h\mathbb{Z} \to \mathbb{C}$. We define the Kravchuk functions, for $a \in h\mathbb{Z}$,

$$\varphi_{n,h}(a) = \alpha_{n,h} k_{n,h}(a) \sqrt{\rho_h(a)} \tag{8}$$

where, with $Nh^2 = 2$ and $k = \frac{1}{h^2} + \frac{a}{h}$ for $a \in A_h$,

$$\rho_h(a) = \frac{1}{h 2^{\frac{2}{h^2}}} \frac{\Gamma(1 + \frac{2}{h^2})}{\Gamma(1 + \frac{1}{h^2} + \frac{a}{h})\Gamma(1 + \frac{1}{h^2} - \frac{a}{h})} = \frac{1}{h 2^N} \binom{N}{k} \tag{9}$$

with the Γ function satisfying $\Gamma(1 + n) = n!$, and $\rho_h(a) = 0$ for $a \notin A_h$, and

$$\alpha_{n,h} = \frac{1}{h^n \sqrt{n!}} \sqrt{\frac{\Gamma(1 + \frac{2}{h^2} - n)}{\Gamma(1 + \frac{2}{h^2})}} = \frac{1}{h^n} \sqrt{\frac{(N-n)!}{N! n!}}. \tag{10}$$

We define the following discrete operator: for all $a \in A_h$ and $u \in \ell^2(h\mathbb{Z})$,

$$\begin{aligned} H_h u(a) = &-\frac{1}{h^2}\sqrt{(1 + ah + h^2)(1 - ah)}\, u(a + h) \\ &- \frac{1}{h^2}\sqrt{(1 - ah + h^2)(1 + ah)}\, u(a - h) + \left(1 + \frac{2}{h^2}\right) u(a), \end{aligned} \tag{11}$$

and the lowering and raising operators

$$\left| \begin{aligned} L_{n,h} u(a) &= \left(nh - \frac{1}{h} + a\right) u(a) + \frac{1}{h}\sqrt{(1 - ah)(1 + ah + h^2)}\, u(a + h), \\ R_{n,h} u(a) &= \left(nh - \frac{1}{h} + a\right) u(a) + \frac{1}{h}\sqrt{(1 + ah)(1 - ah + h^2)}\, u(a - h) \end{aligned} \right. \tag{12}$$

and $H_h(a) = L_n f(a) = R_n u(a) = 0$ for $a \in h\mathbb{Z} \backslash A_h$. Then we have the following result, which gathers and rephrases informations that can be found in [11, 15].

Theorem 1. *We have for all h such that $N = \frac{2}{h^2} \in \mathbb{N}^*$, and all $0 \leq n, m \leq N$,*

$$\left|\begin{array}{l} H_h \varphi_{n,h} = (2n+1)\varphi_{n,h} \\ \langle \varphi_{n,h}, \varphi_{m,h}\rangle_{\ell^2(h\mathbb{Z})} = \delta_{nm} \\ L_{n,h}\varphi_{n,h} = \sqrt{n(2-nh^2+h^2)}\varphi_{n-1,h} \\ R_{n,h}\varphi_{n,h} = \sqrt{(2-nh^2)(n+1)}\varphi_{n+1,h}. \end{array}\right. \tag{13}$$

and the operator relations

$$\left|\begin{array}{l} \langle R_{n,h}u, v\rangle_{\ell^2(h\mathbb{Z})} = \langle u, L_{n,h}v\rangle_{\ell^2(h\mathbb{Z})}, \\ \frac{1}{2}(R_{n-1,h}L_{n,h} + L_{n+1,h}R_{n,h}) = (1 - ah - nh^2)H_h + ((2n+1)ah + (n+1)nh^2)\,\mathrm{Id}. \end{array}\right. \tag{14}$$

We give a complete proof of this result (up to some calculations that are left to the reader) in order to make the paper as self contained as possible.

The second result concerns the approximation of the Hermite function and Hermite operator by the Kravchuk functions. We introduce the natural projection from $H^1(\mathbb{R})$ to $\ell^2(h\mathbb{Z})$ defined by

$$(\pi_h f)(a) = f(a),$$

as f has a continuous representative, and we introduce the weighted Sobolev spaces associated with the domain of the Harmonic oscillator operator

$$\Sigma^n(\mathbb{R}) := \left\{\psi \in L^2(\mathbb{R}) \;\middle|\; \|\psi\|_{\Sigma^n(\mathbb{R})} := \|\psi\|_{H^n(\mathbb{R})} + \|\langle x\rangle^n \psi\|_{L^2(\mathbb{R})} < \infty\right\}$$

for $n \geq 0$, with $\langle x\rangle^2 = 1 + x^2$.

Theorem 2. *We have the following error estimates:*

(i) There exists constants C and N_0 such that for all $N \geq N_0$ and $h = \sqrt{2}N^{-\frac{1}{2}}$, and for all $g \in \Sigma^5(\mathbb{R})$, we have

$$\|\pi_h \circ Hg - H_h \circ \pi_h g\|_{\ell^2(h\mathbb{Z})} \leq Ch^2 \|g\|_{\Sigma^5(\mathbb{R})}.$$

(ii) For all $\delta \in (0,1)$ and $\sigma \geq 0$, there exists constants C and N_0 such that for all $N \geq N_0$ and $h = \sqrt{2}N^{-\frac{1}{2}}$,

$$\left\|\langle a\rangle^\sigma \left(\rho_h(a) - \frac{1}{\sqrt{\pi}}e^{-a^2}\right)\right\|_{\ell^2(h\mathbb{Z})} \leq Ch^{2-\delta}, \tag{15}$$

and the uniform estimate

$$\forall\, n \leq \frac{1}{3}\delta|\log h|, \quad \|\langle a\rangle^\sigma(\varphi_{n,h} - \pi_h\psi_n)\|_{\ell^2(h\mathbb{Z})} \leq Ch^{2-\delta}. \tag{16}$$

The previous proposition shows that for asymptotically large modes $n \lesssim |\log h|$, the Hermite coefficients[2] $c_n(f) = (f, \psi_n)_{L^2}$ are well approximated by the discrete Kravchuck coefficients

$$c_{n,h}(f) = \langle \pi_h f, \varphi_{n,h} \rangle_{\ell^2(h\mathbb{Z})} = h \sum_{a \in A_h} \varphi_n(a) f(a).$$

Our last result, which was already noted in [2], shows that these coefficients can be calculated at a cost equivalent to the evaluation of the exponential of a unitary tridiagonal matrix of size N:

Theorem 3. *Let $N \in \mathbb{N}^*$, $h = \sqrt{2} N^{-\frac{1}{2}}$, and for $k \in \{0, \dots, N\}$, let us set*

$$\phi_n(k) = \varphi_{n,h}(a), \quad a = -\frac{1}{h} + hk.$$

Then we have

$$c_{n,h}(f) = \sum_k \phi_n(k) F(k) \quad \Longleftrightarrow \quad C = LF$$

with $F(k) = hf(a)$, $C = (c_{n,h}(f))_{n=0}^N$, $F = (f(k))_{k=0}^N$ and

$$L = \begin{pmatrix} \phi_0(0) & \phi_0(1) & \dots & \phi_0(N) \\ \phi_1(0) & \phi_1(1) & \dots & \phi_1(N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(0) & \phi_N(1) & \dots & \phi_N(N) \end{pmatrix}. \tag{17}$$

Then we have

$$L = e^{\frac{i\pi(N+1)}{4}} D e^{-\frac{i\pi}{4} A} D^* \tag{18}$$

with

(19)

$$D = \begin{pmatrix} 1 & & & (0) \\ & e^{i\frac{\pi}{2}} & & \\ & & \ddots & \\ (0) & & & e^{i\frac{\pi N}{2}} \end{pmatrix}, \quad \text{and} \quad A = \begin{pmatrix} N+1 & -\beta_1 & & (0) \\ -\beta_1 & N+1 & \ddots & \\ & \ddots & \ddots & -\beta_N \\ (0) & & -\beta_N & N+1 \end{pmatrix},$$

where for all $1 \leq k \leq N$

$$\beta_k = \sqrt{k\,(N-k+1)}.$$

[2] We conjecture that the condition $n \lesssim |\log h|$ can be replaced by $n \lesssim h^{-\delta}$ but this would require a subtle analysis of the asymptotics of the Kravchuk functions, yet to be performed.

Note that in practice the matrix-vector multiplication by the exponential of a unitary tridiagonal matrix, can be easily done by using Padé approximations [10]. The complete analysis of this transform from the numerical point of view, as well as combination with highly oscillatory situations, will be the subject of further studies.

3. Discrete orthogonal Kravchuk polynomials

In this section, we give some fundamental properties of the discrete difference theory in order to introduce the Kravchuk polynomials. Some of the statements we give in the following are also proven for a larger class of discrete orthogonal polynomials in the book of A.F. Nikiforov, S.K. Suslov and V.B. Uvarov [11], however they use there an heavier formalism that we try to avoid here for clearness and conciseness purposes.

We first introduce some notations. Recall that in the following, $N \in \mathbb{N}^*$ and h are linked by the formula $h = \sqrt{2}N^{-\frac{1}{2}}$, and we write $X_N = \{0, \dots, N\}$. We define the application $\tau_h : X_N \to A_h$ (see (7)) by the formula

$$\tau_h(k) = h\left(k - \frac{N}{2}\right) = h\left(k - \frac{1}{h^2}\right).$$

We also define the binomial distribution function on the grid X_N

$$\Pi(k) = \frac{1}{2^N}\binom{N}{k} = \frac{1}{2^N}\frac{N!}{k!(N-k)!}, \tag{20}$$

and we extend this function to $\mathbb{Z}$ by setting $\Pi(k) = 0$ for $k \notin X_N$. The Kravchuk polynomials we consider above are of the form

$$\alpha_{n,h}k_{n,h}(a) = \frac{1}{d_n}K_n(\tau_h^{-1}(a), N), \quad \text{with} \quad \tau_h^{-1}(a) = \frac{1}{h^2} + \frac{a}{h},$$

where $K_n(k, N)$, $n = 0, \dots, N$ are the standard Kravchuk polynomials, and where the constant d_n is equal to

$$d_n = \frac{1}{2^n}\sqrt{\frac{N!}{n!(N-n)!}}, \tag{21}$$

so that

$$k_{n,h}(a) = \frac{1}{\alpha_{n,h}d_n}K_n(\tau_h^{-1}(a), N) = h^n 2^n n! K_n(\tau_h^{-1}(a), N). \tag{22}$$

We describe now the properties of the Kravchuk polynomials $K_n(k, N)$.

3.1. **Discrete difference operators.** Let us recall some classical properties of difference operators. We give only some hints for the proof which are essentially based on polynomial and difference calculus that are mostly left to the reader.

Let $f : \mathbb{Z} \to \mathbb{C}$, we define the operators D_+ and D_- from $\mathbb{C}^{\mathbb{Z}}$ to $\mathbb{C}^{\mathbb{Z}}$ by the formula

$$\mathrm{D}_+ f(k) = f(k+1) - f(k), \quad \text{and} \quad \mathrm{D}_- f(k) = f(k) - f(k-1).$$

They satisfy the following properties, for $k \in \mathbb{Z}$, and $f, g \in \mathbb{C}^{\mathbb{Z}}$,

$$\left| \begin{array}{l} \mathrm{D}_+ f(k) = \mathrm{D}_- f(k+1), \\ \mathrm{D}_+\mathrm{D}_- f(k) = \mathrm{D}_-\mathrm{D}_+ f(k) = f(k+1) + f(k-1) - 2f(k), \\ \mathrm{D}_+ \left[f(k)g(k) \right] = f(k)\mathrm{D}_+ g(k) + g(k+1)\mathrm{D}_+ f(k), \\ \mathrm{D}_- \left[f(k)g(k) \right] = f(k-1)\mathrm{D}_- g(k) + g(k)\mathrm{D}_- f(k). \end{array} \right.$$

We can also prove the *discrete Leibniz rule*

$$\mathrm{D}_+^n \left[f(k)g(k) \right] = \sum_{j=0}^{n} \binom{n}{j} \mathrm{D}_+^j f(k) \mathrm{D}_+^{n-j} g(k+j). \tag{23}$$

where D_+^n is the n-th composition of the operator D_+. This formula can be proved by induction using the previous relation for the derivative of products, and the Pascal formula for the binomial coefficients. The following result is also easy to prove:

Proposition 1. *Let $P : \mathbb{Z} \to \mathbb{C}$ be a polynomial of order n. Then $\mathrm{D}_+ P$ and $\mathrm{D}_- P$ are polynomials of order $n-1$ or less.*

Eventually, the binomial distribution (20) satisfies the following property (called *Pearson equation*, see [11]):

$$\forall k \in \mathbb{Z}, \quad \mathrm{D}_+ \left(k\Pi(k) \right) = (N - 2k)\Pi(k). \tag{24}$$

3.2. **Kravchuk polynomials.** The Kravchuk polynomials (see [15]) are given by the following formula: for all $k \in X_N$,

$$K_n(k, N) = \frac{1}{2^n} \sum_{j=0}^{n} (-1)^{n-j} \binom{k}{j} \binom{N-k}{n-j}, \tag{25}$$

where $\binom{k}{j} = k(k-1)\dots(k-j+1)/j!$ for $k \geq j \geq 1$ and $\binom{k}{0} = 1$. Note that $K_n(k, N)$ can be seen as the n-th coefficient of the polynomial

$$F_{k,N}(X) = \left(1 + \frac{X}{2}\right)^k \left(1 - \frac{X}{2}\right)^{N-k} = \sum_{n=0}^{N} K_n(k, N) X^n. \tag{26}$$

Proposition 2. *For a polynomial $P \in \mathbb{R}[X]$, we denote by $\mathrm{lc}(P) \in \mathbb{R}$ its leading coefficient. Then, for all $0 \leq n \leq N$, $K_n(\,\cdot\,, N)$ is a polynomial of degree n, with leading coefficient*

$$\mathrm{lc}(K_n) = \frac{1}{n!}.$$

Proof. The proof directly comes from the fact that for all $0 \leq j \leq k$,

$$P_j(k) := \binom{k}{j} = \frac{1}{j!}k(k-1)\dots(k-j+1)$$

is a polynomial of degree j in k with leading coefficient $1/j!$, and

$$Q_j(k) := \binom{N-k}{n-j} = \frac{1}{(n-j)!}(N-k)(N-k-1)\dots(N-k-n+j+1)$$

is a polynomial of degree $n-j$ in k, with leading coefficient $(-1)^{n-j}/(n-j)!$. Then we have

$$\mathrm{lc}(K_n) = \frac{1}{2^n}\sum_{j=0}^{n}(-1)^{n-j}\mathrm{lc}(P_j)\mathrm{lc}(Q_j) = \frac{1}{2^n}\sum_{j=0}^{n}\frac{1}{j!(n-j)!} = \frac{1}{n!},$$

which gives the result. □

For instance, the first polynomials are given by

$$K_0(k,N) = 1, \quad K_1(k,N) = k - \frac{N}{2} \quad \text{and} \quad K_2(k,N) = \frac{1}{2}k^2 - \frac{N}{2}k + \frac{N(N-1)}{8}.$$

Directly from the explicit formula (25), we can prove the following:

Proposition 3. *For all $k, n \in \{0, \dots, N\}$,*

$$K_n\left(N-k\right) = (-1)^n K_n(k),$$

and

$$(-1)^n 2^n \binom{N}{k} K_n(k) = (-1)^k 2^k \binom{N}{n} K_k(n). \tag{27}$$

Finally, the polynomials $K_n(\,\cdot\,, N)$ satisfy the following difference equation:

Proposition 4. *For all $k, n \in \{0, \dots, N\}$, $K_n(\,\cdot\,, N)$ satisfies the equation*

$$k\mathrm{D}_+\mathrm{D}_-K_n(k) + (N-2k)\mathrm{D}_+K_n(k) = -2nK_n(k) \tag{28}$$

Proof. We only give the main points. First this equation is equivalent to

$$(N-k)K_n(k+1) - (N-2n)K_n(k) + kK_n(k-1) = 0$$

for all $0 \leq k \leq N$. Differentiating equation (26) with respect to X, we get that

$$F'_{k,N+1}(X) = -\frac{k}{2}F_{k-1,N}(X) + \frac{N+1-k}{2}F_{k,N}(X).$$

We evaluate the coefficients of the monomial X^n in the previous expression, and we find

$$(n+1)K_{n+1}(k,N+1) = -\frac{k}{2}K_n(k-1,N) + \frac{N+1-k}{2}K_n(k,N). \tag{29}$$

On the other hand, using the definition of the polynomials, we have

$$K_n(k+1,N+1) = K_n(k,N) - \frac{1}{2}K_{n-1}(k,N).$$

Shifting N to $N-1$ into this last expression, we have

$$K_n(k+1,N) = K_n(k,N-1) - \frac{1}{2}K_{n-1}(k,N-1). \tag{30}$$

In the same way, we get that

$$K_n(k,N+1) = K_n(k,N-1) + \frac{1}{2}K_{n-1}(k,N),$$

so shifting N to $N-1$ we obtain

$$K_n(k,N) = K_n(k,N-1) + \frac{1}{2}K_{n-1}(k,N-1). \tag{31}$$

Substracting equation (30) to equation (31), we get that

$$K_n(k,N) - K_n(k+1,N) = K_{n-1}(k,N-1). \tag{32}$$

Finally, going back to equation (29), shifting n to $n-1$, N to $N-1$ and multiplying by 2, we have

$$2nK_n(k,N) - (N-k)K_{n-1}(k,N-1) + kK_{n-1}(k-1,N-1) = 0,$$

so using equation (32) for both K_{n-1} we get that

$$2nK_n(k,N) - (N-k)\left(K_n(k,N) - K_n(k+1,N)\right) + k\left(K_n(k-1,N) - K_n(k,N)\right) = 0.$$

Simplifying this equation, we get the result. □

Using (24) we get the following Sturm-Liouville difference equation. From now on we will often omit the N in the notation for the Kravchuk polynomial, and write $K_n(k) = K_n(k,N)$.

Corollary 1. *For all $0 \leq n \leq N$, K_n satisfies the equation*

$$\mathrm{D}_+\left[k\Pi(k)\mathrm{D}_-K_n(k)\right] = 2n\Pi(k)K_n(k). \tag{33}$$

Proof. We multiply equation (28) by $\Pi(k)$ and we use the Pearson equation (24), so that

$$\begin{aligned} &k\Pi(k)\mathrm{D}_+\mathrm{D}_-K_n(k) + (N-2k)\Pi(k)\mathrm{D}_+K_n(k) - \lambda_n K_n(k)\Pi(k) \\ &\qquad = k\Pi(k)\mathrm{D}_+\mathrm{D}_-K_n(k) + \mathrm{D}_-K_n(k+1)\mathrm{D}_+\left[k\Pi(k)\right] - \lambda_n K_n(k)\Pi(k) \\ &\qquad\qquad = \mathrm{D}_+\left[k\Pi(k)\mathrm{D}_-K_n(k)\right] - \lambda_n K_n(k)\Pi(k) = 0. \end{aligned}$$

□

We also have the following orthogonality property:

Proposition 5. *For $0 \leq n, m \leq N$, we have*

$$\sum_{k=0}^{N} K_n(k)K_m(k)\Pi(k) = \delta_{n,m}d_n^2, \tag{34}$$

with the normalization constant d_n given by (21).

Proof. The proof consists in expanding the relation

$$\left[\left(1-\frac{X}{2}\right)\left(1-\frac{Y}{2}\right)+\left(1+\frac{X}{2}\right)\left(1+\frac{Y}{2}\right)\right]^N = 2^N\left(1+\frac{XY}{4}\right)^N$$

using (26). □

The following formula will explain the specific form of the Kravchuk transform:

Proposition 6. *For $0 \leq n, m \leq N$,*

$$\sum_{k=0}^{N} 2^k K_k(n)K_m(k)e^{\frac{i(k-m)\pi}{2}} = 2^{\frac{N}{2}}e^{\frac{in\pi}{4}}e^{-\frac{i\pi N}{4}}K_m(n,N).$$

Proof. The proof consists in expanding the relation

$$\begin{aligned} &\left(1-\frac{X}{2}\right)^N\left(1+i\frac{1+X/2}{1-X/2}\right)^n\left(1-i\frac{1+X/2}{1-X/2}\right)^{N-n} \\ &\qquad\qquad = (1+i)^n(1-i)^{N-n}\left(1+i\frac{X}{2}\right)^n\left(1-i\frac{X}{2}\right)^{N-n}, \end{aligned}$$

by using the definition of the Kravchuk polynomials. □

We finally give the three-term recurrence relation for the Kravchuk polynomials:

Proposition 7. *For all $n \in \mathbb{N}^*$ and for $k \in X_N$, we have*

$$(n+1)K_{n+1}(k) = \left(k-\frac{N}{2}\right)K_n(k) - \frac{N-n+1}{4}K_{n-1}(k). \tag{35}$$

Proof. We denote by a_n and b_n the leading coefficients in the expansion

$$K_n(k) = a_n k^n + b_n k^{n-1} + \dots,$$

and we have (see for instance [11, p. 44])

$$a_n = \frac{1}{n!}, \quad \text{and} \quad b_n = -\frac{N}{2(n-1)!}.$$

Let us now remark that

$$\deg\left(K_{n+1} - \frac{a_{n+1}}{a_n} k K_n\right) \leq n,$$

This shows that

$$K_{n+1} - \frac{a_{n+1}}{a_n} k K_n = \sum_{l=0}^{n} c_l K_l,$$

and by taking the weighted discrete scalar products with weight $\Pi(k)$ and using (34), we can prove that $c_l = 0$ for $l < n-1$ as $\deg(kK_l) < n$. We obtain a relation of the form

$$kK_n = \alpha_n K_{n+1} + \beta_n K_n + \gamma_n K_{n-1},$$

whose coefficients α_n, β_n and γ_n can be found by the formulas

$$\alpha_n = \frac{a_n}{a_{n+1}}, \quad \beta_n = \frac{b_n}{a_n} - \frac{b_{n+1}}{a_{n+1}}, \quad \gamma_n = \frac{a_{n-1}}{a_n} \frac{d_n^2}{d_{n-1}^2}$$

by standard computations, which gives the result. □

We are now going to prove the discrete counterpart of the classical Rodrigues formula for Kravchuk polynomials, as it will be useful for the derivation of the lowering and raising operators. We first need to introduce some notations and properties in the following lemma, which is a consequence of the formula for the discrete derivative of products:

Lemma 1. *Let n, $m \geq 0$, and $k \in \mathbb{Z}$. We denote*

$$\Pi_m(k) = \Pi(k+m) \prod_{j=1}^{m} (k+j), \quad K_n^{(m)} = \mathrm{D}_+^m K_n \quad \textit{and} \quad \mu_n^{(m)} = 2n - 2m.$$

Then, for all $k \in \mathbb{Z}$, $K_n^{(m)}$ satisfies the following Sturm-Liouville difference equation:

$$\mathrm{D}_+ \left[k \Pi_m(k) \mathrm{D}_- K_n^{(m)}(k) \right] + \mu_n^{(m)} \Pi_m(k) K_n^{(m)}(k) = 0.$$

Proof. Differentiating equation (28), we get that

$$\mathrm{D}_+ \left[k \mathrm{D}_- K_n^{(1)}(k) \right] + \mathrm{D}_+ \left[(N - 2k) K_n^{(1)}(k) \right] + \lambda_n K_n^{(1)}(k) = 0,$$

which simplifies in

$$k\mathrm{D}_+\mathrm{D}_-K_n^{(1)}(k)+(N-2k-1)\mathrm{D}_+K_n^{(1)}(k)+(\lambda_n-2)K_n^{(1)}(k)=0.$$

Applying m times this computation, we can prove by induction that $\forall m\geq 0$, that $K_n^{(m)}$ satisfies the following difference equation:

$$k\mathrm{D}_+\mathrm{D}_-K_n^{(m)}(k)+(N-2k-m)\mathrm{D}_+K_n^{(m)}(k)+(\lambda_n-2m)K_n^{(m)}(k)=0.$$

We are now going to show that Π_m satisfies a Pearson-type equation. In fact,

$$\begin{aligned}\mathrm{D}_+\left[k\Pi_m(k)\right] &= (k+1)\Pi(k+1+m)\prod_{j=1}^{m}(k+1+j)-k\Pi(k+m)\prod_{j=1}^{m}(k+j)\\ &=\frac{1}{2^N}\left(\prod_{j=1}^{m}(k+j)\right)\left[(k+1+m)\binom{N}{k+1+m}-k\binom{N}{k+m}\right]\\ &=\frac{1}{2^N}\left(\prod_{j=1}^{m}(k+j)\right)\left[(N-k-m)\binom{N}{k+m}-k\binom{N}{k+m}\right]\\ &=(N-2k-m)\Pi_m(k).\end{aligned}$$

We then just have to reproduce the computation of the proof of Corollary 1 to get the result. □

Proposition 8. ***(Rodrigues formula).*** *For $k\in X_N$, we have*

$$K_n(k)\Pi(k)=\frac{(-1)^n}{2^n n!}\mathrm{D}_+^n\left[\Pi(k)\prod_{j=0}^{n-1}(k-j)\right]. \tag{36}$$

Proof. With the previous notations, it is a direct consequence of Lemma 1 to see that

$$\Pi_m(k)K_n^{(m)}(k)=-\frac{1}{\mu_m^{(n)}}\mathrm{D}_+\left[k\Pi_m(k)\mathrm{D}_-K_n^{(m)}(k)\right]=-\frac{1}{\mu_m^{(n)}}\mathrm{D}_-\left[\Pi_{m+1}(k)K_n^{(m+1)}(k)\right].$$

By induction we get that

$$\Pi(k)K_n(k)=\prod_{j=0}^{n-1}\left(-\frac{1}{\mu_j^{(n)}}\right)\mathrm{D}_-^n\left[\Pi_n(k)K_n^{(n)}(k)\right].$$

As K_n is polynomial of degree n, $K_n^{(n)}=\frac{1}{n!}$ is a constant, so we calculate directly,

$$\Pi(k)K_n(k)=c_n\mathrm{D}_-^n\Pi_n(k)=\frac{(-1)^n}{2^n n!}\mathrm{D}_+^n\left[\Pi(k)\prod_{j=0}^{n-1}(k-j)\right],$$

which gives the result. □

Corollary 2. *For all $n \in \mathbb{N}$ and $k \in X_N$,*

$$2(n+1)K_{n+1}(k) = (n+2k-N)K_n(k) - k\mathrm{D}_- K_n(k).$$

Proof. With $c_n = \frac{(-1)^n}{2^n n!}$, by the Rodrigues formula, we have that

$$K_{n+1}(k)\Pi(k) = c_{n+1}\mathrm{D}_-^{n+1}\Pi_{n+1}(k) = c_{n+1}\mathrm{D}_-^n\left[\mathrm{D}_+\Pi_{n+1}(k-1)\right].$$

Noticing that we can compute

$$\mathrm{D}_+\Pi_{n+1}(k-1) = \mathrm{D}_+\left[\Pi(k+n)\prod_{j=1}^{n+1}(k-1+j)\right] = \mathrm{D}_+\left[k\Pi_n(k)\right] = (N-2k-n)\Pi_n(k),$$

we see that

$$\begin{aligned} K_{n+1}(k)\Pi(k) &= c_{n+1}\mathrm{D}_-^n\left[(N-2k-n)\Pi_n(k)\right] \\ &= c_{n+1}\mathrm{D}_-^{n-1}\left[(N-2k-n)\mathrm{D}_-\Pi_n(k) - 2\mathrm{D}_-\Pi_n(k-1)\right] \\ &= c_{n+1}\left((N-2k-n)\mathrm{D}_-^n\left[\Pi_n(k)\right] - 2n\mathrm{D}_-^{n-1}\left[\Pi_n(k-1)\right]\right) \end{aligned}$$

as we can prove easily by induction. Since

$$\mathrm{D}_- K_n(k) = K_n^{(1)}(k-1) = \frac{c_n}{k\Pi(k)}\mathrm{D}_-^{n-1}\left[\Pi_n(k-1)\right],$$

we obtain

$$K_{n+1}(k) = \frac{c_{n+1}}{c_n}(N-2k-n)K_n(k) - \frac{c_{n+1}}{c_n}\mathrm{D}_- K_n(k)$$

which shows the result. □

3.3. **Kravchuk functions.** We now define the Kravchuk functions $(\phi_n)_n$, such that for all $k \in X_N$,

$$\phi_n(k) = \frac{1}{d_n}K_n(k)\sqrt{\Pi(k)}, \tag{37}$$

and $\phi_n(k) = 0$ elsewhere. From (34) we immediately get that the sequence $(\phi_n)_n$ is orthogonal for the discrete scalar product on X_N:

Proposition 9. *For all $0 \leq n, m \leq N$,*

$$\langle \phi_n, \phi_m \rangle_{\ell^2(\mathbb{Z})} = \sum_{k=0}^{N} \phi_n(k)\phi_m(k) = \delta_{n,m}.$$

Several properties of the Kravchuk polynomials can of course be easily passed to the Kravchuk functions and we omit the proof of the following formulas:

Proposition 10. *For all* $0 \leq k, n \leq N$,

$$(-1)^k \phi_n(k) = (-1)^n \phi_k(n);$$

and for all $0 \leq m, n \leq N$,

$$\phi_m(n) e^{\frac{in\pi}{4}} e^{-\frac{i\pi N}{4}} = \sum_{k=0}^{N} \phi_k(n) \phi_m(k) e^{\frac{i(k-m)\pi}{2}}.$$

3.4. **Kravchuk oscillator.** As Hermite functions for the harmonic oscillator, Kravchuk functions are eigenfunctions for a particular discrete operator denoted $\mathcal{H}$, which also admits a ladder operator description that we explicit in the following.

Proposition 11. ***(Kravchuk oscillator on*** $\mathbb{Z}$***).*** *We define the operator* $\mathcal{H}$ *for* $f \in \ell^2(\mathbb{Z})$ *by*

$$\mathcal{H}f(k) = \sqrt{(k+1)(N-k)} f(k+1) + \sqrt{k(N-k+1)} f(k-1) - N f(k),$$

for $k \in X_N$, *and* $\mathcal{H}f(k) = 0$ *if* $k \notin X_N$. *Then*

$$\mathcal{H}\phi_n = -2n\phi_n.$$

Proof. It comes directly from multiplying equation (28) by $d_n^{-1}\sqrt{\Pi(k)}$, and noticing that formally

$$\frac{\Pi(k)}{\Pi(k+1)} = \frac{k+1}{N-k} \quad \text{and} \quad \frac{\Pi(k)}{\Pi(k-1)} = \frac{N-k+1}{k}.$$

□

Proposition 12. ***(Lowering and raising operators).***
We define the operators $\mathcal{L}$ *and* $\mathcal{R}$ *acting on* $\ell^2(\mathbb{Z})$ *by*

$$\left| \begin{array}{l} \mathcal{L}f(k) = (k-N)f(k) + \sqrt{(N-k)(k+1)} f(k+1), \\ \mathcal{R}f(k) = (k-N)f(k) + \sqrt{k(N-k+1)} f(k-1), \end{array} \right.$$

for $k \in X_N$, $\mathcal{L}f(k) = \mathcal{R}f(k) = 0$ *if* $k \notin X_N$, *and we denote*

$$\mathcal{L}_n = \mathcal{L} + n\mathrm{Id} \quad \text{and} \quad \mathcal{R}_n = \mathcal{R} + n\mathrm{Id},$$

for all $n \geq 0$. *Then, for all* $0 \leq n \leq N$, *we have*

$$\mathcal{L}_n\phi_n = \sqrt{n(N-n+1)}\phi_{n-1} \quad \text{and} \quad \mathcal{R}_n\phi_n = \sqrt{(N-n)(n+1)}\phi_{n+1}. \tag{38}$$

In particular, for all $1 \leq n \leq N$, *we have*

$$\mathcal{R}_{n-1}\mathcal{L}_n\phi_n = n(N-n+1)\phi_n \quad \text{and} \quad \mathcal{L}_{n+1}\mathcal{R}_n\phi_n = n(N-n+1)\phi_n.$$

Proof. We compute

$$\begin{aligned} d_n\mathcal{R}_n\phi_n(k) &= (k+n-N)K_n(k)\sqrt{\Pi(k)} + \sqrt{k(N-k+1)}K_n(k-1)\sqrt{\Pi(k-1)} \\ &= (k+n-N)K_n(k)\sqrt{\Pi(k)} + k\sqrt{\Pi(k)}K_n(k-1) \\ &= (n+2k-N)K_n(k)\sqrt{\Pi(k)} - \sqrt{\Pi(k)}k\mathrm{D}_-K_n(k) \\ &= -2(n+1)K_{n+1}(k)\sqrt{\Pi(k)} \end{aligned}$$

using Corollary 2, so

$$\mathcal{R}_n\phi_n(k) = -2(n+1)\frac{d_{n+1}}{d_n}\phi_{n+1}(k) = \sqrt{(N-n)(n+1)}\phi_{n+1}(k).$$

The calculation for the operator $\mathcal{L}_n$ is entirely similar. ☐

Proposition 13. ***(Self-adjointness of $\mathcal{H}$).***
For all $n \geq 0$, the operators $\mathcal{L}_n$ and $\mathcal{R}_n$ are adjoint, namely for all u, $v \in \ell^2(\mathbb{Z})$,

$$\langle \mathcal{R}_n u, v\rangle_{\ell^2(\mathbb{Z})} = \langle u, \mathcal{L}_n v\rangle_{\ell^2(\mathbb{Z})}.$$

In particular, the operator $\mathcal{H}$ is self-adjoint.

Proof. We compute

$$\langle \mathcal{R}_n u, v\rangle = \sum_{k=0}^{N}(k-N+n)u(k)v(k) + \sum_{k=0}^{N}\sqrt{k(N-k+1)}u(k-1)v(k).$$

In order to make the change of variable $k \mapsto k+1$, we need to remark that the quantity

$$\sqrt{k(N-k+1)} = 0 \text{ when } k=0$$

and

$$\sqrt{(k+1)(N-k)} = 0 \text{ when } k=N,$$

so we can rewrite the secund sum

$$\begin{aligned} \sum_{k=0}^{N}\sqrt{k(N-k+1)}u(k-1)v(k) &= \sum_{k=1}^{N}\sqrt{k(N-k+1)}u(k-1)v(k) \\ &= \sum_{k=0}^{N-1}\sqrt{(k+1)(N-k)}u(k)v(k+1) \\ &= \sum_{k=0}^{N}\sqrt{(k+1)(N-k)}u(k)v(k+1). \end{aligned}$$

The proof for $\mathcal{H}$ is a consequence of the factorization of $\mathcal{H}$ of the next proposition. ☐

Proposition 14. ***(Factorization of $\mathcal{H}$).***
For all $0 \leq n \leq N$ and $k \in X_N$, we have

$$\mathcal{R}_{n-1}\mathcal{L}_n = (k+n-1-N)\left(\mathcal{H}+n\mathrm{Id}\right)+nk\mathrm{Id}$$

and

$$\mathcal{L}_{n+1}\mathcal{R}_n = (k+n+1-N)\left(\mathcal{H}+n\mathrm{Id}\right)+(nk+N)\mathrm{Id},$$

and therefore

$$\begin{aligned}&\frac{1}{2}(\mathcal{R}_{n-1}\mathcal{L}_n+\mathcal{L}_{n+1}\mathcal{R}_n)\\&\qquad=(k+n-N)(\mathcal{H}-1)+\left((n+1)(k+n-N)+nk+\frac{N}{2}\right)\mathrm{Id}.\end{aligned}$$

Proof. We compute

$$\begin{aligned}&\mathcal{L}_{n+1}\mathcal{R}_nf(k)=(k+n+1-N)\mathcal{R}_nf(k)+\sqrt{(N-k)(k+1)}\mathcal{R}_nf(k+1)\\&\quad=(k+n+1-N)(k+n-N)f(k)+(k+n+1-N)\sqrt{k(N-k+1)}f(k-1)\\&\qquad+(k+1+n-N)\sqrt{(N-k)(k+1)}f(k+1)+(N-k)(k+1)f(k)\\&\quad=(k+n+1-N)\left(\mathcal{H}+n\mathrm{Id}\right)f(k)+k(k+n+1-N)f(k)+(k+1)(N-k)f(k)\\&\qquad=(k+n+1-N)\left(\mathcal{H}+n\mathrm{Id}\right)f(k)+(N+nk)f(k).\end{aligned}$$

We compute $\mathcal{R}_{n-1}\mathcal{L}_nf(k)$ the same way:

$$\begin{aligned}&\mathcal{R}_{n-1}\mathcal{L}_nf(k)=(k+n-1-N)\mathcal{L}_nf(k)+\sqrt{k(N-k+1)}\mathcal{L}_nf(k-1)\\&\quad=(k+n-1-N)(k+n-N)f(k)+(k+n-1-N)\sqrt{(k+1)k(N-k)}f(k+1)\\&\qquad+(k+n-1-N)\sqrt{(N-k+1)k}f(k+1)+(N-k+1)kf(k)\\&\quad=(k+n-1-N)\left(\mathcal{H}+n\mathrm{Id}\right)f(k)+k(k+n+1-N)f(k)+(k+1)(N-k)f(k)\\&\qquad=(k+n-1-N)\left(\mathcal{H}+n\mathrm{Id}\right)f(k)+nkf(k).\end{aligned}$$

and thus

$$\begin{aligned}\frac{1}{2}(\mathcal{R}_{n-1}\mathcal{L}_n+\mathcal{L}_{n+1}\mathcal{R}_n)&=(k+n-N)\left(\mathcal{H}+n\mathrm{Id}\right)+\left(nk+\frac{N}{2}\right)\mathrm{Id}\\&=(k+n-N)(\mathcal{H}-1)+(n+1)(k+n-N)\mathrm{Id}+\left(nk+\frac{N}{2}\right)\mathrm{Id}.\end{aligned}$$

□

3.5. **Kravchuk functions and Kravchuk oscillator on $h\mathbb{Z}$.** Theorem 1 is now a consequence of the previous results, using (22). For instance, we get that for all n, $m \geq 0$,

$$h \sum_{a\in h\mathbb{Z}} K_n(\tau_h^{-1}(a))K_m(\tau_h^{-1}(a))\rho_h(a) = \delta_{n,m}d_n^2,$$

as we have $\rho_h(a) = \frac{1}{h}\Pi(\tau_h^{-1}(a))$, see (9). We can also check that with formula (37), we have

$$\varphi_{n,h}(a) = \frac{1}{\sqrt{h}}\phi_n(\tau_h^{-1}(a)).$$

This directly gives that

$$h \sum_{a\in h\mathbb{Z}} \varphi_{n,h}(a)\varphi_{m,h}(a) = \delta_{n,m}.$$

Then we define for $f \in \ell^2(h\mathbb{Z})$,

$$\left| \begin{array}{l} H_h f(a) = (-\mathcal{H}+1)f \circ \tau_h^{-1}(a), \\ L_{n,h} f(a) = h\mathcal{L}_n f \circ \tau_h^{-1}(a), \\ R_{n,h} f(a) = h\mathcal{R}_n f \circ \tau_h^{-1}(a), \end{array} \right.$$

and from the expression of these operators in variable a, we deduce (11) and (12), and Theorem 1 follows. Eventually, Proposition 7 shows that for all $n \in \mathbb{N}^*$, and for all $a \in h\mathbb{Z}$,

$$(n+1)K_{n+1}(\tau_h^{-1}(a)) = \frac{a}{h}K_n(\tau_h^{-1}(a)) - \frac{1}{4}(N-n+1)K_{n-1}(\tau_h^{-1}(a)).$$

As $k_{n,h}(a) = h^n 2^n n! K_n(\tau_h^{-1}(a))$, we calculate that for all $n \in \mathbb{N}^*$ and $a \in h\mathbb{Z}$,

$$k_{n+1,h} = 2ak_{n,h} - 2n\left(1 - h^2\Big(\frac{n-1}{2}\Big)\right)k_{n-1,h},$$

which is (6).

4. Convergence of Kravchuk oscillator

We first show some inequalities between discrete and continuous Sobolev spaces, which will be needed for the proof of Theorem 2.

Lemma 2. *Let $g \in H^1(\mathbb{R})$, then $\pi_h g \in \ell^2(h\mathbb{Z})$ and*

$$\|\pi_h g\|_{\ell^2(h\mathbb{Z})} \leq 2\|g\|_{H^1(\mathbb{R})} \tag{39}$$

as soon as $h \leq \sqrt{2}$.

Proof. Let $a = jh \in h\mathbb{Z}$ with $j \in \mathbb{Z}$. We take $x \in [a, a+h]$. As $g \in H^1(\mathbb{R})$, we can write that

$$(\pi_h g)(a) = g(x) - \int_a^x \partial_x g(y) \mathrm{d}y,$$

so taking the square on this equation, and by Cauchy-Schwarz inequality and Young's inequality for products, we see that

$$|\pi_h g(a)|^2 \leq 2|g(x)|^2 + 2(x-a) \int_a^{a+h} |\partial_x g(y)|^2 \, \mathrm{d}y.$$

Then, integrating (with respect to $\mathrm{d}x$) between a and $a+1$ and summing over $a \in h\mathbb{Z}$, we obtain that

$$h \sum_{a \in h\mathbb{Z}} |\pi_h g(a)|^2 \leq 2 \int_{\mathbb{R}} |g(x)|^2 \mathrm{d}x + h^2 \int_{\mathbb{R}} |\partial_x g(y)|^2 \, \mathrm{d}y,$$

so

$$\|\pi_h g\|^2_{\ell^2(h\mathbb{Z})} \leq 2\|g\|^2_{L^2(\mathbb{R})} + h^2 \|g\|^2_{\dot{H}^1(\mathbb{R})},$$

hence we get the results as soon as $h \leq \sqrt{2}$. □

Remark 1. *Note that in our case, as $h = \sqrt{2/N}$ with $N \geq 1$, we always fulfill the condition $h \leq \sqrt{2}$.*

We now state a lemma that will be useful in the proof of Theorem 2:

Lemma 3. *For all α, $\beta \in \mathbb{N}$ and n such that $\alpha + \beta \leq n-1$, there exists C such that we have for all $g \in \Sigma^n(\mathbb{R})$ with $n \in \mathbb{N}^*$,*

$$\|a^\beta \pi_h \partial_x^\alpha g\|_{\ell^2(h\mathbb{Z})} \leq C\|g\|_{\Sigma^n(\mathbb{R})}.$$

Proof. We first recall a classical lemma from functional analysis, whose complete proof can be found in [7] or [3]: for all α, $\beta \in \mathbb{N}$ such that $\alpha + \beta \leq n$, we have

$$\|x^\alpha \partial_x^\beta g\|_{L^2(\mathbb{R})} \leq C\|g\|_{\Sigma^n(\mathbb{R})}$$

for some constant C independent of g. It naturally follows that if $\alpha + \beta \leq n-1$, then

$$\|x^\beta \partial_x^\alpha g\|_{H^1(\mathbb{R})} \leq C\|g\|_{\Sigma^n(\mathbb{R})}. \tag{40}$$

as

$$\partial_x \left(x^\beta \partial_x^\alpha g\right) = \beta x^{\beta-1} \partial_x^\alpha g + x^\beta \partial_x^{\alpha+1} g.$$

Combining the fact that

$$\pi_h \left(x^\beta \partial_x^\alpha g\right) = a^\beta \pi_h \partial_x^\alpha g$$

with equation (40) and Lemma 2, we then get the result. □

Proof of Theorem 2. Let $g \in \Sigma^5(\mathbb{R})$ and $a \in h\mathbb{Z}$, we have

$$(\pi_h H g)(a) = -g''(a) + a^2 g(a),$$

($g'' \in H^3(\mathbb{R})$ well admits a continuous representative), and

$$\begin{aligned}(H_h \pi_h g)(a) = -\frac{1}{h^2}\sqrt{(1+ah+h^2)(1-ah)}g(a+h) \\ -\frac{1}{h^2}\sqrt{(1-ah+h^2)(1+ah)}g(a-h) + \left(1+\frac{2}{h^2}\right)g(a)\end{aligned}$$

if $a \in A_h = h\mathbb{Z} \cap \left[-\frac{1}{h}, \frac{1}{h}\right]$, and $H_h \pi_h g(a) = 0$ elsewhere. We first compute that

$$(1 \mp ah + h^2)(1 \pm ah) = 1 + h^2(1 - a^2 \pm ah),$$

and we denote

$$R_h^{\pm}(a) := 1 + \frac{h^2}{2}\left(1 - a^2 \pm ah\right) - \sqrt{1 + h^2\left(1 - a^2 \pm ah\right)}$$

for all $a \in A_h$, and $R_h^{\pm}(a) := 0$ elsewhere. We have

$$\begin{aligned}(H_h \pi_h g - \pi_h H)(a) &= g''(a) - \Delta_h g(a) - (a^2-1)g(a) \\ &+ \frac{1}{h^2}R_h^-(a)g(a+h) + \frac{1}{h^2}R_h^+(a)g(a-h) \\ &- (1-a^2+ah)g(a-h) - (1-a^2-ah)g(a+h),\end{aligned}$$

where

$$\Delta_h u(a) = \frac{u(a+h)+u(a-h)-2u(a)}{h^2}.$$

Hence, by a triangular inequality, we get that

$$\|\pi_h H g - H_h \pi_h g\|_{\ell^2(h\mathbb{Z})} \leq \mathcal{S}_1 + \mathcal{S}_2 + \mathcal{S}_3 + \mathcal{S}_4 + \mathcal{S}_5,$$

with

$$\mathcal{S}_1^2 = h \sum_{a \in h\mathbb{Z}} \left|g''(a) - \Delta_h g(a) \mathbf{1}_{A_h}(a)\right|^2,$$

$$\mathcal{S}_2^2 = h \sum_{a \in h\mathbb{Z}} \left|(a^2-1)\left(g(a) - \frac{g(a+h)+g(a-h)}{2}\mathbf{1}_{A_h}(a)\right)\right|^2,$$

$$\mathcal{S}_3^2 = h \sum_{a \in A_h} \left|ah\frac{g(a-h)-g(a+h)}{2}\right|^2,$$

$$\mathcal{S}_4^2 = h \sum_{a \in A_h} \left|\frac{g(a+h)}{h^2}R_h^-(a)\right|^2 \quad \text{and} \quad \mathcal{S}_5^2 = h \sum_{a \in A_h} \left|\frac{g(a-h)}{h^2}R_h^+(a)\right|^2.$$

We first look at $\mathcal{S}_1$, and we split the sum over A_h and $h\mathbb{Z}\backslash A_h$, so that

$$\mathcal{S}_1^2 = h \sum_{a\in A_h} |g''(a) - \Delta_h g(a)|^2 + h \sum_{a\notin A_h} |g''(a)|^2 .$$

For all $a \in A_h$, as $g \in H^5(\mathbb{R}) \hookrightarrow \mathcal{C}^4(\mathbb{R})$ by Taylor formula we get that

$$g(a+h) = g(a) + hg'(a) + \frac{h^2}{2} g''(a) + \frac{h^3}{6} g^{(3)}(a) + \int_a^{a+h} \frac{(a+h-s)^3}{6} g^{(4)}(s)\mathrm{d}s$$

and

$$g(a-h) = g(a) - hg'(a) + \frac{h^2}{2} g''(a) - \frac{h^3}{6} g^{(3)}(a) - \int_{a-h}^{a} \frac{(a-h-s)^3}{6} g^{(4)}(s)\mathrm{d}s,$$

hence by direct cancellations

$$\begin{aligned} g''(a) - \frac{g(a+h)+g(a-h)-2g(a)}{h^2} & \\ = -\frac{1}{6h^2} \left(\int_a^{a+h} (a+h-s)^3 g^{(4)}(s)\mathrm{d}s - \int_{a-h}^{a} (a-h-s)^3 g^{(4)}(s)\mathrm{d}s \right). \end{aligned}$$

By the standard inequality $|a-b|^2 \le 2(|a|^2 + |b|^2)$, we infer that

$$\begin{aligned} |g''(a) - \Delta_h g(a)|^2 & \\ = \frac{1}{18h^4} \left(\left| \int_a^{a+h} (a+h-s)^3 g^{(4)}(s)\mathrm{d}s \right|^2 + \left| \int_{a-h}^{a} (a-h-s)^3 g^{(4)}(s)\mathrm{d}s \right|^2 \right), \end{aligned}$$

so by Cauchy-Schwarz inequality we get, for instance for the first integral, that

$$\begin{aligned} \left| \int_a^{a+h} (a+h-s)^3 g^{(4)}(s)\mathrm{d}s \right|^2 &\le \left(\int_a^{a+h} (a+h-s)^6 \right) \left(\int_a^{a+h} |g^{(4)}(s)|^2 \mathrm{d}s \right) \\ &= \frac{h^7}{7} \int_a^{a+h} |g^{(4)}(s)|^2 \mathrm{d}s, \end{aligned}$$

and the same way,

$$\left| \int_a^{a+h} (a-h-s)^3 g^{(4)}(s)\mathrm{d}s \right|^2 \le \frac{h^7}{7} \int_{a-h}^{a} |g^{(4)}(s)|^2 \mathrm{d}s$$

so finally, as $A_h \subset h\mathbb{Z}$,

$$h \sum_{a\in A_h} |g''(a) - \Delta_h g(a)|^2 \le h \sum_{a\in h\mathbb{Z}} \frac{1}{18h^4} \frac{h^7}{7} \int_{a-h}^{a+h} |g^{(4)}(s)|^2 \mathrm{d}s \le \frac{h^4}{63} \|g^{(4)}\|_{L^2(\mathbb{R})}^2 . \tag{41}$$

On the other hand, as $|a| \geq 1/h$,

$$\sum_{a \notin A_h} |g''(a)|^2 = \sum_{a \notin A_h} \frac{1}{|a|^4} |a|^4 |g''(a)|^2 \leq h^4 \sum_{a \notin A_h} |a|^4 |g''(a)|^2 \leq Ch^3 \|a^2 g''(\cdot)\|^2_{\ell^2(h\mathbb{Z})},$$

using the fact that $h\mathbb{Z} \backslash A_h \subset h\mathbb{Z}$, so

$$\left(h \sum_{a \notin A_h} |g''(a)|^2 \right) \leq Ch^4 \|g\|^2_{\Sigma^5(\mathbb{R})} \tag{42}$$

using Lemma 3, as in particular $\|a^2 g''(\cdot)\|^2_{\ell^2(h\mathbb{Z})} \leq C\|g\|^2_{\Sigma^5(\mathbb{R})}$. Finally, combining estimates (41) and (42), as $\|g^{(4)}\|_{L^2(\mathbb{R})} \leq C\|g\|_{\Sigma^5(\mathbb{R})}$, we get that

$$\mathcal{S}_1 \leq Ch^2 \|g\|_{\Sigma^5(\mathbb{R})}.$$

In the same vein, we see that

$$\mathcal{S}_2^2 = h \sum_{a \in A_h} \left| (a^2 - 1) \left(g(a) - \frac{g(a+h) + g(a-h)}{2} \right) \right|^2 + h \sum_{a \notin A_h} |(a^2 - 1) g(a)|^2.$$

First, for $a \in A_h$, as from Taylor formula

$$\begin{aligned} g(a+h) &= g(a) + hg'(a) + \textstyle\int_a^{a+h} (a+h-s) g''(s) \mathrm{d}s \\ g(a-h) &= g(a) - hg'(a) - \textstyle\int_{a-h}^{a} (a-h-s) g''(s) \mathrm{d}s, \end{aligned}$$

we have

$$g(a) - \frac{g(a+h) + g(a-h)}{2} = -\int_a^{a+h} (a+h-s) g''(s) \mathrm{d}s + \int_{a-h}^{a} (a-h-s) g''(s) \mathrm{d}s.$$

Estimating for instance the first integral, we naturally get that

$$\begin{aligned} \left| \int_a^{a+h} (a+h-s) g''(s) \mathrm{d}s \right|^2 &\leq \left(\int_a^{a+h} (a+h-s)^2 \mathrm{d}s \right) \left(\int_a^{a+h} |g''(s)|^2 \mathrm{d}s \right) \\ &\leq \frac{h^3}{3} \int_a^{a+h} |g''(s)|^2 \mathrm{d}s \end{aligned}$$

from Cauchy-Schwarz inequality, so

$$h \sum_{a \in A_h} |a^2 - 1|^2 \left| g(a) - \frac{g(a+h) + g(a-h)}{2} \right|^2 \leq h^4 \sum_{a \in A_h} \langle a \rangle^2 \int_{a-h}^{a+h} |g''(s)|^2 \mathrm{d}s$$

from the standard inequality $|a^2 - 1|^2 \leq 2(1 + |a|^2) = 2\langle a \rangle^2$. Let $a \geq h$. If $s \in [a, a+h]$, we naturally get that $\langle a \rangle^2 \leq \langle s \rangle^2$, so

$$\langle a \rangle^2 \int_a^{a+h} |g''(s)|^2 \mathrm{d}s \leq \int_a^{a+h} \langle s \rangle^2 |g''(s)|^2 \mathrm{d}s.$$

If $s \in [a-h, a]$, we can write that

$$1 \leq 1 + (a-h)^2 \leq 1 + s^2,$$

so

$$1 + a^2 \leq 1 + s^2 + 2ah - h^2 \leq 3 + s^2 \leq 3\langle s\rangle^2$$

as $a \leq 1/h$ and $0 < h \leq 1$, so

$$\langle a\rangle^2 \int_{a-h}^{a} |g''(s)|^2 \mathrm{d}s \leq 3 \int_{a-h}^{a} \langle s\rangle^2 |g''(s)|^2 \mathrm{d}s.$$

As this bound is obvious for $a = 0$ and entirely symmetrical for $a \leq -h$, we finally get that

$$\left(h \sum_{a \in A_h} \left| (a^2 - 1) \left(g(a) - \frac{g(a+h) + g(a-h)}{2} \right) \right|^2 \right)^{\frac{1}{2}}$$

$$\leq Ch^2 \left(\sum_{a \in A_h} \int_{a-h}^{a+h} \langle s\rangle^2 |g''(s)|^2 \mathrm{d}s \right)^{\frac{1}{2}} \leq Ch^2 \|g\|_{\Sigma^4(\mathbb{R})} \leq Ch^2 \|g\|_{\Sigma^5(\mathbb{R})}.$$

Now, for $a \notin A_h$, we write that

$$|a^2 g(a) - g(a)|^2 \leq 2 \left(|a^2 g(a)|^2 + |g(a)|^2 \right),$$

so as for $\mathcal{S}_1$ we have

$$h \sum_{a \notin A_h} |a^2 g(a)|^2 = h \sum_{a \notin A_h} \frac{1}{a^4} |a|^4 |a^2 g(a)|^2 \leq h^5 \sum_{a \notin A_h} |a^4 g(a)|^2$$

$$\leq h^4 \|a^4 g(\cdot)\|^2_{\ell^2(h\mathbb{Z})} \leq h^4 \|g\|^2_{\Sigma^5(\mathbb{R}},$$

and

$$h \sum_{a \notin A_h} |g(a)|^2 = h \sum_{a \notin A_h} \frac{1}{a^4} |a^2 g(a)|^2 \leq Ch^4 \|g\|_{\Sigma^5(\mathbb{R})}$$

from Lemma 3. So finally we well have

$$\mathcal{S}_2 \leq Ch^2 \|g\|_{\Sigma^5(\mathbb{R})}.$$

Now, looking at $\mathcal{S}_3$, we use the fact that, from the same Taylor formula and Cauchy-Schwarz inequality as before, we have

$$ah \frac{g(a-h) - g(a+h)}{2}$$

$$= -ah^2 g'(a) - \frac{ah}{2} \left(\int_a^{a+h} (a+h-s) g''(s) \mathrm{d}s + \int_{a-h}^{a} (a-h-s) g''(s) \mathrm{d}s \right),$$

so

$$\left|ah\frac{g(a-h)-g(a+h)}{2}+h^2ag'(a)\right|^2 \le Ch^5|a|^2\int_{a-h}^{a+h}|g''(s)|^2\mathrm{d}s$$
$$\le Ch^3\int_{a-h}^{a+h}|g''(s)|^2\mathrm{d}s$$

as $|a|\le 1/h$ for all $a\in A_h$, so

$$\mathcal{S}_3=\left(h\sum_{a\in A_h}\left|ah\frac{g(a-h)-g(a+h)}{2}\right|^2\right)^{\frac12}$$
$$\le\left(h\sum_{a\in A_h}|ah^2g'(a)|^2\right)^{\frac12}+Ch^2\|g''\|_{L^2(\mathbb{R})}\le Ch^2\|g\|_{\Sigma^5(\mathbb{R})}.$$

It now remains to bound S_4 and S_5 in terms of $\|g\|_{\Sigma^5(\mathbb{R})}$. As these two sums are symmetric, we will only show how to control S_4 in the following. Let us first analyze the behavior of the function

$$R_h^-(a)=1+h^2(1-a^2-ah)/2-\sqrt{1+h^2(1-a^2-ah)}=f(h^2(1-a^2-ah))$$

where $f(x)=1+\frac12x-\sqrt{1+x}$. We have that $f''(x)=\frac14(1+x)^{-\frac32}$ which is uniformly bounded on $\mathbb{R}$, and moreover $f(0)=f'(0)=0$, from which we deduce that $|f(x)|\le Cx^2$. Hence

$$h\sum_{a\in A_h}\left|\frac{g(a+h)}{h^2}R_h^-(a)\right|^2\le h\sum_{a\in A_h}\left|g(a+h)h^2(1-a^2-ah)\right|^2$$
$$\le h^4h\sum_{a\in h\mathbb{Z}}\left|g(a)\langle a\rangle^2\right|^2\le Ch^4\|g\|^2_{\Sigma^5(\mathbb{R})},$$

which ends the proof of Theorem 2. □

5. Convergence of Kravchuk functions

The aim of this section is to prove the second part of Theorem 2.

5.1. **Convergence of the binomial law.** We first prove (15). We define the projection of the Gaussian function $x\mapsto e^{-x^2}$ on the grid $h\mathbb{Z}$ by

$$\rho: a\in h\mathbb{Z}\mapsto e^{-a^2}.$$

By definition we have, using (9) and the definition (20) with $N=\frac{2}{h^2}$,

$$\rho_h(a)=\frac1h\Pi_N\left(\tau_h^{-1}(a)\right)=\frac{1}{h4^{1/h^2}}\frac{\Gamma\left(1+\frac{2}{h^2}\right)}{\Gamma\left(1+\frac{1}{h^2}+\frac{a}{h}\right)\Gamma\left(1+\frac{1}{h^2}-\frac{a}{h}\right)},$$

where Γ denotes the usual Gamma function such that $\Gamma(n+1) = n!$ for integers. The Stirling asymptotics (see for instance [1, 6.1.42, p.257]) yields

$$\log\Gamma(z) = \left(z - \frac{1}{2}\right)\log(z) - z + \frac{1}{2}\log(2\pi) + R_0(z) \quad \text{with} \quad |R_0(z)| \leq \frac{c_0}{\langle z \rangle}. \tag{43}$$

for some constant c_0. This asymptotic yields in particular the Stirling formula

$$n! = \Gamma(1+n) \simeq \sqrt{2\pi n}\, n^n e^{-n}.$$

This shows that

$$\begin{aligned}
&\log\rho_h(a) = -\log h - \frac{2}{h^2}\log 2 + \log\Gamma\left(1 + \frac{2}{h^2}\right) \\
&- \log\Gamma\left(1 + \frac{1}{h^2} + \frac{a}{h}\right) - \log\Gamma\left(1 + \frac{1}{h^2} - \frac{a}{h}\right) \\
&= -\log h - \frac{2}{h^2}\log 2 + \left(\frac{2}{h^2} + \frac{1}{2}\right)\log\left(1 + \frac{2}{h^2}\right) - \left(1 + \frac{2}{h^2}\right) + \frac{1}{2}\log(2\pi) \\
&- \left(\frac{1}{h^2} + \frac{a}{h} + \frac{1}{2}\right)\log\left(1 + \frac{1}{h^2} + \frac{a}{h}\right) + \left(1 + \frac{1}{h^2} + \frac{a}{h}\right) - \frac{1}{2}\log(2\pi) \\
&- \left(\frac{1}{h^2} - \frac{a}{h} + \frac{1}{2}\right)\log\left(1 + \frac{1}{h^2} - \frac{a}{h}\right) + \left(1 + \frac{1}{h^2} - \frac{a}{h}\right) - \frac{1}{2}\log(2\pi) \\
&+ R_0\left(1 + \frac{2}{h^2}\right) - R_0\left(1 + \frac{1}{h^2} + \frac{a}{h}\right) - R_0\left(1 + \frac{1}{h^2} - \frac{a}{h}\right),
\end{aligned}$$

so we can write that

$$\begin{aligned}
\log\rho_h(a) = &-\frac{1}{2}\log(2\pi) - \log h - \frac{2}{h^2}\log 2 \\
&- \left(1 + \frac{2}{h^2}\right) + \left(1 + \frac{1}{h^2} + \frac{a}{h}\right) + \left(1 + \frac{1}{h^2} - \frac{a}{h}\right) \\
&+ \left(\frac{2}{h^2} + \frac{1}{2}\right)\left[\log 2 - 2\log h + \log\left(1 + \frac{h^2}{2}\right)\right] \\
&- \left(\frac{1}{h^2} + \frac{a}{h} + \frac{1}{2}\right)\left[-2\log h + \log(1 + ah + h^2)\right] \\
&- \left(\frac{1}{h^2} - \frac{a}{h} + \frac{1}{2}\right)\left[-2\log h + \log(1 - ah + h^2)\right] \\
&+ R_0\left(1 + \frac{2}{h^2}\right) - R_0\left(1 + \frac{1}{h^2} + \frac{a}{h}\right) - R_0\left(1 + \frac{1}{h^2} - \frac{a}{h}\right),
\end{aligned}$$

and thus

(44)
$$\log \rho_h(a) = 1 - \frac{1}{2}\log(\pi) + \left(\frac{2}{h^2} + \frac{1}{2}\right)\log\left(1 + \frac{h^2}{2}\right)$$
$$- \left(\frac{1}{h^2} + \frac{a}{h} + \frac{1}{2}\right)\log(1 + ah + h^2) - \left(\frac{1}{h^2} - \frac{a}{h} + \frac{1}{2}\right)\log(1 - ah + h^2)$$
(45)
$$+ R_0\left(1 + \frac{2}{h^2}\right) - R_0\left(1 + \frac{1}{h^2} + \frac{a}{h}\right) - R_0\left(1 + \frac{1}{h^2} - \frac{a}{h}\right).$$

Let us estimate this term first in the regime $|a| \leq h^{-\delta}$ with $\delta \in (0,1)$. In this case, we have

$$\frac{1}{h^2} \pm \frac{a}{h} = \frac{1}{h^2}(1 + \mathcal{O}(h^{1-\delta})) \geq ch^{-2},$$

for h small enough. This shows that in the previous expression, the terms with R_0 can be estimated with (43) and are of order $\mathcal{O}(h^2)$. We also have $|h^2 \pm ah| \leq Ch^2$ and thus we can expand the log terms by using $\log(1+x) = x - \frac{x^2}{2} + \mathcal{O}(|x|^3)$ and we obtain

$$\begin{aligned}\log \rho_h(a) = {} & 1 - \frac{1}{2}\log(\pi) \\ & + \left(\frac{2}{h^2} + \frac{1}{2}\right)\left(\frac{h^2}{2} - \frac{h^4}{4} + \mathcal{O}(h^6)\right) \\ & - \left(\frac{1}{h^2} + \frac{a}{h} + \frac{1}{2}\right)\left(ah + h^2 - \frac{1}{2}(ah + h^2)^2 + \mathcal{O}(h^6)\right) \\ & - \left(\frac{1}{h^2} - \frac{a}{h} + \frac{1}{2}\right)\left(-ah + h^2 - \frac{1}{2}(-ah + h^2)^2 + \mathcal{O}(h^6)\right) \\ & + \mathcal{O}(h^2)\end{aligned}$$

and thus

$$\begin{aligned}\log \rho_h(a) = {} & 1 - \frac{1}{2}\log(\pi) + 1 + \mathcal{O}(h^2) \\ & - \left(\frac{1}{h^2} + \frac{a}{h} + \frac{1}{2}\right)\left(ah + h^2 - \frac{1}{2}a^2h^2 - ah^3\right) \\ & - \left(\frac{1}{h^2} - \frac{a}{h} + \frac{1}{2}\right)\left(-ah + h^2 - \frac{1}{2}a^2h^2 + ah^3\right),\end{aligned}$$

yielding

$$\begin{aligned}\log\rho_h(a) &= 2-\frac{1}{2}\log(\pi)+\mathcal{O}(h^2)\\ &\quad-\left(\frac{a}{h}+a^2+ah+1+ah+\frac{h^2}{2}-\frac{1}{2}a^2-\frac{1}{2}a^3h-\frac{1}{4}a^2h^2-ah-a^2h^2\right)\\ &\quad-\left(-\frac{a}{h}+a^2-ah+1-ah+\frac{h^2}{2}-\frac{1}{2}a^2+\frac{1}{2}a^3h-\frac{1}{4}a^2h^2+ah-a^2h^2\right)\end{aligned}$$

or

$$\begin{aligned}\log\rho_h(a) &= 2-\frac{1}{2}\log(\pi)-2\left(a^2+1-\frac{1}{2}a^2-\frac{5}{4}a^2h^2\right)+\mathcal{O}(h^2)\\ &= -\frac{1}{2}\log(\pi)-a^2+\mathcal{O}(h^{2-\delta}).\end{aligned}$$

We thus obtain that

$$\left|\rho_h(a)-\frac{1}{\sqrt{\pi}}e^{-a^2}\right|\le Ch^{2-\delta}e^{-a^2},\quad a\in h\mathbb{Z}\cap[-h^{-\delta},h^{-\delta}],$$

from which we deduce that

$$\begin{aligned}h\sum_{a\in h\mathbb{Z},|a|\le h^{-\delta}}\langle a\rangle^{2\sigma}\left|\rho_h(a)-\frac{1}{\sqrt{\pi}}e^{-a^2}\right|^2 &\le Ch^{4-2\delta}h\sum_{a\in h\mathbb{Z},|a|\le h^{-\delta}}\langle a\rangle^{2\sigma}e^{-a^2}\\ &\le Ch^{4-2\delta}h\sum_{a\in h\mathbb{Z}}\langle a\rangle^{2\sigma}e^{-a^2}\le C_\sigma h^{4-2\delta}.\end{aligned}$$

Now from (44), we have that for $|a|\ge h^{-\delta}$ and $\beta>0$, by using the fact that the R_0 terms are uniformly bounded in h,

$$\begin{aligned}\log e^{\beta a^2}\rho_h(a) &= \beta a^2+\left(\frac{2}{h^2}+\frac{1}{2}\right)\log\left(1+\frac{h^2}{2}\right)+\mathcal{O}(1)\\ &\quad-\left(\frac{1}{h^2}+\frac{a}{h}+\frac{1}{2}\right)\log(1+ah+h^2)-\left(\frac{1}{h^2}-\frac{a}{h}+\frac{1}{2}\right)\log(1-ah+h^2).\end{aligned}$$

In the case $a \in [h^{-\delta}, h^{-1}]$, we write $a = h^{-1}(1-b)$, $b \in [0, h^{1-\delta}]$ and obtain

$$\begin{aligned}
\log e^{\beta a^2}\rho_h(a) &= \frac{\beta}{h^2}(1-b)^2 - \left(\frac{2-b}{h^2} + \frac{1}{2}\right)\left(\log 2 + \log\left(1 - \frac{b}{2} + \frac{h^2}{2}\right)\right) \\
&\quad - \left(\frac{b}{h^2} + \frac{1}{2}\right)\log(b + h^2) + \mathcal{O}(1) \\
&= \frac{\beta}{h^2}(1-b)^2 - \frac{1}{h^2}\left(2\log 2 + \mathcal{O}\left(h^{1-\frac{\delta}{2}}\right)\right) \\
&= \frac{1}{h^2}\left(\beta - 2\log 2 + \mathcal{O}(h^{1-\delta}\right) \leq 0
\end{aligned}$$

for $\beta = 1 < 2\log 2$ and h small enough. By symmetry, we deduce that

$$\forall\, a \in [h^{-\delta}, h^{-1}], \quad |\rho_h(a)| \leq e^{-a^2}$$

Hence

$$\begin{aligned}
h \sum_{a \in h\mathbb{Z} \cap [h^{-\delta}, h^{-1}]} \langle a \rangle^{2\sigma} |\rho_h(a)|^2 &\leq h \sum_{a \in h\mathbb{Z} \cap [h^{-\delta}, h^{-1}]} \langle a \rangle^{2\sigma} e^{-2a^2} \\
&\leq e^{-\beta h^{-\delta}} h \sum_{a \in h\mathbb{Z} \cap [h^{-\delta}, h^{-1}]} \langle a \rangle^{2\sigma} e^{-a^2} \leq C_\sigma e^{-\beta h^{-\delta}} h = \mathcal{O}(h^2).
\end{aligned}$$

As the same bounds holds for the Gaussian e^{-a^2}, we obtain the result.

5.2. **Convergence of the Kravchuk functions.** We now prove (16). Recall that the Hermite polynomials are defined by the relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad H_0(x) = 1, \tag{46}$$

while the scaled Kravchuk polynomials are defined by the relation

$$K_{n+1,h}(x) = 2xK_{n,h}(x) - 2n\left(1 - h^2\binom{n-1}{2}\right)K_{n-1,h}(x), \quad K_{0,h}(x) = 1.$$

The Hermite functions are then defined by the formula

$$\psi_n(x) := \frac{1}{\pi^{\frac{1}{4}} 2^{\frac{n}{2}} \sqrt{n!}} e^{-\frac{x^2}{2}} H_n(x),$$

and let us recall that Cramér's inequality states that

$$\forall\, x \in \mathbb{R}, \quad \forall\, n \geq 0, \quad |\psi_n(x)| \leq \pi^{-\frac{1}{4}},$$

which shows in particular that

$$\forall\, x \in \mathbb{R}, \quad \forall\, n \geq 0, \quad |H_n(x)| \leq e^{\frac{x^2}{2}} 2^{\frac{n}{2}} \sqrt{n!}. \tag{47}$$

Lemma 4. *For any given N and $h = \sqrt{2}N^{-\frac{1}{2}}$, we denote by $(k_{n,h})_n$ the Kravchuk polynomials given by the relation (6). We then have the following bounds: there exists C such that for all N and $h = \sqrt{2}N^{-\frac{1}{2}}$, for all $\delta \in (0,1)$,*

$$\forall\, n \leq \frac{1}{3}\delta|\log h|, \quad \forall\, x \in \mathbb{R}, \quad |H_n(x) - k_{n,h}(x)| \leq Ch^{2-\delta}e^{\frac{x^2}{2}}2^{\frac{n}{2}}\sqrt{n!} \tag{48}$$

and

$$\forall\, n \leq \frac{1}{3}\delta|\log h|, \quad \forall\, x \in \mathbb{R}, \quad |k_{n,h}(x)| \leq Ch^{-\delta}e^{\frac{x^2}{2}}2^{\frac{n}{2}}\sqrt{n!}. \tag{49}$$

Proof. We first remark that (48) and (47) imply (49), so we only need to prove (48). Let us define

$$H(x,t) = \sum_{n\geq 0}\frac{t^n}{n!}H_n(x) \quad \text{and} \quad K_h(x,t) = \sum_{n\geq 0}\frac{t^n}{n!}k_{n,h}(x).$$

Multiplying (46) by $\frac{t^n}{n!}$ we can prove that the function $H(t,x)$ satisfies the equation $\partial_t H(t,x) = (2x-2t)H(t,x)$ and we obtain the classical relation

$$H(x,t) = e^{2xt-t^2},$$

valid for all $x \in \mathbb{R}$ and $t \in \mathbb{C}$. Moreover, relation (6) yields

$$\sum_{n\geq 0}\frac{t^n}{n!}k_{n+1,h}(x) = 2xk_h(x,t) - 2\sum_{n\geq 0}n\frac{t^n}{n!}k_{n-1,h}(x) + h^2\sum_{n\geq 0}n(n-1)\frac{t^n}{n!}k_{n-1,h}(x)$$

or

$$\begin{aligned}\partial_t K_h(x,t) &= 2xK_h(x,t) - 2tK_h(x,t) + h^2t^2\sum_{n\geq 2}\frac{t^{n-2}}{(n-2)!}k_{n-1,h}(x)\\ &= 2xK_h(x,t) - 2tK_h(x,t) + h^2t^2\partial_t K_h(x,t),\end{aligned}$$

and we find

$$(1-h^2t^2)\partial_t K_h(x,t) = (2x-2t)K_h(x,t)$$

from which we deduce that

$$\begin{aligned}K_h(x,t) &= \exp\left(\int_0^t \frac{2x-2s}{1-h^2s^2}\mathrm{d}s\right)\\ &= \exp\left(2x\frac{1}{h}\int_0^{ht}\frac{1}{1-s^2}\mathrm{d}s\right)\exp\left(\frac{1}{h^2}\int_0^{ht}\frac{-2s}{1-s^2}\mathrm{d}s\right)\\ &= \exp\left(2x\frac{1}{h}\mathrm{artanh}(ht)\right)\exp\left(\frac{1}{h^2}\log(1-(ht)^2)\right)\\ &= \left(\frac{1+ht}{1-ht}\right)^{\frac{x}{h}}\left(1-h^2t^2\right)^{\frac{1}{h^2}}.\end{aligned}$$

Remark 2. *This formula shows in particular that for $n > N$, the Kravchuk polynomials vanish.*

This shows that for $t \in \mathbb{C}$, $|t| \leq R$ with $R > 1$, we have for h small enough

$$\begin{aligned} |H(x,t) - K_h(x,t)| &= |e^{2xt-t^2}||1 - e^{2x(\frac{1}{h}\operatorname{artanh}(ht)-1)}e^{\frac{1}{h^2}\log(1-(ht)^2)+t^2}| \\ &= |e^{2xt-t^2}||1 - e^{2x(\mathcal{O}(h^2|t|^3)+\mathcal{O}(h^2|t|^4)}| \\ &\leq Ch^2(|x|R^3 + R^4)e^{2|x|R+R^2}. \end{aligned}$$

By Cauchy estimates on the disk $|t| \leq R$, we obtain

$$\forall\, n \in \mathbb{N}, \quad |H_n(x) - k_{n,h}(x)| \leq n! R^{-n} C h^2 (|x|R^3 + R^4)e^{2|x|R+R^2}.$$

We take $R^2 = n$. This yields using Stirling expansions

$$\begin{aligned} e^{-\frac{x^2}{2}}|H_n(x) - k_{n,h}(x)| &\leq Ch^2(|x|n^{\frac{3}{2}} + n^2)n^n e^{-n} n^{\frac{1}{2}} n^{-\frac{n}{2}} e^{2|x|\sqrt{n}+n} e^{-\frac{x^2}{2}} \\ &\leq Ch^2(|x|n^{\frac{3}{2}} + n^2)n^{\frac{n}{2}} e^{-n} n^{\frac{1}{2}} e^{-\frac{1}{2}(x-2\sqrt{n})^2+3n}. \end{aligned}$$

Now we remark that

$$|x|e^{-\frac{1}{2}(x-2\sqrt{n})^2} \leq |x - 2\sqrt{n}|e^{-\frac{1}{2}(x-2\sqrt{n})^2} + 2\sqrt{n}e^{-\frac{1}{2}(x-2\sqrt{n})^2} \leq C\sqrt{n}$$

for $n \geq 1$. Hence we have

$$\begin{aligned} e^{-\frac{x^2}{2}}|H_n(x) - k_{n,h}(x)| &\leq Ch^2 2^{\frac{n}{2}} n^{\frac{n}{2}} e^{-\frac{n}{2}} n^{\frac{1}{4}} \left(n^{\frac{1}{4}} n^2 2^{-\frac{n}{2}} e^{-\frac{n}{2}} e^{3n}\right) \\ &\leq Ch^2 2^{\frac{n}{2}} \sqrt{n!}(n^{\frac{9}{4}} e^{(\frac{5}{2}-\frac{1}{2}\log 2)n}) \\ &\leq Ch^2 2^{\frac{n}{2}} \sqrt{n!} e^{\frac{5}{2}n} \end{aligned}$$

and this yields the result as $e^{\frac{5}{2}n} \leq e^{-\frac{5}{6}\delta \log h} \leq h^{-\delta}$. □

Now let us recall that the Kravchuk functions are given by the formula

$$\begin{aligned} \varphi_{n,h}(a) := \frac{1}{d_n h^n 2^n n!} k_{n,h}(a)\sqrt{\rho_h(a)} &= \frac{1}{h^n}\sqrt{\frac{(N-n)!}{N!n!}} k_{n,h}(a)\sqrt{\rho_h(a)} \\ &= \frac{1}{h^n\sqrt{n!}}\sqrt{\frac{\Gamma(1+\frac{2}{h^2}-n)}{\Gamma(1+\frac{2}{h^2})}} k_{n,h}(a)\sqrt{\rho_h(a)}. \end{aligned}$$

Using (43), we have

$$\log \frac{\Gamma(1+\frac{2}{h^2}-n)}{\Gamma(1+\frac{2}{h^2})} = \left(\frac{2}{h^2}-n+\frac{1}{2}\right)\log\left(1+\frac{2}{h^2}-n\right) - 1 - \frac{2}{h^2} + n + \frac{1}{2}\log(2\pi)$$
$$- \left(\frac{2}{h^2}+\frac{1}{2}\right)\log\left(1+\frac{2}{h^2}\right) + \frac{2}{h^2} + 1 - \frac{1}{2}\log(2\pi)$$
$$+ R_0\left(1+\frac{2}{h^2}-n\right) - R_0\left(1+\frac{2}{h^2}\right) - R_0(1+n)$$

and thus

$$\log \frac{\Gamma(1+\frac{2}{h^2}-n)}{\Gamma(1+\frac{2}{h^2})} = \left(\frac{2}{h^2}-n+\frac{1}{2}\right)\left(\log 2 - 2\log h + \log\left(1-h^2\frac{(n-1)}{2}\right)\right)$$
$$+ n - \left(\frac{2}{h^2}+\frac{1}{2}\right)\left(\log 2 - 2\log h + \log\left(1+\frac{h^2}{2}\right)\right)$$
$$+ R_0\left(1+\frac{2}{h^2}-n\right) - R_0\left(1+\frac{2}{h^2}\right).$$

Now let us assume that $n \leq h^{-\beta}$, we can write that

$$\log \frac{\Gamma(1+\frac{2}{h^2}-n)}{\Gamma(1+\frac{2}{h^2})} = n - n\log 2 + 2n\log h - (n-1) - 1 + \mathcal{O}(h^{2-\beta}),$$

and thus we have

$$\sqrt{\frac{\Gamma(1+\frac{2}{h^2}-n)}{\Gamma(1+\frac{2}{h^2})}} = \frac{h^n}{2^{\frac{n}{2}}}(1+\mathcal{O}(h^{2-\beta})).$$

Hence we have for $n \leq h^{-\beta}$,

$$\varphi_n(a) = \frac{h^n}{2^{\frac{n}{2}}}(1+\mathcal{O}(h^{2-\beta}))\frac{1}{\pi^{\frac{1}{4}}h^n\sqrt{n!}}k_{n,h}(a)\sqrt{\sqrt{\pi}\rho_h(a)}$$
$$= \frac{1}{2^{\frac{n}{2}}\pi^{\frac{1}{4}}\sqrt{n!}}k_{n,h}(a)\sqrt{\sqrt{\pi}\rho_h(a)}(1+\mathcal{O}(h^{2-\beta})).$$

By using the previous bound, we thus obtain the result.

6. Time-dependent scheme

We consider now the time-dependent discrete Schrödinger equation

$$i\partial_t\psi = H_h\psi, \tag{50}$$

with $\psi(0,\cdot)=\psi_0\in\ell^2(h\mathbb{Z})$. We define

$$\begin{aligned}E(\psi)&=\frac{1}{h}\sum_{a\in A_h}\left(-\sqrt{(1-ah+h^2)(1+ah)}\,\mathrm{Re}(\psi(a)\overline{\psi}(a-h))+|\psi(a)|^2\left(1+\frac{h^2}{2}\right)\right)\\&=\langle\psi,H_h\psi\rangle_{\ell^2(h\mathbb{Z})},\end{aligned}$$

where A_h is defined in (7). We first show the conservation of mass and energy property of the discrete harmonic oscillator:

Proposition 15. *For all* $t\in\mathbb{R}$,

$$\|\psi(t)\|_{\ell^2(h\mathbb{Z})}=\|\psi_0\|_{\ell^2(h\mathbb{Z})}\quad\text{and}\quad E(\psi(t))=E(\psi_0).\tag{51}$$

Proof. We multiply (50) by $\overline{\psi}$ and we sum over $h\mathbb{Z}$:

$$\begin{aligned}\sum_{a\in h\mathbb{Z}}i\overline{\psi}(a)\partial_t\psi(a)=\sum_{a\in h\mathbb{Z}}&\left(-\frac{1}{h^2}\sqrt{(1+ah+h^2)(1-ah)}\psi(a+h)\overline{\psi}(a)\right.\\&\left.-\frac{1}{h^2}\sqrt{(1-ah+h^2)(1+ah)}\psi(a-h)\overline{\psi}(a)+\left(1+\frac{h^2}{2}\right)|\psi(a)|^2\right)\mathbf{1}_{-\frac{1}{h}\le a\le\frac{1}{h}},\end{aligned}$$

so

$$\begin{aligned}i\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{a\in h\mathbb{Z}}|\psi(a)|^2\right)&=-\frac{1}{h^2}\sum_{a\in A_h}\left(\sqrt{(1+ah+h^2)(1-ah)}\psi(a+h)\overline{\psi}(a)\right)\\&\quad-\sum_{a\in h\mathbb{Z}}\left(\sqrt{(1-ah+h^2)(1+ah)}\psi(a-h)\overline{\psi}(a)\right)+\left(1+\frac{h^2}{2}\right)\sum_{a\in A_h}|\psi(a)|^2.\end{aligned}$$

By a change of variable $a\mapsto a-h$ in the first part of the middle sum of the previous equation, we see that

$$\begin{aligned}&\sum_{a\in A_h}\left(\sqrt{(1+ah+h^2)(1-ah)}\psi(a+h)\overline{\psi}(a)\right.\\&\qquad\left.+\sqrt{(1-ah+h^2)(1+ah)}\psi(a-h)\overline{\psi}(a)\right)\\&=\sum_{a\in A_h}\left(\psi(a)\overline{\psi}(a-h)+\psi(a-h)\overline{\psi}(a)\right)\sqrt{(1-ah+h^2)(1+ah)}\\&=2\sum_{a\in A_h}\mathrm{Re}\left(\psi(a)\overline{\psi}(a-h)\right)\sqrt{(1-ah+h^2)(1+ah)},\end{aligned}$$

so multiplying the previous equation by h and taking the imaginary part, we get the mass conservation. The second statement is classical using the symmetry of H_h. □

Now we are going to analyze time-dependent scheme (50) and compare it with solutions of the corresponding equation $i\partial_t\psi = H\psi$ for the harmonic oscillator. Using (4) recall that if $f \in L^2(\mathbb{R})$, then we can decompose f on the Hermite-Gauss basis $(\psi_n)_{n\in\mathbb{N}}$ by

$$f(x) = \sum_{n\geq 0} c_n\psi_n(x)$$

for all $x \in \mathbb{R}$, with

$$c_n = \langle f, \psi_n\rangle_{L^2(\mathbb{R})} = \int_{\mathbb{R}} f(x)\psi_n(x)\mathrm{d}x,$$

so that the solution of $i\partial_t\psi = H\psi$ with initial condition $\psi(0,\cdot) = f$ can be written, for all $t \geq 0$,

$$\psi(t,\cdot) = e^{-itH} f = \sum_{n\geq 0} c_n e^{-i(2n+1)}\psi_n$$

We now denote by $u := (\pi_h f)\,\mathbf{1}_{A_h}$ the projection of f on A_h, then we can decompose u on the finite basis $(\varphi_{n,h})_{0\leq n\leq n_{\max}}$ of $\ell^2(A_h)$, where $n_{\max} \in \mathbb{N}^*$ is a fixed integer:

$$u(a) = \sum_{n\geq 0} c_{n,h}\varphi_{n,h}(a)$$

for all $a \in A_h$, where the scalars $(c_{n,h})_{0\leq n\leq n_{\max}}$ are defined through the relation

$$c_{n,h} = \langle u, \varphi_{n,h}\rangle_{\ell^2(h\mathbb{Z})} = h\sum_{a\in h\mathbb{Z}} u(a)\varphi_{n,h}(a).$$

Then, as in the continuous case, we can express the solution ψ_h of (50) by

$$\psi_h(t,\cdot) = \sum_{n=0}^{n_{\max}} c_{n,h}e^{-i(2n+1)t}\varphi_{n,h}.$$

Theorem 4. *Assume that f is smooth. Then there exists C such that for all s, there exists C_s such that for all h sufficiently small and all $n_max \in \mathbb{N}$ such that $\frac{1}{4}\delta|\log h| \leq n_{\max} \leq \frac{1}{3}\delta|\log h|$, for all $t \geq 0$,*

$$\|\pi_h\psi(t,\cdot) - \psi_h(t,\cdot)\|_{\ell^2(h\mathbb{Z})} \leq Ch^{2-\delta} + \frac{C_s}{|\log h|^s}$$

for all $\delta > 0$.

Proof. We directly compute, for all $a \in A_h$, with the notation $\lambda_n = 2n+1$,

$$\begin{aligned}\pi_h\psi(t,a) - \psi_h(t,a) &= \sum_{n\geq 0} c_n e^{-i\lambda_n t}\psi_n(a) - \sum_{n=0}^{n_{\max}} c_{n,h} e^{-i\lambda_n t}\varphi_{n,h}(a) \\ &= \sum_{n\geq n_{\max}+1} c_n e^{-i\lambda_n t}\psi_n(a) + \sum_{n=0}^{n_{\max}} e^{-i\lambda_n t}\left(c_n\psi_n(a) - c_{n,h}\varphi_{n,h}(a)\right)\end{aligned}$$

so that

$$\|\pi_h\psi(t,\cdot) - \psi_h(t,\cdot)\|_{\ell^2(h\mathbb{Z})} \leq \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3,$$

where

$$\mathcal{E}_1 := \left\| \sum_{n\geq n_{\max}+1} c_n e^{-i\lambda_n t}\psi_n(a)\right\|_{\ell^2(h\mathbb{Z})}, \quad \mathcal{E}_2 := \sum_{n=0}^{n_{\max}} |c_n - c_{n,h}|\|\psi_n\|_{\ell^2(h\mathbb{Z})}$$

and

$$\mathcal{E}_3 := \sum_{n=0}^{n_{\max}} |c_{n,h}|\|\psi_n - \varphi_{n,h}\|_{\ell^2(h\mathbb{Z})}.$$

We assume that the first term is smooth in the sense that it belongs to all space $\Sigma^s(\mathbb{R})$, $s \geq 0$. Classically, this is equivalent to say that the coefficients c_n decay like $C_N\langle n\rangle^{-N}$ for all N, with constant depending on N. This shows that for all s, there exists C_s such that

$$\mathcal{E}_1 \leq C_s\langle n_{\max}\rangle^{-s} \leq \frac{C_s}{|\log h|^s}$$

as $|\log h| \lesssim n_{\max}$. In order to bound $\mathcal{E}_2$, by definition of c_n and $c_{n,h}$ we see that

$$|c_{n,h} - c_n| \leq \left|\langle f,\psi_n\rangle_{L^2(\mathbb{R})} - \langle u,\psi_n\rangle_{\ell^2(h\mathbb{Z})}\right| + \left|\langle u,\psi_n - \varphi_{n,h}\rangle_{\ell^2(h\mathbb{Z})}\right|,$$

where

$$\left|\langle u,\psi_n - \varphi_{n,h}\rangle_{\ell^2(h\mathbb{Z})}\right| \leq \|u\|_{\ell^2(h\mathbb{Z})}\|\psi_n - \varphi_{n,h}\|_{\ell^2(h\mathbb{Z})} \leq C_{n_{\max}} h^{2-\delta}\|f\|_{L^2(\mathbb{R})}$$

for all $\delta > 0$ by using (16), and because $n_{\max} \leq \frac{1}{3}\delta|\log h|$. The error $\mathcal{E}_3$ is estimated similarly, by noticing that

$$|c_{n,h}| \leq \|u\|_{\ell^2(h\mathbb{Z})}\|\varphi_{n,h}\|_{\ell^2(h\mathbb{Z})} \leq C_{n_{\max}}\|f\|_{H^1(\mathbb{R})},$$

so $\mathcal{E}_3 = \mathcal{O}\left(h^{2-\delta}\right)$.

□

Remark 3. *The error term in* $\log h$ *could be refined by a better frequency estimate in* (16)*, like for example* $n \leq h^{-\delta}$ *but this would require a better bound for the asymptotics of the Kravchuk functions which is out of the scope of this work.*

7. Kravchuk Transform

We now prove Theorem 3, which can also be found in [2]. For a vector $x \in \mathbb{R}^{N+1}$, we define the transformation $\tilde{x} = \mathcal{K}x$ by the formula

$$\tilde{x}_k = \sum_{j=0}^{N} e^{i\frac{\pi}{2}(j-k-N/2)} \phi_k(j) x_j$$

for all $0 \le k \le N$, corresponding to the multiplication by the matrix

$$K = e^{-\frac{i\pi N}{4}} \times \begin{pmatrix} \phi_0(0) & e^{\frac{i\pi}{2}}\phi_0(1) & \dots & e^{\frac{i\pi(N-1)}{2}}\phi_0(N-1) & e^{\frac{i\pi N}{2}}\phi_0(N) \\ e^{-\frac{i\pi}{2}}\phi_1(0) & \phi_1(1) & \dots & e^{\frac{i\pi(N-2)}{2}}\phi_1(N-1) & e^{\frac{i\pi(N-1)}{2}}\phi_1(N) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ e^{-\frac{i\pi N}{2}}\phi_N(0) & e^{-\frac{i\pi(N-1)}{2}}\phi_N(1) & \dots & e^{-\frac{i\pi}{2}}\phi_N(N-1) & \phi_N(N) \end{pmatrix}.$$

Recall that here $\phi_n(k)$ denote the functions (37) corresponding to the function $\varphi_{n,h}$ after scaling. With the notation (17) and (19), we obtain

$$K = e^{-\frac{i\pi N}{4}} D^* L D.$$

As a direct consequence of the fact that the $(\phi_n)_{0\le n\le N}$ are orthogonal, we get that the matrix L and K are unitary:

$$K^* K = L^* L = \mathrm{Id}.$$

Proposition 16. *The matrix K satisfies*

$$K = e^{\frac{i\pi}{4}} e^{-\frac{i\pi}{4}A},$$

where A is the matrix defined in (19).

Proof. We are going to show that both matrices K^* and $e^{-\frac{i\pi}{4}} e^{\frac{i\pi}{4}A}$ have the same image on a particular basis of $\mathbb{R}^{N+1}$, the basis formed by the $N+1$-vectors $v_n := (\phi_n(0), \phi_n(1), \dots, \phi_n(N))^\top$ for $0 \le n \le N$. We first compute that for all $0 \le k \le N$,

$$(Av_n)_k = (N+1)\phi_n(k) - \sqrt{k(N-k+1)}\phi_n(k-1) - \sqrt{(k+1)(N-k)}\phi_n(k+1),$$

hence from Proposition 11 we get that

$$(Av_n)_k = (2n+1)\,\phi_n(k),$$

so the matrix A is diagonal in the basis $(v_0, v_1, \dots, v_n)$, and

$$e^{-\frac{i\pi}{4}} e^{\frac{i\pi}{4}A} v_n = e^{-\frac{i\pi}{4}} \sum_{k\geq 0} \frac{1}{k!} \left(\frac{i\pi}{4}\right)^k (2n+1)^k v_n = e^{-\frac{i\pi}{4}} e^{\frac{i\pi}{2}\left(n+\frac{1}{2}\right)} v_n$$
$$= e^{i\frac{n\pi}{2}} v_n.$$

On the other hand, using Proposition 10, we compute

$$(K^* v_n)_m = \left(e^{\frac{i\pi N}{4}} D^* L^* D v_n\right)_m = e^{\frac{i\pi N}{4}} \sum_{k=0}^{N} \phi_n(k)\phi_k(m) e^{i\frac{k-m}{2}\pi} = e^{i\frac{n}{2}\pi}\phi_n(m),$$

so

$$K^* = e^{-\frac{i\pi}{4}} e^{\frac{i\pi}{4}A}$$

and we get the result. □

8. Numerical simulations of Kravchuk functions

In this section we are going to present some plots and numerical simulations of some of the previous properties of the Kravchuk functions $(\varphi_{n,h})_n$. First we illustrate the convergence result (15) on the grid X_N for $N = 50$. We plot both functions ρ_h and $\rho/\sqrt{\pi}$ in Figure 1. We observe than even if the number of space discretization points is rather low, the accuracy of the approximation of the Gaussian function is pretty good. This is highlighted by Figure 2, where we plot the $\ell^2(h\mathbb{Z})$, the $\ell^\infty(h\mathbb{Z})$ and the $h^1(h\mathbb{Z})$ norms[3] of the difference $\rho_h - \rho/\sqrt{\pi}$ in logarithmic scale with respect to $N = 2/h^2$, and we get a leading coefficient of -1 for these three lines, which corresponds to the $O(h^{2-\delta})$ for $\delta > 0$ as small as we want in (15).

In the same way, we illustrate Theorem 2 by plotting $(\varphi_{n,h})_{1\leq n\leq 6}$ with $N = 50$ and comparing these functions to the first Hermite functions $(\psi_n)_{1\leq n\leq 6}$ in Figure 3, then by computing the $\ell^2(h\mathbb{Z})$, $\ell^\infty(h\mathbb{Z})$ and $h^1(h\mathbb{Z})$ errors of the differences $\varphi_{10,h} - \psi_{10}$ for $n = 10$ in logarithmic scale, where we observe a convergence in $-\log(N)$ which well corresponds to the $O(h^{2-\delta})$ for $\delta > 0$ of Theorem 2.

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[3]The $h^1(h\mathbb{Z})$ norm is defined by $\|u\|^2_{h^1(h\mathbb{Z})} = \|v\|^2_{\ell^2(h\mathbb{Z}} + \langle v, \Delta_h v\rangle_{\ell^2(h\mathbb{Z})}$ where Δ_h is the discrete Laplacian.

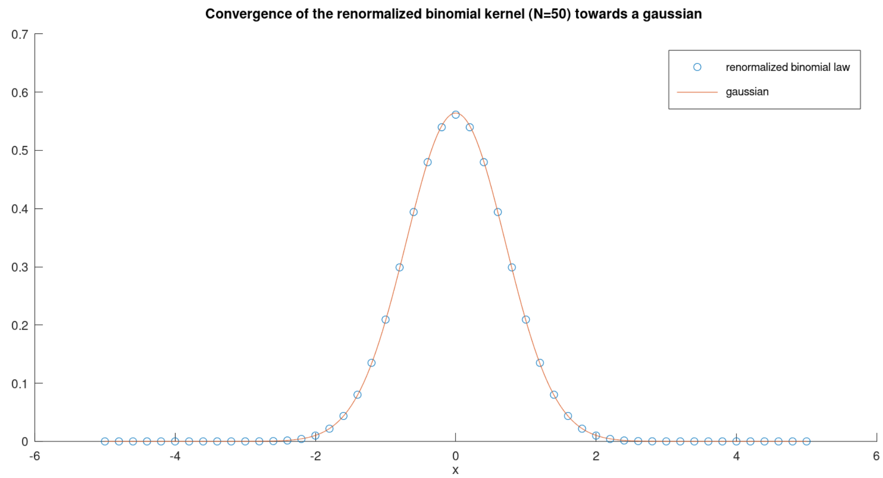

FIGURE 1. Convergence of the binomial law ρ_h to the Gaussian $\rho/\sqrt{\pi}$.

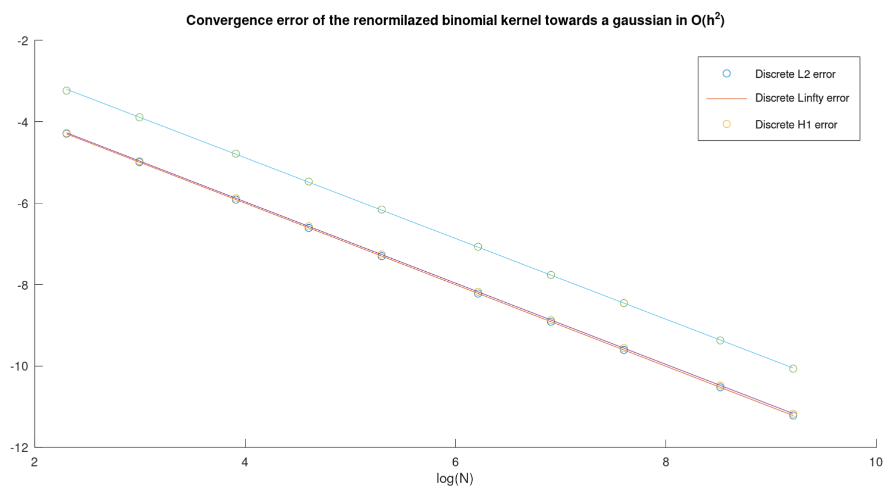

FIGURE 2. $\ell^2(h\mathbb{Z})$, $\ell^\infty(h\mathbb{Z})$ and $h^1(h\mathbb{Z})$ convergence error of the binomial law ρ_h to the Gaussian $\rho/\sqrt{\pi}$.

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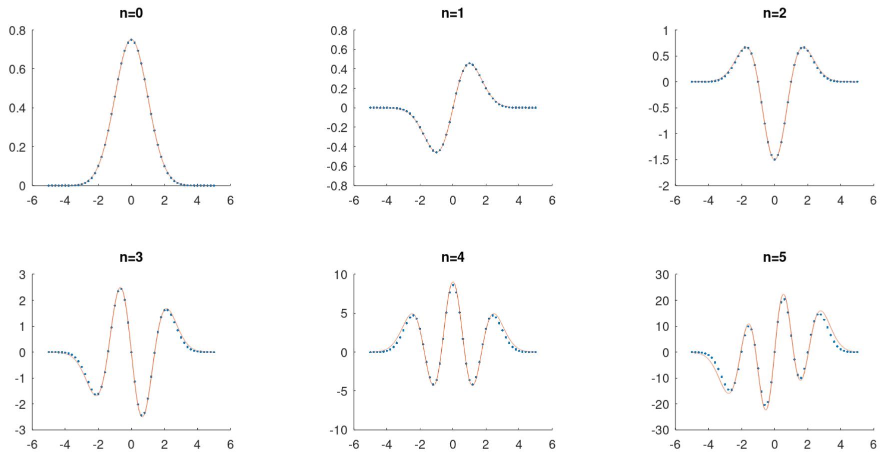

FIGURE 3. Convergence of the Kravchuk functions $(\varphi_{n,h})_{1\leq n\leq 6}$ to the Hermite functions $(\psi_n)_{1\leq n\leq 6}$.

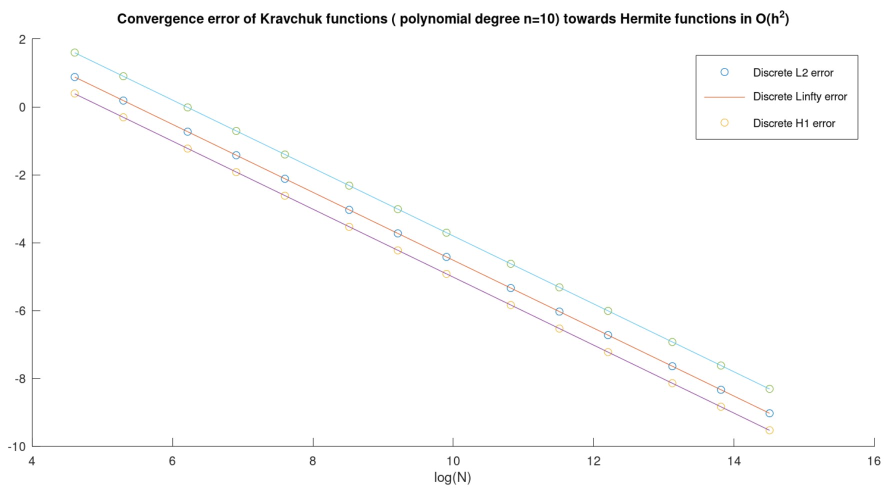

FIGURE 4. $\ell^2(h\mathbb{Z})$, $\ell^\infty(h\mathbb{Z})$ and $h^1(h\mathbb{Z})$ convergence error of the Kravchuk functions $(\varphi_{n,h})_{1\leq n\leq 6}$ to the Hermite functions $(\psi_n)_{1\leq n\leq 6}$.

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