Quantum mechanics and umbral calculus

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Abstract

In this paper we present the first steps for obtaining a discrete Quantum Mechanics making use of the Umbral Calculus. The idea is to discretize the continuous Schrödinger equation substituting the continuous derivatives by discrete ones and the space-time continuous variables by well determined operators that verify some Umbral Calculus conditions. In this way we assure that some properties of integrability and symmetries of the continuous equation are preserved and also the solutions of the continuous case can be recovered discretized in a simple way. The case of the Schrödinger equation with a potential depending only in the space variable is discussed.

1 Introduction

In the last years the interest in physics for discrete space-time theories has increased mainly in relation with quantum gravity \cite{1}. In a scenario where the physical space-time may be discrete (i.e. there is a fundamental length in the space-time –let \(\sigma\) be the fundamental space length and \(\tau\) the fundamental time length – that could be related with Planck’s constant), continuous theories would only be approximations to the reality. Hence, it seems interesting the study of discrete physical theories such that in the limit of \(\sigma\) going to zero we recover the well known and established continuous physical theories. One way to do that is to discretize continuous physical theories, in particular quantum theories. It is obvious, that after discretization some properties will be conserved and other ones will disappear. A detailed study about when, how and why this happens would be pertinent and very interesting. This is the aim of this work: to study how to discretize a physical theory in such a way that properties related with symmetries in the continuous case can be preserved in the process, and so, to analyse the behaviour of quantum mechanics after discretization.

The Umbral Calculus is the mathematical tool that we will use to discretize Quantum Mechanics. It has been used recently to provide discrete representations of canonical commutation relations (i.e. \([\partial_x, x] = 1\)) in order to discretize linear differential equations \cite{2}-\cite{9}, in such a way that the continuous point symmetries are preserved the most cases.

In this paper we will consider a fixed lattice and use the umbral correspondence to obtain discrete solutions maintaining certain commutation relations \cite{9}.
The history of the Umbral Calculus goes back to the 17th century: Taylor, Newton, Barrow, Vandermonde, etc. [10] found some theorems and expressions relating powers with polynomials. However, in the second half of the 19th century through Sylvester, Cayley and Blissard [11]–[13] appeared the terms ‘umbrae’ (shadow in Latin) and ‘Umbral Calculus’ for the first time in relation with a set of ‘magic’ rules of lowering and raising indices. Some mathematical developments, like the theory of Sheffer polynomials (called Appell polynomials or more generally polynomials of type zero) [14]–[17] and the theory of abstract linear operators by Pincherle [15], converged to Umbral Calculus. Finally, in the second half of the 20th century Rota, Roman and collaborators [18]–[23] developed the Umbral Calculus as a linear algebra of operators. Thus, they formulated the theory of the umbral algebra and its dual in the space of formal series. A large bibliography about Umbral Calculus and its applications can be found in Ref. [24].

About recent results, we can mention that new methods in Umbral Calculus have been introduced for computation of series by integration [25]. Also Ref. [26]–[30] study the symmetries of nonlinear difference equations or multidimensional ones related with Quantum Mechanics.

This paper is organised as follows. In the next section we introduce the basic concepts of Umbral Calculus in terms of the theory of linear operators. In section 3 we show the main facts relative to the discretization of the (continuous) Quantum Mechanics. The most usual representations for the discrete derivative operator (right, left and symmetric discrete derivatives) are analysed in section 4. In order to see how the above umbral correspondences work we present in section 5 their action on some non-polynomial functions: the exponential and the trigonometric functions. The next section is devoted to present the basis for constructing a discrete Quantum Mechanics founded on the Umbral Calculus. Thus we present an umbral version of the Schrödinger equation for some potentials. Finally some conclusions close the paper.

2 Introduction to Umbral Calculus

This introductory exposition of the modern theory of the Umbral Calculus, developed mainly by Rota and Roman, follows mainly Ref. [23]. The umbral algebra, $\mathcal{L}$, is the algebra of linear operators acting on the algebra, $\mathcal{F}$, of formal power series in a variable or acting on the algebra of real or complex polynomials in a variable, $\mathcal{P}$. The elements of $\mathcal{F}$ are of the form

$$f(x) = \sum_{n=0}^{\infty} a_n x^n, \quad a_n \in \mathbb{F},$$

and those of $\mathcal{P}$ are

$$p_n(x) = \sum_{i=0}^{n} a_i x^i, \quad a_i \in \mathbb{F}, \quad n \in \mathbb{N},$$

being $\mathbb{F}$ a field of characteristic zero (in our case it will be identified with the real numbers $\mathbb{R}$, but it could be, for example, the complex numbers).
The linear operators of \( L \) called *shift operator*, \( T \), and *coordinate operator*, \( X \), act on the elements of \( F \) or \( P \) as follows
\[
T_\sigma \cdot p(x) = p(x + \sigma), \quad X \cdot p(x) = x \cdot p(x). \tag{1}
\]
All the results of this work can be extended to separable equations of any number of variables. For non separable equations the method is the same but the results may be quite different.

An operator \( O \in L \) is said *shift invariant* if and only if commutes with the shift operator, i.e.,
\[
[O, T_\sigma] = OT_\sigma - T_\sigma O = 0, \quad \forall \sigma \in F.
\]

The so-called *delta operators*, \( \Delta \), are those operators of \( L \) such as
\[
\Delta \cdot x = c \neq 0, \quad c \in F, \quad [\Delta, T_\sigma] = \Delta T_\sigma - T_\sigma \Delta = 0, \quad \forall \sigma \in F, \tag{2}
\]
where \( c \in F \) is any fixed constant. It is easy to prove that
\[
\Delta \cdot a = 0, \quad \forall \ a \in F.
\]

For every delta operator \( \Delta \) there is a *series of basic polynomials* \( \{p_0(x), p_1(x), p_2(x), \ldots, p_n(x)\} \) of \( P \) verifying
\[
p_0(x) = 1,
\]
\[
p_n(0) = 0, \quad \forall n > 0, \tag{3}
\]
\[
\Delta \cdot p_n(x) = n \cdot p_{n-1}(x).
\]

We see that \( \Delta \) acts as a lowering (index) operator on its associated polynomial. A very important fact of the theory is that each pair \( \{\Delta, p_n(x)\} \) defines a unique realization or representation of the umbral algebra. There is a bijective correspondence \( J \), between basic series of polynomials and their \( \Delta \) operators. Hence, \( J \) may be defined with only one element of the pair.

The commutator of an operator \( O \) with the coordinate operator \( X \)
\[
O' = [O, X] = OX - XO \tag{4}
\]
is called the *Pincherle derivative* of \( O \).

Given a delta operator \( \Delta \) we can find an associated operator \( \xi \) such that
\[
[\Delta, \xi] = 1. \tag{5}
\]
This operator \( \xi \) is not shift invariant and together with \( \Delta \) and \( 1 \) close the Heisenberg-Weyl algebra or, in other words, expression (5) is a Heisenberg-like relation between \( \Delta \) and its conjugate \( \xi \). It is worthy to note that \( \xi \) is associated with the corresponding basic series of the operator \( \Delta \) by
\[
\xi^n \cdot 1 = p_n(x).
\]
Although only in a determined correspondence $\xi^n \cdot 1$ coincides with the Pockhammer symbol $x^{(n)}$, from now on we will use the following notation

$$\xi^n \cdot 1 = p_n(x) \equiv x^{(n)},$$

which is easy to prove taking into account that

$$[\Delta, \xi^n] = n \xi^{n-1}.$$  

Obviously, there is only one way to define $\xi$ if its associated polynomial series obeys all the relations (3). Given an operator $\Delta$ its associated operator $\xi$ must be

$$\xi = X \beta,$$

where $\beta^{-1}$ is the first Pincherle derivative of $\Delta$. It is easy to demonstrate that $\beta^{-1}$ is invertible and $\beta$ is shift invariant.

Let $\Delta_1$ and $\Delta_2$ be two delta operators with associated $\xi$-operators $\xi_1$ and $\xi_2$, respectively. A map $R : \mathcal{L} \to \mathcal{L}$ is called an umbral correspondence if

$$R : \xi_1^n \to \xi_2^n, \quad \forall n \in \mathbb{N}.$$  

The umbral correspondence also induces a correspondence $R$ between two delta operators. Summarising, the following diagram is commutative

$$\begin{array}{ccc}
\xi_1^n & \xrightarrow{R} & \xi_2^n \\
\downarrow \mathcal{J} & & \downarrow \mathcal{J} \\
\Delta_1 & \xrightarrow{R} & \Delta_2 \\
\downarrow \mathcal{J} & & \downarrow \mathcal{J} \\
\xi_1^n \cdot 1 = x_1^{(n)} & \xrightarrow{R} & \xi_2^n \cdot 1 = x_2^{(n)}
\end{array}$$

From the above diagram one easily sees that there is a triplet $\{\Delta, \xi, p_n(x)\}$ that defines a unique representation of the umbral algebra. Moreover through $\mathcal{J}$ we can go in a bijective way from one element to another of the triplet in such a way that only one of these elements is necessary and sufficient to define the umbral representation. The bijective application $R$ bring us from a umbral representation to another one.

### 3 Umbral correspondence and discretized quantum mechanics

As we mentioned before, the main goal of this work is the application of the umbral correspondence to discretize Quantum Mechanics. In fact, the 1-dimensional Quantum Mechanics is an umbral realization via the identification

$$\Delta = \partial_x, \quad \xi = X, \quad p_n(x) = x^n.$$  

Since we are interested in the discretization of Quantum Mechanics we will use the umbral correspondence to relate the triplet $(\partial_x, \ X, \ x^n)$ with another one defined on the lattice field $\mathbb{F}_\sigma = \{x \in \mathbb{R} \mid x = m\sigma, \ m \in \mathbb{Z}\}$ with lattice parameter $\sigma \in \mathbb{R}$. 
Let us start defining a general difference operator, $\Delta$, as a delta operator such that in the limit when $\sigma$ goes to zero becomes the differential operator $\partial_x$. Supposing that $\Delta$ is a linear difference operator then it will have a polynomial dependence on the shift operator $T$, i.e.,

$$\Delta = \frac{1}{N\sigma} \sum_{n=-j}^{k} a_n T^n,$$

(7)

where $N \in \mathbb{N}$, $a_n \in \mathbb{R}$ and $\sigma \in \mathbb{R}$ is the lattice parameter. Imposing condition (2a), i.e. $\Delta \cdot x = 1$, since condition (2b) is trivially verified we get

$$\sum_{n=-j}^{k} a_n = 0,$$

$$\sum_{n=-j}^{k} na_n = N.$$

(8)

These conditions (8) guarantee that in the limit when $\sigma$ goes to zero $\Delta$ goes to $\partial_x$ as it is easy to prove.

Recalling that the pair of Quantum Mechanics operators $(\partial_x, X)$ verifies the Heisenberg relation

$$[\partial_x, X] = 1,$$

we call discrete position operator to a non-shift invariant operator $\xi$ such that with the difference operator $\Delta$ verifies a similar Heisenberg relation, i.e.,

$$[\Delta, \xi] = 1.$$

The umbral correspondence allows us to relate continuous linear equations $h$ and their solutions $f$ if they can be developed in power series, with umbral discrete versions $\hat{h}$ and $\hat{f}$, respectively, as follows

$$h(\partial_x^n f(x), x^s) = 0 \iff \hat{h}(\Delta^n \hat{f}(\xi), \xi^s) \cdot 1 = 0, \quad n, s \in \mathbb{N};$$

$$f(x) = \sum_{n=0}^{\infty} f_n x^n \iff \hat{f}(\xi) \cdot 1 = \sum_{n=0}^{\infty} f_n x^{(n)}.$$

(9)

This is the main result of Umbral Calculus that we will exploit here for ours purposes. Umbral Calculus allows us not only to discretize continuous differential equations obtaining discrete equations but also to get solutions of these equations if their continuous counterparts are polynomial solutions or may be developed in power series which converge after the correspondence. Note, however, that with the umbral correspondence we obtain an operator which must be applied to 1 to get a difference equation or its solution.

For the particular case of a symmetric difference operator, i.e., a difference operator $\Delta_{\sigma}$ such that

$$\Delta_{\sigma} \cdot f(x) = -\Delta_{-\sigma} \cdot f(x),$$

we have that the general expression (7) reduces to

$$\Delta_{\sigma} = \frac{1}{N\sigma} \sum_{n=1}^{j} a_n (T^n - T^{-n}).$$

(10)
4 Differential operators for discretized quantum mechanics

In the following we will use some particular expressions (or representations) for the differential operator $\Delta$, all of them of low (first and second) order on the shift operator $T$. Let us consider the two possible representations for $\Delta$ of first order, the right discrete derivative $\Delta_+$ and the left discrete derivative $\Delta_-$, and the (only) symmetric discrete derivative of second order $\Delta_s$.

The right-correspondence is determined by the couple of operators $(\Delta_+, \xi_+)$ given by

$$\Delta_+ := \frac{1}{\sigma} (T - 1), \quad \beta_+ = T^{-1},$$

and the left-correspondence $(\Delta_-, \xi_-)$ by

$$\Delta_- := \frac{1}{\sigma} (1 - T^{-1}), \quad \beta_- = T.$$

Note that both are connected by the change $\sigma \leftrightarrow -\sigma$.

The basic polynomial series of the right-correspondence is related with the Pochhammer symbols. Its explicit expression is

$$(X\beta_+)^n \cdot 1 = x_+^{(n)} = x(x - \sigma)(x - 2\sigma)\ldots(x - (n - 1)\sigma)$$

$$= \prod_{i=0}^{n-1} (x - i\sigma) = \sigma^n \prod_{i=0}^{n-1} (m - i)$$

$$= \begin{cases} 
(-\sigma)^n \frac{(-m + n - 1)!}{(-m - 1)!} & \text{if } m < 0 \\
0 & \text{if } \begin{cases} m \geq 0 \\
m < n \\
m \geq n
\end{cases} \\
\sigma^n \frac{m!}{(m - n)!} & \text{if } \begin{cases} m \geq 0 \\
m < n \\
m \geq n
\end{cases}
\end{cases} \quad \text{(11)}$$

where $x = m\sigma$ with $m \in \mathbb{Z}$. This series of polynomials has some interesting properties. First of all we can see that the $n$-th order zero of $x^n$ splits into $n$ first order zeros of $x_+^{(n)}$ at the right of the origin. If the right-correspondence is applied to a Taylor power series then, for the positive points of the domain, it will be truncated and therefore will converge, but not for the negative ones, and therefore could diverge.

The left-correspondence $\{\Delta_-, \xi_-\}$ is nearly similar to the right one. The basic sequence is related with the rising factorial (instead of the falling factorial of the previous case), and it is mirror symmetric respect to the $y$-axis to the right-correspondence: in fact, the negative points of a Taylor series discretized in this way, always converge.

According to the formula (10) there is only one symmetric representation of second order on $T$ ($S$-representation) determined by the pair $\{\Delta_s, \xi_s\}$, where

$$\Delta_s = \frac{1}{2\sigma} (T - T^{-1}), \quad \beta_s = 2(T + T^{-1})^{-1},$$
and its basic sequence is

\[(X\beta)^n \cdot 1 = x_s^{(n)} = x[x - (n - 2)\sigma][x - (n - 4)\sigma] \ldots [x + (n - 4)\sigma][x + (n - 2)\sigma] = x \prod_{i=0}^{n-2} [x + (2i - (n - 2))\sigma] = \sigma^n m \prod_{i=0}^{n-2} [m + 2i - (n - 2)]\]

\[= \begin{cases} 
\frac{(\text{sign}(m)\sigma)^m |m + n - 2|!!}{(|m| - n)!!} & \text{if } n \leq |m| \\
0 & \text{if } \begin{cases} n > |m| \\ p(n - m) = +1 \end{cases} \\
(-1)^{\frac{1}{2}(n - |m| - 1)}(\text{sign}(m)\sigma)^m m \times (|m| + n - 2)!!(n - |m| - 2)!! & \text{if } \begin{cases} n > |m| \\ p(n - m) = -1 \end{cases}
\end{cases}\]

where \(p(n) = (-1)^n\) is the parity function and the double factorial is defined as \(n!! = n(n-2)!!\) with \(n!! = 1\) when \(n\) is 0 or 1.

The behaviour of this basic sequence is much more complicated than those of the right and left-correspondences. The zero at the origin of order \(n\) of the continuous power function of degree \(n\) splits into \(n\) simple zeros after discretization. These zeros appear at the points \(x = m\sigma\) with the conditions

\[p(n - m) = +1, \quad n > |m|.\]  \hspace{1cm} (13)

Thus, applying the \(S\)-correspondence to a Taylor series we find that at the points obeying the conditions (13) there is a cut-off in the series and, hence, the sums will always converge in case the function has a well defined parity.

In the following diagram we display the basis elements \((\xi^n, \Delta, x^{(n)})\) of the three usual representations:

\[
\begin{array}{ccc}
\text{Right representation} & \text{Left representation} & \text{Symmetric representation} \\
\xi^+_n = (XT^{-1})^n & \xi^+_n = (XT)^n & \xi^+_n = \left(2X (T + T^{-1})^{-1}\right)^n \\
\Delta^+_n = \frac{1}{\sigma} (T - 1) & \Delta^+_n = \frac{1}{\sigma} (1 - T^{-1}) & \Delta^+_n = \frac{1}{2\sigma} (T - T^{-1}) \\
x^+_n = \prod_{i=0}^{n-1} (x - i\sigma) & x^+_n = \prod_{i=0}^{n-1} (x + i\sigma) & x^+_n = x \prod_{i=0}^{n-2} (x + (2i - n + 2)\sigma).
\end{array}
\]
Figure 1: Represented in dashed line the continuous powers and in dots the powers for the discrete position with red circles for $x^2$ and blue squares for $x^3$. The number of zeros is equal to the power $n$ for the right and the left cases.

5 The discretized exponential function and the trigonometric functions

We start with the exponential function which in some sense, is the simplest case. The continuous exponential function, as it is well known, is defined through the following differential equation
\[
\frac{d}{dx} y_k = ky_k, \quad y_k(0) = 1, \quad k \in \mathbb{R},
\]
and its power expansion series around the origin is
\[
y_k(x) = e^{kx} = \sum_{n=0}^{\infty} \frac{(kx)^n}{n!}.
\]

As we mentioned before, the umbral correspondence gives rise to the same function either by solving the discrete difference equation, obtained by applying the umbral correspondence to the continuous differential equation, or by applying the umbral correspondence to its solutions as long as their power series converge. Hence, we have to calculate
\[
\exp_U(k, x) = \sum_{n=0}^{\infty} \frac{k^n}{n!} x^n \cdot 1. \tag{14}
\]
If we use the right-correspondence (11) the umbral-exponential (14) becomes
\[ \exp_+(k, \sigma m) = \begin{cases} \sum_{n=0}^{m} (k\sigma)^n \frac{m!}{n!(m-n)!} & \text{if } m > 0 \\ \sum_{n=0}^{\infty} (-k\sigma)^n \frac{(-m+n-1)!}{n!(-m-1)!} & \text{if } m < 0 \end{cases} = (1 + k\sigma)^m. \]

For the left-correspondence we get
\[ \exp_-(k, \sigma m) = \begin{cases} \sum_{n=0}^{\infty} (k\sigma)^n \frac{(m+n-1)!}{n!(m-1)!} & \text{if } m > 0 \\ \sum_{n=0}^{-m} (-k\sigma)^n \frac{(-m)!}{n!(-m-n)!} & \text{if } m < 0 \end{cases} = (1 - k\sigma)^{-m}. \]

In Fig. 2(a) it is displayed the continuous exponential function together with its discrete version by the right-correspondence. It is worthy to note that if in the continuous case we found that \( \exp(k x) = \exp((-k)(-x)) \), now in the discrete case we have that \( \exp_+(k, x) = \exp_-(k, -x) \).

Another possibility is to apply the \( S \)-correspondence (12). So, we obtain
\[ \exp_s(k, \sigma m) = \sum_{n=0}^{\infty} (k\sigma)^n \frac{m!}{n!(m-n)!} \prod_{i=0}^{n-2} (m+2i-(n-2)) = \left( k\sigma + \sqrt{(k\sigma)^2 + 1} \right)^m. \]

These discrete exponentials only converge when the continuous variable \( k \) obeys, \( (k\sigma)^2 < 1 \), for all the three correspondences studied in the previous sections.

Also, we can easily study the trigonometric functions (as well as the hyperbolic functions) taking into account their expressions in terms of the exponential functions. In this way, we can obtain the discrete trigonometric functions from the discrete exponential function. We display in Fig. 2(b) the sine function.

We can see that the symmetric discrete trigonometric functions maintain the periodic behaviour of the continuous ones. However the period \( \lambda_\sigma \) is different to the continuous function \( \lambda = 2\pi/k \). We find it easier in the case of the sine function through \( \sin_s(k, l\sigma) = \sin_s(k, 0\sigma) \). We have fixed \( \lambda = l\sigma \) with \( l \in \mathbb{Z} \), but it can be generalized without problems to \( l \in \mathbb{R} \).

\[ \sin_s(k, l\sigma) = \frac{1}{2i} \left( \left( \sqrt{1-(k\sigma)^2+i\sigma} \right)^l - \left( \sqrt{1-(k\sigma)^2-i\sigma} \right)^l \right) = 0 = \sin_s(k, 0\sigma) \]
\[ \Rightarrow \left( \sqrt{1-(k\sigma)^2+i\sigma} \right)^l = \left( \sqrt{1-(k\sigma)^2-i\sigma} \right)^l \]

to solve this identity we define
\[ \sqrt{1-(k\sigma)^2+i\sigma} = re^{i\theta} = \begin{cases} \theta = \arctan \left( \frac{k\sigma}{\sqrt{1-(k\sigma)^2}} \right) \\ r = 1 \end{cases} \]
and this guide us to the solution
\[ \sin(\theta l) = 0 \Rightarrow \theta_n = \frac{n\pi}{l} \Rightarrow k_n = \frac{1}{\sigma} \sin \frac{n\pi}{l}. \]
As there are two zeros in each period of the function, we can find the relation between the number of waves and the wavelength. We have added a superscript to remark that these relations are different for each representation, then

\[ k^s = \frac{1}{\sigma} \sin \left( \frac{2\pi}{l} \right), \quad \lambda^s = \frac{2\pi \sigma}{\arcsin(k^s \sigma)}. \] (15)

It is easy to demonstrate the periodic behaviour of the symmetric trigonometric functions, in fact introducing (15) into the symmetric sinus

\[ \sin_s(k^s, m\sigma) = \sin \left( m \frac{2\pi}{l} \right). \]

For the right and left correspondences the trigonometric functions are not periodic. However the extremums of the functions and the intersection points with the abscissa axis appear periodically and then we can define a wave function through this property. With a similar computation than in the symmetric case, we find

\[ k^+ = \frac{1}{\sigma} \tan \left( \frac{2\pi}{l} \right), \quad \lambda^+ = \frac{2\pi \sigma}{\arctan(k^+ \sigma)}. \] (16)

The wave length is bigger in the right and left discretizations and smaller in the symmetric discretization than in the continuous trigonometric functions. Also in these three correspondences the trigonometric functions have a minimum period, it appears in the convergence limit, when \( k\sigma = 1 \). For the right and the left discretizations we have \( \lambda^+_{\min} = 8\sigma \), in fact it is a 8 point wave, and for the symmetric one \( \lambda^s_{\min} = 4\sigma \), in fact it is a 4 point wave.

We set \( \lambda = l\sigma \) and without loss of generality we fix \( l \) integer. Then it is easy to calculate the change in the amplitude in the right and left correspondences through (16)

\[ \sin_+(k^+, m\sigma) = \frac{1}{2i} \left( (1 + ik^+ \sigma)^m - (1 - ik^+ \sigma)^m \right) = \cos^{-m} \left( \frac{2\pi}{l} \right) \sin \left( m \frac{2\pi}{l} \right) \]

and

\[ \sin_+(k, m\sigma)A_n(l) = \sin_+(k, (m + nl)\sigma) \]

Hence, the non periodic part is then the multiplicative factor

\[ A_n(l) = \left( \sec^l \left( \frac{2\pi}{l} \right) \right)^n. \] (17)

This is also true for the cosine function and for any \( l \in \mathbb{R} \). Although we have a wave length \( \lambda = l\sigma \) for the trigonometric functions in the right and left representations, we can see that they are not periodic.

It is important to note that all the properties that obey the exponential and the trigonometric functions are maintained after the discretization with an exception: any property that includes two or more different constants \( k \), because they give similar effects than a different lattice spacing \( \sigma \), nor a different \( x \) like in the continuous case. Thus, for example

\[ \exp_U(k, m\sigma) \exp_U(k, n\sigma) = \exp_U(k, (m + n)\sigma), \]

\[ \exp_U(k, m\sigma) \exp_U(k', m\sigma) \neq \exp_U(k + k', m\sigma). \]
Let us go to discretize the Schrödinger equation with a potential $V(x)$. We will profit the well known fact that if the potential is independent of the time then the continuous Schrödinger equation is separable. Thus, from the Schrödinger equation
\[ i\hbar \partial_t \phi(x,t) = -\frac{\hbar^2}{2m} \partial_x^2 \phi(x,t) + V(x)\phi(x,t), \]
and considering $\phi(x,t) = \psi(x)\varphi(t)$ we obtain two uncoupled ordinary differential equations
\[-\frac{\hbar^2}{2m} \partial_x^2 \psi(x) + V(x)\psi(x) = E\psi(x),\]
\[ i\hbar \partial_t \varphi(t) = E\varphi(t), \]
that we can rewrite with natural units as
\[ \partial_x^2 \psi(x) + V(x)\psi(x) = E\psi(x), \]
\[-i\partial_t \varphi(t) = E\varphi(t). \]
The solution of the equation (18b) is
\[ \varphi(t) = Ce^{iEt}. \] (19)

6.1 Constant potential

In relation with the first equation of (18), the simplest case appears when the potential is constant \( V(x) = V_0 \). The solution is

\[ \psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{if } E > V_0, \]
\[ \psi(x) = Ae^{ikx} + Be^{-kx} \quad \text{if } E < V_0, \] (20)

with \( k = \sqrt{|E - V_0|} \). Therefore, the solution \( \phi(x,t) \) is a linear combination of trigonometric or exponential functions and, hence, their discretizations have been studied in section 5.

The energy, for a fixed momentum \( k \), is the same than in the continuous case for any discretization as we can see:

\[
H\psi = (-\Delta^2 + V_0) \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} (A + (-1)^n B) \xi^n = \]
\[
= (k^2 + V_0) \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} (A + (-1)^n B) \xi^n = (k^2 + V_0) \psi.
\]

In spite of this result, the relation between the momentum and the wave length \( \lambda = l\sigma \) is different in the discrete case:

\[ k = \frac{2\pi}{\lambda}, \quad k_\pm = \frac{1}{\sigma} \tan \left( \frac{2\pi}{l} \right), \quad k_s = \frac{1}{\sigma} \sin \left( \frac{2\pi}{l} \right). \]

Then the phase velocity changes, although the group velocity is the same as in the continuous case and, for this reason, the relation between the energy and the velocity.

Let be \( t = \tilde{\tau} \) where \( \tilde{\tau} \in \mathbb{Z} \) the discrete time, and \( \tau \) the fundamental time length. Following the limits of convergence of the discrete exponentials we find two upper limits for the energy, one in relation with the temporal part of the wave function (19) and the other one in relation with the spatial part of the wave function (20).

\[ E_{\text{max}_t} = \frac{\hbar}{\tau}, \quad E_{\text{max}_l} = \frac{\hbar^2}{2m\sigma^2}. \] (21)

In fact, we have to take the minor of them in each situation. Taking \( \sigma \approx l_{\text{Planck}} = 1.62 \times 10^{-35} m \) and \( \tau \approx l_{\text{Planck}} = 5.39 \times 10^{-44} s \) we find values of the maximum energy for the time wave \( E_{\text{max}_t} \) and for the spatial wave for a proton \( E_{p^+ , \text{max}_l} \) and an electron \( E_{e^- , \text{max}_l} \)

\[
E_{\text{max}_t} \approx E_{\text{Planck}} = 1.22 \times 10^{38} eV, \quad E_{\text{max}_l} = 1.38 \times 10^{20} \frac{1}{m} eV
\]
\[
E_{p^+ , \text{max}_l} = 7.94 \times 10^{46} eV, \quad E_{e^- , \text{max}_l} = 1.46 \times 10^{50} eV.
\]
Remark that these are non-relativistic effects. We can study also the change in the amplitude for the right and left correspondences. The factor of expansion or contraction is

\[ A_n(l) = \left( \sec \left( \frac{2\pi}{l} \right) \right)^n \approx \left( 1 + \frac{2\pi^2}{l} \right)^n \]

where \( l \) is the number of points into the wave length and \( n \) is the number of wave lengths along the wave. For the temporal part of the wave function of a particle which travel into the LEP, that is during 9 \( 10^{-5} \) s with an energy of 1.99 \( 10^{14} \) eV, we find that the factor is \( A_n(l) \sim 10^{10^5} \). For the spatial part of the same particle, an electron, the factor is of order \( A_n(l) \sim 3 \). These factors grow a lot with the energy or the mass of the particle. As at this energy the relativistic effects are important and we are using now non relativistic quantum mechanics, it is comprehensible to find these too big numbers.

### 6.2 Infinite potential well

A little more complicated is the infinite potential well, although it is very similar to a constant potential, it reduces the space to a finite region and due to this fact new differences will appear between the continuous and the discrete case. The potential is

\[ V(x) = \begin{cases} 
0 & \text{if } x \in [0, L] \\
\infty & \text{if } x \notin [0, L]
\end{cases} \]

The wave functions must obey the boundary conditions \( \psi(0) = \psi(L) = 0 \) which lead to a countable number of solutions:

\[ \psi_n(x) = \sin \left( \frac{n\pi x}{L} \right), \quad k = \frac{n\pi}{L}, \quad n \in \mathbb{Z}, \]

in the same way we apply the boundary conditions to all our discretizations. We can find the quantum rule for both the right and left correspondences following the computation of (15). So

\[ k^+_n = \frac{1}{\sigma} \tan \pi \frac{n}{M} \]

where \( L = M\sigma \). Therefore there are only \( M/2 \) possible states instead of the infinite states of the continuous case, with a degeneration relative to the parity. The energy is \( E_n = k^2_n \) and it is bounded at \( n = (M - 1)/2 \). So the maximum energy is

\[ E_{\text{max}}^+ = \frac{\hbar^2}{2m^2\sigma^2} \tan^2 \left( \pi \frac{M - 1}{2M} \right) \]

At \( n = M/2 \) we find a non physical state of infinite energy and infinite wave function amplitude. We can do a small computation finding that an electron in an infinite well of wide the Bohr radius \( M \sim 10^{27} \) will have a maximum state energy of \( E_{\text{max}}^+ \sim 10^{77} \) eV. The maximum energy grows when increasing the number of points \( M \) and also when decreasing the mass of the particle. But the wave function, as we saw previously, has a convergence range that limits the number of states to \( n \in (-M/4, M/4) \) because \( k < 1/\sigma \). Hence, the maximum energy is much more smaller.
We have that the quantum rule for the $S$-correspondence is

$$k^s_n = \frac{1}{\sigma} \sin \pi \frac{n}{M}. $$

Again we have a finite number of states, $M/2$, rounding down, with a degeneration relative to the parity also. The energy is always bounded by $\hbar/(2m\sigma^2)$, just as we found with the convergence condition

$$E^s_n = (k^s_n)^2 = \frac{1}{\sigma^2} \sin^2 \pi \frac{n}{M}. $$

In Figure 3 are drawn the energy levels and the wave functions of the ground state and the two first excited states for the continuous case and the three discretizations. We can see the great fit of the symmetric one for the first excited states, but remarking that as its number of states is finite, $M/2$, then upper these wave functions there are not more states. The right and the left ones have an asymmetry to the left and right directions of the space and then are much more different to the continuous wave functions.

![Energy levels and wave functions](image)

Figure 3: Energy levels and wave functions of the infinite well. The energy levels are in the left, ones in solid line for the continuous case and dashed for the discrete case, the shorter red lines are the right/left case energies and the longer blue lines are the symmetric case energies. Wave functions are in the right, in black solid line are for the continuous case, blue circled points are for the $S$-correspondence, red triangled ones for the right correspondence and green squared ones the left correspondence.
7 Conclusions

In this paper we have shown how to apply the techniques of the Umbral Calculus for the discretization of equations preserving the point symmetries. We can see the advantage of a tool that may be used not only on the equations, but also over their solutions. Due to this fact we have not to solve difference equations because we alternatively can sum series. Moreover, in the most difficult cases we can use numerical methods to get a solution.

In the umbral discretization we can choose between infinite umbral representations. However, still in the simplest cases they present very different behaviours. We can separate all of them in two classes, one preserving the parity of the equations and solutions (like the $S$-representation) and the other one that does not (like the right and left representations). From the point of view of the local symmetries in Ref (2–9, [26]) it was proved that independently of the correspondence we get the same discrete point symmetries.

The study of the discrete Schrödinger equation together with other potentials (Coulomb, harmonic oscillator, . . . ) are in progress [31–32] and the results will be published elsewhere.

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