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Umbral calculus, discretization, and quantum mechanics on a lattice

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Abstract. 'Umbral calculus' deals with representations of the canonical commutation relations. We present a short exposition of it and discuss how this calculus can be used to discretize continuum models and to construct representations of Lie algebras on a lattice. Related ideas appeared in recent publications and we show that the examples treated there are special cases of umbral calculus. This observation then suggests various generalizations of these examples. A special umbral representation of the canonical commutation relations given in terms of the position and momentum operator on a lattice is investigated in detail.

1. Introduction

Umbral calculus§ is an analysis of certain representations of the commutation relations

$$[Q_i, \hat{\boldsymbol{x}}_j] = \delta_{ij}\mathbb{1} \qquad [Q_i, Q_j] = 0 = [\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_j] \tag{1.1}$$

in terms of operators on the algebra of polynomials in variables $x_i, i = 1, \dots, n$ (see [1, 2] for reviews). In particular, it provides us with representations by operators acting on polynomials of *discrete* variables. Let us assume that $Q_i, \hat{\boldsymbol{x}}_j$ is such a representation and let $A(y_i, \partial/\partial y_j) f(y_k) = 0$ be a differential equation on $\mathbb{R}^n$ with a polynomial solution f‖. Introducing multiplication operators $\boldsymbol{y}_i$, we can write it in the form¶

$$A(\boldsymbol{y}_i, \partial/\partial y_j) f(\boldsymbol{y}_k) 1 = 0. \tag{1.2}$$

The operators $\boldsymbol{y}_i$ and $\partial/\partial y_j$ do satisfy the commutation relations (1.1), of course. The verification that $f(y_k)$ solves the original differential equation is now translated into an algebraic problem which only requires the abstract commutation relations (1.1), i.e. it does not depend on the specific choice of representation. Defining $\tilde{f}(x_k) := f(\hat{\boldsymbol{x}}_k)1$, then also

$$A(\hat{\boldsymbol{x}}_i, Q_j)\tilde{f}(x_k) = 0 \tag{1.3}$$

holds which is a *difference* equation. We have simply substituted

$$\boldsymbol{y}_i \mapsto \hat{\boldsymbol{x}}_i \qquad \frac{\partial}{\partial y_j} \mapsto Q_j. \tag{1.4}$$

§ This terminology goes back to the nineteenth-century mathematician Sylvester who used the Latin word *umbra* to denote something which would nowadays be called a linear functional. See also [1].
‖ Here and in the following an expression such as $f(y_k)$ stands for $f(y_1, \dots, y_n)$.
¶ In this expression the 1 plays the role of a 'state' on which we act with an operator algebra to generate an irreducible representation of the latter.

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If $f(y_k)$ solves the original differential equation, then $\tilde{f}(x_k)$ is a solution of the corresponding difference equation.

For differential equations possessing polynomial solutions, the notion of quasi-exact solvability has been introduced [3]. Several examples are provided by eigenvalue problems in quantum mechanics. A corresponding example for the above discretization procedure appeared recently in [4]. In section 4 we show that its underlying structure is umbral calculus.

The above operator substitution yields a mapping of an eigenvalue equation for a differential operator to an eigenvalue equation for a difference operator together with a 'formal' mapping of solutions. It seems that we have a general procedure for 'isospectral discretization' of differential operator eigenvalue problems. The problem, however, is that (besides for polynomials) the mapping of solutions in general only works at the level of formal power series, but does not respect convergence properties.

Also, in the above-mentioned treatment [4] of eigenvalue problems one does not really get a discretization of the original quantum mechanical problem since that involves non-polynomial functions. For serious applications, therefore, we need an extension of the procedure sketched above beyond polynomials and formal power series. Such a discretization method could then be of interest for solving differential equations numerically.

The commutation relations of differential operators $A(\boldsymbol{y}_i, \partial/\partial y_j)$ and $B(\boldsymbol{y}_i, \partial/\partial y_j)$ are preserved under the substitution (1.4). In this way one obtains representations of operator algebras, in particular Lie and Hopf algebras, by operators acting on functions on a lattice. An example appeared recently in [5] where representations of the Poincaré and the κ-deformed Poincaré algebra [6] on a lattice were constructed. In section 5 we explain how it fits into the umbral framework.

All this raises the question whether it is possible to understand (some of the) umbral maps (1.4) on algebras of non-polynomial functions. In view of possible applications to quantum mechanics, it would be of interest to have $Q_i, \hat{\boldsymbol{x}}_j$ defined on the Hilbert space of square summable functions on a lattice. Is it possible that $\hat{\boldsymbol{x}}_i$ and $-\mathrm{i}Q_j$ (which as a consequence of (1.1) satisfy the canonical commutation relations of quantum mechanics) are selfadjoint operators and is (1.4) perhaps a unitary equivalence? Our work intends to contribute to the clarification of such questions. An example of particular interest is suggested by the work in [5]. The representation of the canonical commutation relations which appeared there is investigated in detail in section 6.

Section 2 contains a brief introduction to our understanding of umbral calculus. It by no means intends to cover the whole subject. An example treating symmetries on a lattice is then presented in section 3. Another application is discussed in section 4, partly motivated by [4]. In section 5 we slightly generalize the umbral framework of section 2. We also comment on a representation of the Poincaré algebra on a lattice which appeared in [5]. Its underlying representation of the canonical commutation relations is the subject of section 6. It leads us to a framework for quantum mechanics on a lattice. Some conclusions are collected in section 7.

2. A brief introduction to umbral calculus

In this section we recall some notions and results from umbral calculus. We refer to [2, 1] for the corresponding proofs and further results. For simplicity, we restrict our considerations to the case of a single 'coordinate' x. All results extend to several (commuting) variables in an obvious way.

An operator O acting on the algebra (over a field of characteristic zero, like $\mathbb{R}$ or $\mathbb{C}$)

of polynomials in x is *shift-invariant* if it commutes (for all a in the field) with the shift operators S_a (defined by $S_a f(x) = f(x+a)$).

The *Pincherle derivative* of an operator O is defined as the commutator

$$O' := [O, \boldsymbol{x}] = O\boldsymbol{x} - \boldsymbol{x}O \tag{2.1}$$

where $\boldsymbol{x}$ is the multiplication operator, acting on polynomials in x by multiplication with x. The Pincherle derivative of a shift-invariant operator is again a shift-invariant operator. The *umbral algebra* is the algebra of all shift-invariant operators. The Pincherle derivative is a derivation of the umbral algebra.

A *delta operator* Q is a linear operator, acting on the algebra of polynomials in x, which is shift-invariant and for which Qx is a non-zero constant. It can be shown that Q'^{-1} exists (as a linear operator on the space of polynomials) and commutes with Q. If we define

$$\hat{\boldsymbol{x}} := \boldsymbol{x}\, Q'^{-1} \tag{2.2}$$

it follows that

$$[Q, \hat{\boldsymbol{x}}] = \mathbb{1} \tag{2.3}$$

where $\mathbb{1}$ stands for the identity operator. In this way each delta operator Q provides us with a representation of the canonical commutation relations on the algebra of polynomials in x.

A *polynomial sequence* $q_k(x)$, $k = 0, 1, 2 \ldots$, is a sequence of polynomials where $q_k(x)$ is of degree k. A polynomial sequence is called *basic* for a delta operator Q if $q_0(x) = 1$, $q_k(0) = 0$ whenever $k > 0$, and

$$Qq_k = kq_{k-1}. \tag{2.4}$$

It turns out that basic sequences are of *binomial type*, i.e. they satisfy

$$q_k(x+y) = \sum_{\ell=0}^{k} \binom{k}{\ell} q_\ell(x) q_{k-\ell}(y). \tag{2.5}$$

The basic polynomial sequence for Q is given by

$$q_k(x) = \hat{\boldsymbol{x}} q_{k-1}(x) = \hat{\boldsymbol{x}}^k 1 \tag{2.6}$$

which is known as the *Rodrigues formula*.

An operator which maps a basic polynomial sequence into another basic polynomial sequence is called an *umbral operator* ([2], p 28). Defining

$$\tilde{f}(x) := f(\hat{\boldsymbol{x}})1 \tag{2.7}$$

for a polynomial f, (2.6) shows that the operator $\tilde{}$ is an umbral operator.

An associative and commutative product is defined by

$$\tilde{f}(x) * \tilde{h}(x) := f(\hat{\boldsymbol{x}})h(\hat{\boldsymbol{x}})1. \tag{2.8}$$

In particular, $q_k(x) * q_\ell(x) = q_{k+\ell}(x)$. The delta operator Q is a derivation with respect to the $*$-product, i.e.

$$Q[p(x) * q(x)] = (Qp(x)) * q(x) + p(x) * Qq(x) \tag{2.9}$$

for polynomials p and q.

Example 1. For $Q = \mathrm{d}/\mathrm{d}x$ we have $Q' = \mathbb{1}$ and therefore $q_k(x) = x^k$ which is the simplest polynomial sequence. □

Example 2. Let $Q = D/(D-1)$ with $D := \mathrm{d}/\mathrm{d}x$. Then $Q' = -(D-1)^{-2}$ and $q_k(x) = [-\boldsymbol{x}(D-1)^2]^k 1$ are the *basic Laguerre polynomials* [2]. □

As pointed out in the introduction, we are particularly interested in the case where the algebra of polynomials in x can be realized as an algebra of functions on a discrete set. In the following two examples we may choose x to be the canonical coordinate function on an infinite lattice with spacings a (where a is a positive real number). In the way outlined in the introduction, both examples provide us with a prescription to translate functions on $\mathbb{R}$ and differential operators into corresponding functions and operators on a lattice. The interesting aspect is that this prescription not only maps a differential equation into a corresponding difference equation, but it also allows us, in principle, to calculate the solutions of the difference equation from those of the differential equation (see sections 4 and 6).

Example 3. Let $Q = \partial_+$ where ∂_+ is the *forward discrete derivative* operator,

$$(\partial_+ f)(x) = \frac{1}{a}[f(x+a) - f(x)] \tag{2.10}$$

acting on a function f. We find $(Q' f)(x) = f(x+a)$ and therefore $Q' = S_a$, the shift operator. Hence,

$$q_k(x) = (\boldsymbol{x} S_a^{-1})^k 1 = x(x-a)\cdots(x-(k-1)a) = x^{(k)} \tag{2.11}$$

where $x^{(k)}$ is the kth (falling) *factorial function*†. Some formulae for the $*$-product associated with the discrete derivative delta operator can be found in the appendix. Analogous formulae hold for the *backward* discrete derivative operator ∂_- which is formally obtained from ∂_+ replacing a by $-a$. □

Example 4. For the *central difference operator* [7]

$$Q = \frac{1}{2a}(S_a - S_{-a}) = \tfrac{1}{2}(\partial_+ + \partial_-) \tag{2.12}$$

we have $Qf(x) = [f(x+a) - f(x-a)]/(2a)$. Solving (2.4), one finds the basic sequence

$$q_k(x) = x \prod_{n=1}^{k-1}(x + ka - 2na) \qquad (k > 1) \tag{2.13}$$

and $q_0(x) = 1, q_1(x) = x$. Furthermore,

$$Q' = \tfrac{1}{2}(S_a + S_{-a}) \qquad Q'' = a^2 Q. \tag{2.14}$$

Using the Rodrigues formula,

$$Q'^{-1} q_k(x) = \prod_{n=1}^{k}[x + (k+1)a - 2na] \qquad (k > 0) \tag{2.15}$$

which shows that Q'^{-1} is indeed well-defined on polynomials in x. The operator Q'^{-1} also exists as a selfadjoint operator in the Hilbert space $\ell_2(a\mathbb{Z})$, see section 6. □

Example 5. Over a finite field there are finite-dimensional representations of the commutation relation (2.3). Over $\mathbb{Z}_3$ the matrices

$$\boldsymbol{x} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad Q = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \tag{2.16}$$

provide us with an example which generalizes in an obvious way to the Galois fields $GF(p^n)$ (where p is a prime and $n \in \mathbb{N}$). Though in this case we leave the usual umbral framework since we consider a field which is not of characteristic zero, some basic constructions and results remain valid. □

† For $a = 1$ and $x \in \mathbb{N}$ it counts the number of injective maps from a set of n elements to a set of x elements.

As long as we restrict our considerations to operators acting on polynomials, everything works smoothly. We are, however, also interested in more general classes of functions and in particular power series. In general, an umbral operator like $\tilde{}$ does not preserve convergence of such a series. The result of the application of an umbral operator to a power series *a priori* only makes sense as a *formal* power series. A problem is then to determine its domain of convergence (which may be empty) and a possible continuation. It seems that little is known about the convergence of power series obtained via umbral maps.

3. Symmetry operators on a lattice: an example

In this section we generalize the example 3 of section 2 to n-dimensions. As an application of the umbral method, a representation of the Lie algebra of $SO(3)$ on a lattice is then presented. Let $x_1, \ldots, x_n$ be the canonical coordinate functions on an n-dimensional (hypercubic) lattice with spacings a_i. We define delta operators

$$(Q_i f)(x) := \frac{1}{a_i}[f(x_1, \ldots, x_{i-1}, x_i + a_i, x_{i+1}, \ldots, x_n) - f(x)] \tag{3.1}$$

acting on functions of $x = (x_1, \ldots, x_n)$. The corresponding Pincherle derivatives are the shift operators S_i acting on functions as follows,

$$(S_i f)(x) := f(x_1, \ldots, x_{i-1}, x_i + a_i, x_{i+1}, \ldots, x_n). \tag{3.2}$$

The operators $\hat{\boldsymbol{x}}_i = \boldsymbol{x}_i S_i^{-1}$ and Q_j then satisfy the commutation relations (1.1) on the algebra of polynomials in the variables $x_1, \ldots, x_n$.

As outlined in the introduction, given a representation of a Lie algebra in terms of the operators $\boldsymbol{y}_i$ and $\partial/\partial y_j$ acting on functions on $\mathbb{R}^n$, (1.4) maps it into a representation by operators acting on functions on a lattice. For the angular momentum operators in three dimensions this means

$$L_i = -\mathrm{i} \sum_{j,k} \epsilon_{ijk} \boldsymbol{y}_j \frac{\partial}{\partial y_k} \mapsto \tilde{L}_i := -\mathrm{i} \sum_{j,k} \epsilon_{ijk} \hat{\boldsymbol{x}}_j Q_k \tag{3.3}$$

where

$$\tilde{L}_i f(x) = -\mathrm{i} \sum_{j,k} \epsilon_{ijk} x_j (Q_k f)(x - a_j) \tag{3.4}$$

using the notation $x - a_j = (x_1, \ldots, x_{j-1}, x_j - a_j, x_{j+1}, \ldots, x_n)$.

What are the corresponding 'spherically symmetric' functions on the lattice? We have to find the solutions of $\tilde{L}_i f(x) = 0$. From the corresponding solution in the continuum case, we know that f should depend on x_k only through $\sum_{k=1}^3 \hat{\boldsymbol{x}}_k^2 1 = \sum_{k=1}^3 x_k(x_k - a_k)$ or $*$-products of this expression. The set of lattice points determined by the equation $\sum_{k=1}^3 x_k(x_k - a_k) =$ constant therefore constitutes the analogue of the 2-sphere in the continuum case. Of course, only for special values of the constant it will be non-empty. For a lattice with equal spacings in all dimensions, the mappings $x_k \leftrightarrow x_\ell$ and $x_k \mapsto a - x_k$ leave the above expression invariant and thus help to construct the 'lattice spheres'.

4. Isospectral discretization of eigenvalue equations via umbral calculus?

In [3] differential equations were called 'quasi-exactly solvable' if there is at least one polynomial solution and 'exactly solvable' if there is a complete set of polynomial solutions. The relevance for physics has been established in a series of papers [8] where quantum mechanical eigenvalue problems were collected which can be reduced to equations having polynomial eigenfunctions via an *ansatz* of the form

$$\psi(y) = \phi(y) f(y) \tag{4.1}$$

with a fixed non-polynomial function f on $\mathbb{R}$. The most familiar example is provided by the (one-dimensional) harmonic oscillator. In this case

$$\psi(y) = \phi(y)\mathrm{e}^{-y^2/2} \tag{4.2}$$

converts the Schrödinger equation into a differential equation for ϕ which has the Hermite polynomials as a complete set of solutions. Another example is the radial part of the Schrödinger equation for a hydrogen atom.

In [4] a discretization procedure has been proposed for a differential operator eigenvalue equation possessing polynomial solutions such that the resulting difference equation has the same spectrum. It corresponds to an umbral map in the sense of section 2 with the choice $Q = \partial_+$, the forward discrete derivative operator†. However, the procedure does not work well, in general, when applied to the original eigenvalue problem which we started with. Though we do get a discrete eigenvalue problem in this way which is naively‡ isospectral, problems arise when we try to translate the non-polynomial solutions. This will be illustrated with the following examples.

Example 1. We apply the umbral map to a simple differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}y} f(y) = kf(y) \mapsto Q\tilde{f}(x) = k\tilde{f}(x). \tag{4.3}$$

From the solution $f(y) = \exp(ky)$ of the differential equation the corresponding solution of the difference equation on the r.h.s. of (4.3) is then obtained as follows,

$$\tilde{f}(x) = f(\hat{\boldsymbol{x}})1 = \sum_{\ell=0}^{\infty} \frac{k^\ell}{\ell!} x^{(\ell)}. \tag{4.4}$$

Though we would like to choose x as the canonical coordinate function on the lattice $a\mathbb{Z}$, it may be helpful at this point to consider it as a coordinate function on $\mathbb{R}$ in view of a possible analytic continuation of the power series obtained from the umbral procedure. *A priori*, we obtain $\tilde{f}$ only as a *formal* power series. For *real* k, the series in (4.4) (which is a special case of a *Newton series*) converges everywhere on the real line if $|ka| < 1$. For $|ka| > 1$ the series is everywhere divergent, except for non-negative integer multiples of a (see [11], for example). The difference equation on the r.h.s. of (4.3) has no non-vanishing solution for $k = -1/a$. For all other values of $k \in \mathbb{C}$ the solutions are given by

$$\tilde{f}(na) = \tilde{f}(0)(1 + ka)^n. \tag{4.5}$$

With $\tilde{f}(0) = 1$ this extends the series obtained above (for $k > -1/a$). □

Example 2. Let us now apply the umbral map to the Hamiltonian of the harmonic oscillator,

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \tfrac{1}{2}\boldsymbol{y}^2 \mapsto \tilde{H} = -\tfrac{1}{2}Q^2 + \tfrac{1}{2}\hat{\boldsymbol{x}}^2. \tag{4.6}$$

† The umbral framework provides us with several alternatives, of course, which have not been considered in [4].
‡ In order to formulate a well-defined eigenvalue problem, we have to specify a suitable function space in which we are looking for solutions. Each eigenfunction of a differential operator is mapped to an eigenfunction of the corresponding discrete operator (or at least a formal power series which satisfies the discrete eigenvalue equation). Note, however, that the discrete equation may have additional solutions. In particular, this is the origin of boson or fermion doubling in lattice-field theories (cf [9, 10]).

The eigenvalue equation for H is then translated into the following eigenvalue equation for $\tilde{H}$,

$$\tilde{H}\tilde{\psi}(x) = \tfrac{1}{2}[-Q^2\tilde{\psi}(x) + x(x-a)\tilde{\psi}(x-2a)] = E\tilde{\psi}(x) \tag{4.7}$$

which is a difference equation ($Q = \partial_+$). From the solution $\psi_0(y) = \exp(-y^2/2)$ of the original eigenvalue problem we obtain the solution

$$\tilde{\psi}_0(x) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{2^\ell \ell!} x^{(2\ell)} \tag{4.8}$$

of the difference equation (4.7) with $E = \frac{1}{2}$ as a formal power series. Using

$$\frac{x^{(2\ell+2)}}{2^{\ell+1}(\ell+1)!} = \frac{(x-2\ell a)(x-2\ell a-a)}{2(\ell+1)} \frac{x^{(2\ell)}}{2^\ell \ell!} \tag{4.9}$$

the quotient criterion shows that the series is everywhere divergent, except at values of x which are non-negative integer multiples of a (where the series terminates). Equation (4.8) thus only determines a solution of the difference equation

$$x(x-a)\tilde{\psi}(x-2a) = \frac{1}{a^2}[\tilde{\psi}(x) - 2\tilde{\psi}(x+a) + \tilde{\psi}(x+2a)] + \tilde{\psi}(x) \tag{4.10}$$

on the non-negative part of $a\mathbb{Z}$. The l.h.s. of (4.10) vanishes for $x = 0$ and $x = a$. Also the r.h.s. vanishes if we calculate the corresponding values of $\tilde{\psi}$ using (4.8). Our solution can therefore be extended to the whole of $a\mathbb{Z}$. But the extension is not unique since $\tilde{\psi}(-a)$ and $\tilde{\psi}(-2a)$ can be chosen arbitrarily. This shows that the difference equation has more independent solutions than the differential equation we started with. The umbral-mapping of ψ_0 can, however, be completed to yield a solution of the difference equation which exists everywhere on $a\mathbb{Z}$. This is done by expanding ψ_0 into power series about negative multiples of a and acting with $\tilde{}$ on these series.

The higher eigenfunctions of the harmonic oscillator are products of Hermite polynomials with ψ_0,

$$\psi_n(y) = \mathcal{H}_n(y)\psi_0(y). \tag{4.11}$$

Now $\tilde{\psi}_n(x)$ is obtained by replacing the ordinary product by the $*$-product (cf the appendix), $\psi_0(y)$ by $\tilde{\psi}_0(x)$ as given above, and the Hermite polynomials by the 'discrete Hermite polynomials'. The latter are obtained from the generating function

$$\tilde{F}(x,s) = \sum_{\ell=0}^{\infty} \frac{\tilde{\mathcal{H}}_\ell(x)}{\ell!} s^{(\ell)} = \sum_{\ell=0}^{\infty}\sum_{k=1}^{\ell} \frac{2^{\ell-k}(-1)^k}{k!(\ell-k)!} s^{(\ell+k)} x^{(\ell-k)} \tag{4.12}$$

by $\tilde{\mathcal{H}}_n(x) = (\mathrm{d}/\mathrm{d}s)^n \tilde{F}(x,s)|_{s=0}$. □

5. Some more umbral calculus

There is a generalization of the calculus described in section 2. Given a representation of the commutation relation (2.3) by operators Q and $\hat{\boldsymbol{x}}$ as in section 2, and given an operator A on the space of polynomials which commutes with Q, then the new operator $\hat{\boldsymbol{x}} + A$ together with Q also satisfies the commutation relation. In the following, let $\hat{\boldsymbol{x}}$ denote such a more general choice (than the special one in (2.2)). Defining

$$s_k(x) := \hat{\boldsymbol{x}}^k 1 \tag{5.1}$$

one finds

$$Qs_k = ks_{k-1} \tag{5.2}$$

by use of the commutation relation (2.3). Such a polynomial sequence s_k is called a *Sheffer set* for the delta operator Q in the umbral literature. The basic polynomial sequence q_k for a delta operator Q is a special Sheffer set. If s_k is a Sheffer set for Q, then there is an invertible shift-invariant operator which maps the Sheffer polynomials s_k to the basic polynomials q_k. Furthermore,

$$s_n(x) = \sum_{k=0}^{n} \binom{n}{k} s_k(0) q_{n-k}(x). \tag{5.3}$$

We refer to [2] for proofs and further results. Again, we define $\tilde{f}(x) := f(\hat{\boldsymbol{x}})1$.

We have to stress that not all umbral results established for the special choice (2.2) for $\hat{x}$ translate to the more general case considered in this section. In general, $s_k(0) \neq 0$ and the s_k are not binomial.

A particularly interesting choice for $\hat{\boldsymbol{x}}$ turns out to be

$$\hat{\boldsymbol{x}} = \tfrac{1}{2}(\boldsymbol{x}Q'^{-1} + Q'^{-1}\boldsymbol{x}). \tag{5.4}$$

From umbral calculus we know that Q'^{-1} commutes with Q. One can then easily verify that $[Q, \hat{\boldsymbol{x}}] = \mathbb{1}$. The advantage of (5.4) over (2.2) is that it is more symmetric and thus opens the chance to turn $\hat{\boldsymbol{x}}$ and $\mathrm{i}Q$ into Hermitian operators on a Hilbert space†. For $Q = \mathrm{d}/\mathrm{d}x$ we have $s_k(x) = q_k(x)$. In case of the (forward) discrete derivative operator one finds

$$s_k(x) = \frac{1}{2^k}(\boldsymbol{x}S_a^{-1} + S_a^{-1}\boldsymbol{x})^k 1 = (x - \tfrac{1}{2}a)(x - \tfrac{3}{2}a)\cdots\left(x - \frac{2k-1}{2}a\right). \tag{5.5}$$

Another realization of (5.4), involving the central difference operator, will be the subject of the following examples and the next section. In that case, we have

$$s_0(x) = 1, s_1(x) = x, s_2(x) = x^2 - \frac{a^2}{2}, \ldots \tag{5.6}$$

using (2.14) and $Q1 = 0$.

Example 1. Let us consider again the example of the harmonic oscillator. Using (5.4) and the central difference operator (2.12), the corresponding Schrödinger equation is umbral mapped to

$$\mathrm{i}\frac{\partial}{\partial t}\tilde{\psi}(x) = \frac{1}{2}\left[-Q^2 + Q'^{-2}\left(\boldsymbol{x}^2 - \frac{a^2}{2}\right) + 2a^2 Q'^{-3}Q\boldsymbol{x} + \frac{5}{4}a^4 Q'^{-4}Q^2\right]\tilde{\psi}(x) \tag{5.7}$$

where on the r.h.s. we have naively commuted all the non-local operators Q'^{-1} to the left. Acting with Q'^4 on this equation results in a finite difference equation (with respect to the space coordinates). However, if we discretize the time‡ in order to solve the initial value problem for the above equation on a computer, calculation of the wavefunction at the next time step requires Q'^{-1}. But to explore an equation of the type above numerically, we have to use an approximation with a *finite* lattice. Choosing periodic boundary conditions (i.e. a periodic lattice), there are convenient formulae for Q'^{-1}. On a periodic lattice with $N = 2m$ sites where m is odd, the equation

$$Q'^{-1} = \sum_{k=0}^{m-1}(-1)^k S_a^{2k+1} \tag{5.8}$$

† If $\boldsymbol{x}$ is Hermitian and Q anti-Hermitian, then Q' and Q'^{-1} are Hermitian and thus also the operator in (5.4).

‡ This can be achieved via an umbral map, of course.

holds†. For odd N one finds instead

$$Q'^{-1} = \sum_{k=0}^{(N-1)/2} (-1)^{k+(N-1)/2} S_a^{2k} + \sum_{k=0}^{(N-1)/2-1} (-1)^k S_a^{2k+1}. \tag{5.9}$$

In the following section, the quantum mechanical setting behind (5.7) is investigated more rigorously. □

Example 2. In section 3 we determined the 'lattice spheres' with respect to some umbral representation. Instead of (2.2) here we choose

$$\hat{\boldsymbol{x}}_i := \boldsymbol{x}_i (S_i + S_i^{-1})^{-1} + (S_i + S_i^{-1})^{-1} \boldsymbol{x}_i \tag{5.10}$$

with the shift operators defined in (3.2). This means that we consider (5.4) generalized to several dimensions with central difference operators

$$Q_i = \frac{1}{2a_i}(S_i - S_i^{-1}). \tag{5.11}$$

Using $Q_i'' = a_i^2 Q_i$ and $Q_i 1 = 0$, we find the following equations for 'lattice spheres' in three dimensions,

$$\sum_{i=1}^{3} (\hat{\boldsymbol{x}}_i)^2 1 = \sum_{i=1}^{3} \left[(x_i)^2 - \frac{a_i^2}{2} \right] = \text{constant}. \tag{5.12}$$

A spherically symmetric potential on the lattice is then a function which only depends on $*$-products of $\sum_{i=1}^{3} [(x_i)^2 - a_i^2/2]$. □

Example 3. A familiar representation of the Poincaré algebra is

$$P_\mu = -\mathrm{i}\frac{\partial}{\partial y_\mu} \qquad M_i = \sum_{j,k} \epsilon_{ijk} \boldsymbol{y}_j P_k \qquad L_i = y_0 P_i - \kappa \boldsymbol{y}_i P_0. \tag{5.13}$$

These operators act on functions on $\mathbb{R}^4$ (with canonical coordinates y_μ). The commutation relations are then preserved when we perform in the expressions (5.13) the substitutions

$$\boldsymbol{y}_i \mapsto \hat{\boldsymbol{x}}_i \qquad \frac{\partial}{\partial y_i} \mapsto Q_i \qquad i = 1, 2, 3 \tag{5.14}$$

with the operators defined in (5.10) and (5.11). In this way we obtain a representation of the Poincaré algebra on a lattice with spacings a_i (and continuous time as long as y_0 and P_0 are kept unchanged)‡. The quadratic Casimir operator of the Poincaré algebra in this representation is

$$C = -\partial_t^2 + \sum_k Q_k^2 \tag{5.15}$$

where $\partial_t := \partial/\partial x_0$. There is, however, a drawback of the representation presented above and also those given in [5]. As pointed out in [9], the Klein–Gordon equation built with the operator (5.15) suffers from a boson doubling problem analogous to the more familiar fermion doubling problem in lattice-field theory (see [10], for example). This leaves us with a Poincaré-invariant theory with eight species of bosons. If the time dimension is also discretized, one obtains 16 species. The relation between this Klein–Gordon equation and the Dirac equation for 'naive lattice fermions' is the same as in the continuum,

$$(\mathrm{i}\gamma^0\partial_t + \mathrm{i}\gamma^k Q_k - m)(\mathrm{i}\gamma^0\partial_t + \mathrm{i}\gamma^k Q_k + m) = -\partial_t^2 + \sum_k Q_k^2 - m^2. \tag{5.16}$$

† For even m, Q' is not invertible.

‡ See also [5]. A representation on a four-dimensional space–time lattice is obtained by extending the map (5.14) to y_0 and $\partial/\partial y_0$.

The representation of the Poincaré algebra acting on continuum spinor fields is mapped via (5.14) to a representation on the lattice which leaves the lattice Dirac equation invariant. □

6. Via umbral calculus to quantum mechanics on a lattice

In this section we investigate the umbral discretization method with the central difference operator $Q = (S_a - S_{-a})/(2a)$ and the symmetric operator (5.4). It will be shown that they define selfadjoint operators on the Hilbert space $\ell_2(a\mathbb{Z})$, the space of square summable functions on the infinite lattice with spacings a. We thus have a rigorous framework to explore the 'umbral map'.

By standard arguments $\boldsymbol{x}$ is selfadjoint with domain $[f \in \ell_2(a\mathbb{Z}) | \boldsymbol{x} f \in \ell_2(a\mathbb{Z})]$. The Fourier transformation $f \mapsto F$ where

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\pi/a}^{\pi/a} F(k) \mathrm{e}^{\mathrm{i}kx} \, \mathrm{d}k \tag{6.1}$$

is an isomorphism $\ell_2(a\mathbb{Z}) \to L^2_{\pi/a}$. Here and in the following L^2_b stands for $L^2([-b, b])$, the space of square-integrable functions on the interval $[-b, b]$. It is more convenient for us to define the domain of $\boldsymbol{x}$ now as follows,

$$\mathcal{D}_{\boldsymbol{x}} = \left\{ f \in \ell_2(a\mathbb{Z}) | F \text{ abs. cont.}, F\left(-\frac{\pi}{a}\right) = F\left(\frac{\pi}{a}\right), \frac{\mathrm{d}F}{\mathrm{d}k} \in L^2_{\pi/a} \right\}. \tag{6.2}$$

The action of $\boldsymbol{x}$ on $\ell_2(a\mathbb{Z})$ then corresponds to the action of $\mathrm{i}\,\mathrm{d}/\mathrm{d}k$ on the domain in $L^2_{\pi/a}$ specified above†. Its spectrum is $[na | n \in \mathbb{Z}]$.

Next we note that $-\mathrm{i}Q$ is a bounded selfadjoint operator on $\ell_2(a\mathbb{Z})$. In $L^2_{\pi/a}$ it acts by multiplication with $\sin(ak)/a$. Concerning the umbral map we can conclude the following,

$$\begin{aligned}
&\text{operator}: \ -\mathrm{i}\,\mathrm{d}/\mathrm{d}y \mapsto -\mathrm{i}Q \\
&\text{spectrum}: \mathbb{R}\{\lambda \in \mathbb{R} | |\lambda| \leqslant \tfrac{1}{a}\} \\
&\text{eigenfunctions}: \ f_\lambda(y) = \exp(\mathrm{i}\lambda y) \mapsto \tilde{f}_\lambda(x) = \exp[\mathrm{i}(x/a) \arcsin\,(\lambda a)].
\end{aligned}$$

The eigenfunctions of $-\mathrm{i}Q$ can indeed be calculated directly from the power series expansions for those of $-\mathrm{i}\,\mathrm{d}/\mathrm{d}y$ (with the help of [7], section 6.5). The spectrum of $-\mathrm{i}Q$ is bounded, however, in accordance with the boundedness of the operator. Only in the limit $a \to 0$ we recover the full spectrum of the continuum momentum operator.

For $f \in \mathcal{D}_{\boldsymbol{x}}$ we have $Qf \in \mathcal{D}_{\boldsymbol{x}}$. The operator $Q' = [Q, \boldsymbol{x}] = (S_a + S_{-a})/2$ is then defined on $\mathcal{D}_{\boldsymbol{x}}$. It is bounded and can be extended to a selfadjoint operator on $\ell_2(a\mathbb{Z})$. $Q'f = 0$ for $f \in \ell_2(a\mathbb{Z})$ implies $f = 0$. Hence Q'^{-1} exists on $\mathcal{D}_{Q'^{-1}} = Q'(\ell_2(a\mathbb{Z}))$ and is selfadjoint (lemma XII.1.6 in [12]). The Fourier transform of Q' acts in $L^2_{\pi/a}$ by multiplication with $\cos(ak)$. The operator Q'^{-1} therefore acts by multiplication with $1/\cos(ak)$ on the domain $\{F \in L^2_{\pi/a} | F(k)/\cos(ak) \in L^2_{\pi/a}\}$.

It remains to investigate the operator $\hat{\boldsymbol{x}} = (\boldsymbol{x}Q'^{-1} + Q'^{-1}\boldsymbol{x})/2$ which is Hermitian on the dense domain

$$\mathcal{D}_{\hat{\boldsymbol{x}}} = [f \in \mathcal{D}_{\boldsymbol{x}} \cap \mathcal{D}_{Q'^{-1}} | \boldsymbol{x} f \in \mathcal{D}_{Q'^{-1}}, Q'^{-1} f \in \mathcal{D}_{\boldsymbol{x}}]. \tag{6.3}$$

Without any calculations we can immediately conclude the following. The operator $\hat{\boldsymbol{x}}^2$ can be defined on a dense domain on which it commutes with complex conjugation. According to theorem XII.4.18 and corollary XII.4.13(a) in [12] this operator has selfadjoint extensions. Let us recall a theorem due to Rellich and Dixmier (see Theorem 4.6.1 in [13]).

† The latter is a standard textbook example of a selfadjoint operator. Via Fourier transformation it is mapped to a selfadjoint operator on $\mathcal{D}_{\boldsymbol{x}} \subset \ell_2(a\mathbb{Z})$.

Theorem. Let $\boldsymbol{q}$ and $\boldsymbol{p}$ be closed Hermitian operators on a Hilbert space $\mathcal{H}$ such that

(1) $[\boldsymbol{p}, \boldsymbol{q}] = -\mathrm{i}$ on a subset $\Omega \subset \mathcal{D}_{\boldsymbol{q}} \cap \mathcal{D}_{\boldsymbol{p}}$ dense in $\mathcal{H}$ which is invariant under $\boldsymbol{q}$ and $\boldsymbol{p}$,

(2) $\boldsymbol{p}^2 + \boldsymbol{q}^2$ on Ω is essentially selfadjoint.

Then $\boldsymbol{p}$ and $\boldsymbol{q}$ are selfadjoint and unitarily equivalent to a direct sum of Schrödinger representations. □

An isomorphism $\ell_2(a\mathbb{Z}) \cong L^2(\mathbb{R})$ maps the operators $\hat{\boldsymbol{x}}$ and $-\mathrm{i}Q$ to corresponding operators in $L^2(\mathbb{R})$. These operators cannot be unitarily equivalent to those of the Schrödinger representation since the latter are both unbounded. Besides (2), the operator $\hat{\boldsymbol{x}}$ (which has a closed Hermitian extension [12]) and $-\mathrm{i}Q$ fulfil all assumptions of the last theorem. Taking into account that $(-\mathrm{i}Q)^2$ is selfadjoint and bounded, it follows that $\hat{\boldsymbol{x}}^2$ is not essentially selfadjoint. Together with our previous result this means that $\hat{\boldsymbol{x}}^2$ has inequivalent selfadjoint extensions.

We now turn to a closer inspection of the operator $\hat{\boldsymbol{x}}$ which, via Fourier transformation, is translated into the operator

$$X := \tfrac{\mathrm{i}}{2}\left(\frac{1}{\cos(ak)}\frac{\mathrm{d}}{\mathrm{d}k} + \frac{\mathrm{d}}{\mathrm{d}k}\frac{1}{\cos(ak)}\right) \tag{6.4}$$

with domain $\mathcal{D}_X \subset L^2_{\pi/a}$ determined by (6.3). This operator is singular at $k = \pm\pi/(2a)$ and functions in $\mathcal{D}_X$ vanish at these points. This suggests to look for selfadjoint extensions of X for which all the functions in their domains share this property†. Such selfadjoint extensions of X are then sums of selfadjoint extensions of the following two operators,

(a) $X^{(1)}$ is X restricted to

$$\mathcal{D}_{X^{(1)}} := \left\{F \in L^2_{\pi/2a} \left| \frac{F(k)}{\cos(ak)} \text{ abs. cont., } F\left(-\frac{\pi}{(2a)}\right) = 0 = F\left(\frac{\pi}{(2a)}\right), XF \in L^2_{\pi/2a}\right.\right\}$$

(b) $X^{(2)}$ is X restricted to

$$\mathcal{D}_{X^{(2)}} := \left\{F \in L^2_{\cup} \left| \frac{F(k)}{\cos(ak)} \text{ abs. cont., } F\left(-\frac{\pi}{(2a)}\right) = 0 = F\left(\frac{\pi}{(2a)}\right),\right.\right.$$
$$\left. F\left(-\frac{\pi}{a}\right) = F\left(\frac{\pi}{a}\right), XF \in L^2_{\cup}\right\}$$

where

$$L^2_{\cup} := L^2\left(\left[-\frac{\pi}{a}, -\frac{\pi}{(2a)}\right] \cup \left[\frac{\pi}{(2a)}, \frac{\pi}{a}\right]\right).$$

In both cases we perform a change of coordinate

$$p = \frac{1}{a}\sin(ak). \tag{6.5}$$

Then, with the separation

$$F(k) = \sqrt{|\cos(ak)|}\,\chi(p) \tag{6.6}$$

we find for $\ell = 1, 2$,

$$(X^{(\ell)}F)(k) = \mathrm{i}\sqrt{|\cos(ak)|}\frac{\mathrm{d}}{\mathrm{d}p}\chi(p). \tag{6.7}$$

† The following elementary analysis does not exhaust the selfadjoint extensions of X. The problem under consideration constitutes a special case to which the general theory developed in [14] can be applied. We are grateful to one of the referees for pointing out these references. The following steps leading to (6.11) should actually be reversed, i.e. starting from the class of selfadjoint operators (6.11) we obtain selfadjoint extensions of X. Our presentation displays the heuristics which is here (as often) contragredient to the mathematical logic.

The two operators $X^{(\ell)}$ now both translate into the more familiar one†

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}p} \qquad \text{on} \quad \left\{\chi \in L^2_{1/a} \middle| \chi \text{ abs. cont.}, \chi\left(-\frac{1}{a}\right) = 0 = \chi\left(\frac{1}{a}\right), \frac{\mathrm{d}\chi}{\mathrm{d}p} \in L^2_{1/a}\right\}. \tag{6.8}$$

Let $F_{(1)}$ and $F_{(2)}$ denote the restrictions of $F \in \mathcal{D}_X$ to $[-\pi/a, \pi/a]$ and $[-\pi/a, -\pi/(2a)] \cup [\pi/(2a), \pi/a]$, respectively. Then

$$(F, F') = \int_{-\pi/a}^{\pi/a} F(k)^* F'(k)\,\mathrm{d}k = (\chi_{(1)}, \chi'_{(1)}) + (\chi_{(2)}, \chi'_{(2)}) \tag{6.9}$$

where

$$(\chi_{(\ell)}, \chi'_{(\ell)}) = \int_{-1/a}^{1/a} \chi_{(\ell)}(p)^* \chi'_{(\ell)}(p)\,\mathrm{d}p \qquad (\ell = 1, 2). \tag{6.10}$$

The selfadjoint extensions of the operator (6.8) are known to be given by

$$D_\alpha = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}p} \qquad \text{on } \mathcal{D}_\alpha := \left\{\chi \in L^2_{1/a} \middle| \chi \text{ abs. cont.}, \chi\left(\frac{1}{a}\right) = \mathrm{e}^{2\pi\mathrm{i}\alpha}\chi\left(-\frac{1}{a}\right), \frac{\mathrm{d}\chi}{\mathrm{d}p} \in L^2_{1/a}\right\} \tag{6.11}$$

where $\alpha \in [0, 1)$ [15]. A complete orthonormal set of eigenfunctions of D_α is

$$\chi_n^\alpha(p) := \sqrt{\frac{a}{2}}\exp[-\mathrm{i}(\alpha + n)\pi a p] \qquad n \in \mathbb{Z} \tag{6.12}$$

and D_α has a pure point spectrum $[(\alpha + n)\pi a | n \in \mathbb{Z}]$. A selfadjoint extension of the operator $\hat{\boldsymbol{x}}$ is now obtained by choosing any pair from the set of operators D_α. It then defines operators $X^{(1)}_{\alpha_1}$ and $X^{(2)}_{\alpha_2}$ and in this way a selfadjoint extension $\hat{\boldsymbol{x}}_{\alpha_1,\alpha_2}$ of $\hat{\boldsymbol{x}}$ with spectrum $[(\alpha_1 + n)\pi a | n \in \mathbb{Z}] \cup [(\alpha_2 + n)\pi a | n \in \mathbb{Z}]$. The operator $\hat{\boldsymbol{x}}_{\alpha_1,\alpha_2}$ has the complete set of eigenfunctions

$$f^{(\alpha_1)}_{n,1}(x) = \frac{1}{2}\sqrt{\frac{a}{\pi}}\int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} \sqrt{\cos(ak)}\exp[-\mathrm{i}(\alpha_1 + n)\pi\sin(ak) + \mathrm{i}kx]\,\mathrm{d}k \tag{6.13}$$

$$f^{(\alpha_2)}_{n,2}(x) = \frac{1}{2}\sqrt{\frac{a}{\pi}}\left(\int_{-\frac{\pi}{a}}^{-\frac{\pi}{2a}} + \int_{\frac{\pi}{2a}}^{\frac{\pi}{a}}\right)\sqrt{|\cos(ak)|}\exp[-\mathrm{i}(\alpha_2 + n)\pi\sin(ak) + \mathrm{i}kx]\,\mathrm{d}k \tag{6.14}$$

in $\ell_2(a\mathbb{Z})$. For the umbral map we can draw the following conclusions,

$$\begin{aligned} &\text{operator}: \boldsymbol{y} \mapsto \hat{\boldsymbol{x}}_{\alpha_1,\alpha_2} \\ &\text{spectrum}: \mathbb{R}\{(\alpha_\ell + n)\pi a | n \in \mathbb{Z}, \ell = 1, 2\} \\ &\text{eigenfunctions}: f_\lambda(y) = \delta(y - \lambda) f^{(\alpha_1)}_{n,1}, f^{(\alpha_2)}_{n,2}. \end{aligned}$$

Of course, in this case we have no method to calculate eigenfunctions of $\hat{\boldsymbol{x}}_{\alpha_1,\alpha_2}$ directly from the generalized eigenfunctions $\delta(y - \lambda)$ of the Schrödinger operator $\boldsymbol{y}$.

Slightly more complicated is the case of the operator $\hat{\boldsymbol{x}}^2$. Following our treatment of the operator $\hat{\boldsymbol{x}}$ itself, a set of two selfadjoint extensions of the operator $-\mathrm{d}^2/\mathrm{d}p^2$ determines a selfadjoint extension of $\hat{\boldsymbol{x}}^2$. The domains of selfadjoint extensions of $-\mathrm{d}^2/\mathrm{d}p^2$ in $L^2_{1/a}$ have the form

$$\mathcal{D}_{b.c.} = \left\{\chi \in L^2_{1/a} \middle| \chi\,\text{diff.}, \frac{\mathrm{d}\chi}{\mathrm{d}p} \text{ abs. cont.}, \frac{\mathrm{d}^2\chi}{\mathrm{d}p^2} \in L^2_{1/a}, b.c.\right\} \tag{6.15}$$

where $b.c.$ stands for a certain choice of boundary conditions, such as $\chi(-1/a) = 0 = \chi(1/a)$ (see [15] for other choices).

† Via this transformation the operator Q is mapped to the 'position operator' in $L^2_{1/a}$.

Example. Let us consider the equation $\boldsymbol{a}\psi_0 = \kappa\psi_0$ where $\boldsymbol{a} = \partial/\partial y + \boldsymbol{y}$ is the annihilation operator for the one-dimensional harmonic oscillator, and $\kappa \in \mathbb{C}$. The umbral map replaces $\boldsymbol{a}$ by $Q + \hat{\boldsymbol{x}}$. Choosing for $\hat{\boldsymbol{x}}$ a selfadjoint extension, we have to consider

$$(Q + \hat{\boldsymbol{x}}_{\alpha_1,\alpha_2})\tilde{\psi}_0 = \kappa\tilde{\psi}_0. \tag{6.16}$$

We write the Fourier transform of $\tilde{\psi}_0$ as $\Psi_0(k) = \sqrt{|\cos(ak)|}\chi_0(p)$ with p given by (6.5), separately on $[-\pi/(2a), \pi/(2a)]$ and $[-\pi/a, -\pi/(2a)] \cup [\pi/(2a), \pi/a]$. Now (6.16) translates on both subsets of $[-\pi/a, \pi/a]$ to $(p + \mathrm{d}/\mathrm{d}p)\chi_0 = \kappa\chi_0$ with the solution $\chi_0(p) = C\exp(\kappa p - p^2/2)$ where C is a constant. For $C \neq 0$ one finds $\chi_0 \in \mathcal{D}_\alpha$ with $\alpha = -\mathrm{i}\kappa/(\pi a)$. This restricts κ since $\alpha \in [0, 1)$. Furthermore, $\alpha_1 = \alpha_2 = \alpha$. Application of the (umbral mapped) creation operator $-Q + \hat{\boldsymbol{x}}_{\alpha,\alpha}$ to $\tilde{\psi}_0$ leaves $\mathcal{D}_{\hat{\boldsymbol{x}}_{\alpha,\alpha}}$ since $p\chi_0(p)$ is not in $\mathcal{D}_\alpha$. The algebraic construction of the eigenfunctions for the harmonic oscillator therefore does not survive after the umbral mapping. The problem actually appears already in rewriting the Hamiltonian as

$$\tilde{H}_\alpha = \tfrac{1}{2}(-Q^2 + \hat{\boldsymbol{x}}^2_{\alpha,\alpha}) = \tfrac{1}{2}(-Q + \hat{\boldsymbol{x}}_{\alpha,\alpha})(Q + \hat{\boldsymbol{x}}_{\alpha,\alpha}) + \tfrac{1}{2}[Q, \hat{\boldsymbol{x}}_{\alpha,\alpha}]. \tag{6.17}$$

The point is that $[Q, \hat{\boldsymbol{x}}_{\alpha,\alpha}] = \mathbb{1}$ does not hold on the domain of $\hat{\boldsymbol{x}}_{\alpha,\alpha}$. As a consequence, there is no simple relation between the spectra of $\tilde{H}_\alpha$ and $\frac{1}{2}(-Q + \hat{\boldsymbol{x}}_{\alpha,\alpha})(Q + \hat{\boldsymbol{x}}_{\alpha,\alpha})$.

In the way described above, the eigenvalue problem for a selfadjoint extension of the Hamiltonian $\tilde{H} = (-Q^2 + \hat{\boldsymbol{x}}^2)/2$ reduces in p-space to (twice) the eigenvalue problem for the Hamiltonian of the ordinary harmonic oscillator restricted to the finite interval $[-1/a, 1/a]$ with the respective boundary conditions. A choice among the many different selfadjoint extensions of $\tilde{H}$ should be determined by the specification of the physical system (on the lattice) which we intend to describe. It is not obvious for us, however, what a natural choice could be. □

An interesting aspect of the representation of the canonical commutation relations considered in this section is the fact that it is solely composed of the two operators $\boldsymbol{x}$ and Q which both receive a physical meaning if we interprete $\ell_2(a\mathbb{Z})$ as the space of functions on a (physical) space lattice. $\boldsymbol{x}$ is the position operator and $-\mathrm{i}Q$ the natural candidate for the momentum operator (see also [16]). This is the basis for a discrete version of quantum mechanics. Whereas ordinary quantum mechanics has a continuous position space, discrete quantum mechanics lives on a lattice. Quantum mechanical models on a lattice should then be modelled with the selfadjoint operators $\boldsymbol{x}$ and $-\mathrm{i}Q$. These satisfy commutation relations which are different from the canonical ones. Still missing, however, is a general recipe to quantize a (discrete) mechanical system, analogous to canonical quantization. But what is the meaning of the representation given by $\hat{\boldsymbol{x}}$ and $-\mathrm{i}Q$? Basically it just offers us a way to get, apparently, close to the results of ordinary quantum mechanics within the framework of discrete quantum mechanics. That this representation is not equivalent to the Schrödinger representation means that, within the framework of discrete quantum mechanics, we cannot reproduce ordinary quantum mechanics rigorously, at least not in the way attempted in this section. In fact, we have found rather drastic deviations, in particular a kind of spectrum doubling, a familiar problem in lattice field theories [9, 10].

7. Conclusions

In this paper we have pointed out that there is an apparently widely unknown mathematical scheme, called umbral calculus, behind recent work [4, 5] on discretization of differential equations and physical continuum models. Using several examples we have discussed its prospects and shortcomings. By choosing delta operators different from those used in these papers, alternative discretizations can be obtained. They have not been worked out in detail yet.

Discretization of a continuum theory breaks the continuous spacetime symmetries which play a crucial role in (non-gravitational) quantum field theory. There have been attempts to find a discrete analogue of spacetime symmetries for lattice theories such that essential features of the continuum group structures are maintained. Discretizations of Lorentz transformations were considered in [17], for example. In [18] the Poincaré group acts on an ensemble of lattices (see also [19] for a related point of view). Umbral calculus offers a different way to implement symmetries on lattices (see also [5]).

Umbral calculus provides us with certain classes of representations of the canonical commutation relations. It is therefore of potential interest for quantum mechanics and quantum field theory. Among the variety of umbral maps which we have at our disposal, the one determined by (5.4) with the central difference operator is of special interest (see also [5]). In this case we have a representation of the canonical commutation relations constructed from the position and the momentum operator on a lattice. This suggested a kind of embedding of ordinary quantum mechanics into a formalism for quantum mechanics on a lattice and thus a discretization of quantum mechanical systems which is different from conventional ones (see [20], for example). The representation of the canonical commutation relations obtained in this way is, however, not unitarily equivalent to the Schrödinger representation. As a consequence, the image of ordinary quantum mechanics under the umbral map cannot reproduce the results of the former rigorously. We revealed a kind of spectrum doubling similar to what is known in lattice field theories. This may be regarded as a negative feature. In any case, we believe that this is an interesting example of a representation of the canonical commutation relations by selfadjoint operators which is not equivalent to the Schrödinger representation. Furthermore, our analysis sheds some light on the work in [5] where this representation has been used. The umbral framework yields many more examples, of course, which can be analysed analogously to the example which we selected in section 6.

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Appendix. On the $*$-product associated with the forward discrete derivative delta operator

Let x be the canonical coordinate function on a lattice with spacings a. A function $f(x)$ for which the finite difference analogue of the Taylor series expansion (Gregory–Newton formula) exists can be written as follows,

$$f(x) = \sum_{n=0}^{\infty} f_n x^n = \sum_{k=0}^{\infty} F_k x^{(k)} \tag{A.1}$$

where we have used

$$x^n = \sum_{k=0}^{n} S(n,k) a^{n-k} x^{(k)}. \tag{A.2}$$

The coefficients $S(n, k)$ are the Stirling numbers of the second kind ($S(n, 0) = 0$ when $n > 0$, $S(n, n) = 1$). The coefficients F_k in (A.1) are given by

$$F_k = \sum_{m=0}^{\infty} f_{k+m} S(k+m, k) a^m. \tag{A.3}$$

The equation (A.1) can also be expressed as

$$f(x) = \tilde{F}(x) \tag{A.4}$$

where

$$F(\hat{\boldsymbol{x}}) = \sum_{k=0}^{\infty} F_k \hat{\boldsymbol{x}}^k. \tag{A.5}$$

The $*$-product of two functions of x is then given by

$$(f * h)(x) = (\widetilde{FH})(x) = \sum_{k,\ell=0}^{\infty} F_k H_\ell x^{(k+\ell)} \tag{A.6}$$

and the r.h.s. can be written as a power series in x with the help of

$$x^{(n)} = \sum_{k=0}^{n} s(n, k) a^{n-k} x^k \tag{A.7}$$

where $s(n, k)$ are the Stirling numbers of the first kind.

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