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Exact Finite Differences for Quantum Mechanics

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Additional information is available at the end of the chapter

Abstract

We introduce a finite difference derivative, on a non-uniform partition, with the characteristic that the derivative of the exponential function is the exponential function itself, times a constant, which is similar to what happens in the continuous variable case. Aside from its application to perform numerical computations, this is particularly useful in defining a quantum mechanical discrete momentum operator.

Keywords: exact finite differences derivative, discrete quantum mechanical momentum operator, time operator

1. Introduction

Even though the calculus of finite differences is an interesting subject on its own [1–4] that scheme is mainly used to perform numerical computations with the help of a computer. Finite differences methods give approximate expressions for operators like the derivative or the integral of functions, and it is expected that we get a good approximation when the separation between the points of the partition is small; the smaller it becomes the better.

The momentum operator of Quantum Mechanics, when considering continuous variables, is related to the derivative of functions, but its form, when the variable takes discrete values, is not known yet (an approach is found in Ref. [5]); we need an exact expression for the momentum operator in discrete Quantum Mechanics. Thus, to have an expression for the quantum mechanical momentum operator on a mesh of points, we need an exact expression for the derivate on a mesh of points. In this chapter, we intend to modify the usual finite differences definition of the derivative on a partition to propose an operator that can be used as a momentum operator for discrete Quantum Mechanics.

2. Exact first-order finite differences derivatives of functions

In this section, we intend to introduce a finite differences derivative, which has the same eigenfunction as for the continuous variable case. We start with results valid for any function, but we will concentrate, later in the chapter, on the exponential function because that function is used to perform translations along several directions in the quantum realm. The resulting derivative operator will depend on the point at which it is evaluated as well as on the partition of the interval and on the function of interest. This is the trade-off for having exact finite differences derivatives.

2.1. Backward and forward finite differences derivatives

An exact, backward, finite differences derivative of an absolutely continuous function $g(x)$ (this class of functions is the domain of the momentum operator in Quantum Mechanics), on a partition $P = \{x_1, , x_2, \cdots, x_N\}$ of N non-uniformly spaced points $\{x_j\}_1^N$, is defined through the requirement that

$$(D_b g)(x_j) := \frac{g(x_j) - g(x_j - \Delta_{j-1})}{\chi_2(j-1)} = g'(x_j), \tag{1}$$

where $\Delta_j = x_{j+1} - x_j$ and the spacing function $\chi_2(j)$, which is a replacement for the usual spacing function Δ_j, is obtained by solving the above equality for $\chi_2(j)$,

$$\chi_2(j-1) := \frac{g(x_j) - g(x_j - \Delta_{j-1})}{g'(x_j)} = \frac{1}{g'(x_j)} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} g^{(k)}(x_j) \Delta_{j-1}^k. \tag{2}$$

This is an expression which is valid for points x_j different from the zeroes of $g'(x)$.

A definition for forward finite differences at x_j is

$$(D_f g)(x_j) := \frac{g(x_j + \Delta_j) - g(x_j)}{\chi_1(j)} = g'(x_j), \tag{3}$$

where

$$\chi_1(j) := \frac{g(x_j + \Delta_j) - g(x_j)}{g'(x_j)} = \frac{1}{g'(x_j)} \sum_{k=1}^{\infty} \frac{1}{k!} g^{(k)}(x_j) (\Delta_j)^k, \tag{4}$$

valid for points different from the zeroes of $g'(x)$.

These definitions coincide with the usual finite differences derivative when the function to which they act on is the linear function $g(x) = a_0 + a_1 x$, $a_0, a_1 \in \mathbb{C}$. An exact finite differences derivative of other functions need of more terms than the one found in the usual definition of a finite differences derivative, as can be seen in Eqs. (2) and (4).
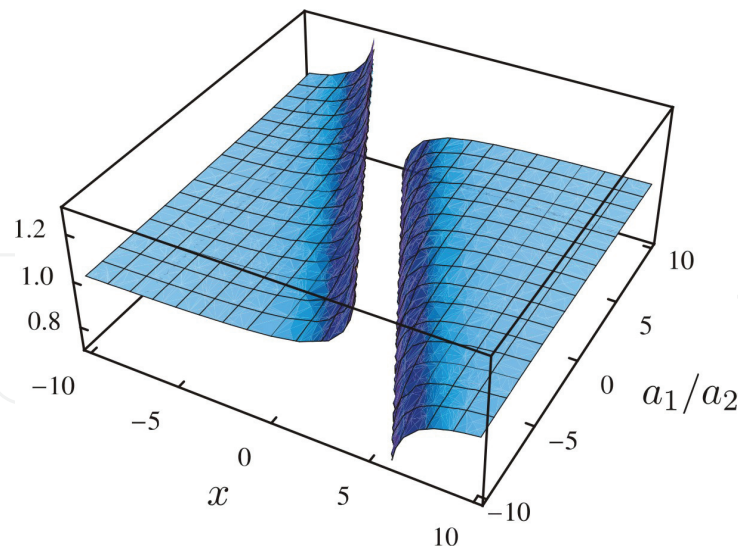
Figure 1. Three-dimensional plot of $\chi_2(x, j)$ for the quadratic function $g(x) = a_0 + a_1 x + a_2 x^2$ with $\Delta_j = 1$.

Example. For the quadratic function $g(x) = a_0 + a_1 x + a_2 x^2$, $a_0, a_1, a_2 \in \mathbb{C}$, the spacing function $\chi_2(x, j)$ becomes

$$\chi_2(x, j) = \Delta_j - \frac{\Delta_j^2}{\frac{a_1}{a_2} + 2x},\tag{5}$$

where $x \neq -a_1/2a_2$. A plot of this function is shown in **Figure 1** for $\Delta_j = 1$.

In the remaining part of this chapter, we only consider the derivative of the exponential function; this choice fixes the form of the spacing functions $\chi_1(j)$ and $\chi_2(j)$.

3. Exact first-order finite differences derivative for the exponential function

Let us consider the exact backward and forward finite differences derivatives of $e^{v\,x}$, at x_j, given by

$$\left(D_b e^{v\,x}\right)_j := \frac{e^{v\,x_j} - e^{v\,x_{j-1}}}{\chi_2(v, j-1)} = v\,e^{v\,x_j} \text{ and } \left(D_f e^{v\,x}\right)_j := \frac{e^{v\,x_{j+1}} - e^{v\,x_j}}{\chi_1(v, j)} = v\,e^{v\,x_j},\tag{6}$$

where $v \in \mathbb{C}$ can be a pure real or pure imaginary constant, and the spacing functions $\chi_1(v, j)$ and $\chi_2(v, j)$ are defined as

$$\chi_1(v, j) := \frac{e^{v\,\Delta_j} - 1}{v} \cong \Delta_j + \frac{v}{2}\Delta_j^2 + O\left(\Delta_j^3\right),\tag{7}$$

and

$$\chi_2(v,j) := \frac{1 - e^{-v\,\Delta_j}}{v} \cong \Delta_j - \frac{v}{2}\Delta_j^2 + O\left(\Delta_j^3\right). \tag{8}$$

Note that we recover the usual definitions of a finite differences derivative in the limit $\Delta_j \to 0$ ($N \to \infty$) in which case $\chi_1(v,j) = \chi_2(v,j) \to \Delta_j$. Hereafter, the exact finite differences derivatives that we will consider are

$$(D_b g)_j := \frac{g_j - g_{j-1}}{\chi_2(v,j-1)} \quad \text{and} \quad (D_f g)_j := \frac{g_{j+1} - g_j}{\chi_1(v,j)}, \tag{9}$$

with $\chi_1(v,j)$ and $\chi_2(v,j)$ given in Eqs. (7) and (8), and some properties of these definitions follow. There is a plot of $\chi_1(v,j)$ in **Figure 2**. The spacing function $\chi_1(v,j)$ is defined for finite values of v and Δ_j.

The summation of a derivative. As is the case for continuous systems, the summation is the inverse operation to the derivative,

$$\sum_{j=n}^{m} \chi_1(v,j)(D_f g)_j = \sum_{j=n}^{m} \left(g_{j+1} - g_j\right) = g_{m+1} - g_n, \tag{10}$$

where $1 \le n < m < N$, and

$$\sum_{j=n}^{m} \chi_2(v,j-1)(D_b g)_j = g_m - g_{n-1}, \tag{11}$$

where $1 < n < m \le N$.

The exponential function is also an eigenfunction of the summation operation. The usual integral of the exponential function also has its equivalent expression in exact finite differences terms
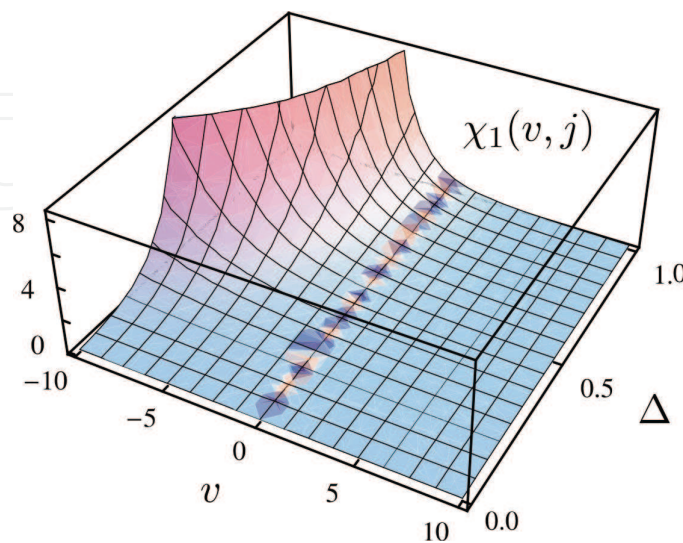

Figure 2. Three-dimensional plot of $\chi_1(v,j)$ for the exponential function $e^{v\,x}$.

$$\sum_{j=n}^{m} \chi_1(v,j) v\, e^{v\, x_j} = \sum_{j=n}^{m} \chi_1(v,j)\left(D_f e^{v\, x}\right)_j = e^{v\, x_{m+1}} - e^{v\, x_n}, \tag{12}$$

where $1 \le n < m < N$, and

$$\sum_{j=n}^{m} \chi_2(v,j-1) v\, e^{v\, x_j} = e^{v\, x_m} - e^{v\, x_{n-1}}, \tag{13}$$

where $1 < n < m \le N$.

Chain rule. The finite differences versions of the chain rule are

$$\begin{aligned}
\left(D_f g(h(x))\right)_j &= \frac{g\left(h(x_{j+1})\right) - g\left(h(x_j)\right)}{\chi_1(v,j)} = v\frac{g\left(h(x_{j+1})\right) - g\left(h(x_j)\right)}{e^{v\,\left(h(x_{j+1})-h(x_j)\right)} - 1}\frac{e^{v\,\left(h(x_{j+1})-h(x_j)\right)} - 1}{v\,\chi_1(v,j)} \\
&= \left(D_f g\right)_j \frac{\chi_1(v,\Delta_{h,j})}{\chi_1(v,j)},
\end{aligned} \tag{14}$$

where

$$\left(D_f g\right)_j := v\frac{g\left(h(x_{j+1})\right) - g\left(h(x_j)\right)}{e^{v\,\left(h(x_{j+1})-h(x_j)\right)} - 1}, \tag{15}$$

$\chi_1\left(v,\Delta_{h,j}\right) = \dfrac{e^{v\,\left(h(x_{j+1})-h(x_j)\right)} - 1}{v}$ and $\Delta_{h,j} = h(x_{j+1}) - h(x_j)$, and

$$\left(D_b g(h(x))\right)_j = \left(D_b g\right)_j \frac{\chi_2\left(v,\Delta_{h,j-1}\right)}{\chi_2(v,j-1)}, \tag{16}$$

where $\chi_2\left(v,\Delta_{h,j-1}\right) = \left(1 - e^{-v\,\left(h(x_j)-h(x_{j-1})\right)}\right)/v$,

$$\left(D_b g\right)_j := v\frac{g\left(h(x_j)\right) - g\left(h(x_{j-1})\right)}{1 - e^{-v\,\left(h(x_j)-h(x_{j-1})\right)}}. \tag{17}$$

and $h(x)$ is any absolutely continuous complex function on $[a,b]$.

The derivative of a product of functions. The exact finite differences derivative of a product of functions is

$$\begin{aligned}
\left(D_f gh\right)_j &= \frac{g_{j+1}h_{j+1} - g_j h_j}{\chi_1(v,j)} = g_{j+1}\frac{h_{j+1} - h_j}{\chi_1(v,j)} + \frac{g_{j+1} - g_j}{\chi_1(v,j)}h_j \\
&= g_{j+1}\left(D_f h\right)_j + h_j\left(D_f g\right)_j = e^{-v\,\Delta_j} g_{j+1}\left(D_b h\right)_{j+1} + h_j\left(D_f g\right)_j,
\end{aligned} \tag{18}$$

where $1 \le j < N$. Also, for the backwards derivative, we have

$$(D_b gh)_j = g_j(D_b h)_j + h_{j-1}(D_b g)_j = g_j(D_b h)_j + e^{v\,\Delta_{j-1}} h_{j-1}(D_f g)_{j-1}, \tag{19}$$

where $1 < j \le N$.

The derivative of the ratio of two functions. For the finite differences, backward derivative of the ratio of two functions we have

$$
\begin{aligned}
\left(D_b \tfrac{g}{h}\right)_j &= \frac{1}{\chi_2(v,j-1)}\left(\frac{g_j}{h_j} - \frac{g_{j-1}}{h_{j-1}}\right) = \frac{1}{\chi_2(v,j-1)}\left(-\frac{g_j(h_j - h_{j-1})}{h_j h_{j-1}} + \frac{(g_j - g_{j-1})h_j}{h_j h_{j-1}}\right) \\
&= \frac{(D_b g)_j}{h_{j-1}} - g_j\frac{(D_b h)_j}{h_j h_{j-1}},
\end{aligned} \tag{20}
$$

$$\left(D_b \frac{g}{h}\right)_j = \frac{(D_b g)_j}{h_j} - g_{j-1}\frac{(D_b h)_j}{h_j h_{j-1}}, \tag{21}$$

$$\left(D_f \frac{g}{h}\right)_j = \frac{(D_f g)_j}{h_{j+1}} - g_j\frac{(D_f h)_j}{h_j h_{j+1}}, \tag{22}$$

$$\left(D_f \frac{g}{h}\right)_j = \frac{(D_f g)_j}{h_j} - g_{j+1}\frac{(D_f h)_j}{h_j h_{j+1}}. \tag{23}$$

Additional properties. A couple of equalities that will be needed below are

$$\frac{1}{\chi_2(v,j)} - \frac{1}{\chi_1(v,j)} = v, \text{ and } \frac{\chi_1(v,j)}{\chi_2(v,j)} = e^{v\,\Delta_j}. \tag{24}$$

For instance, these equalities imply that

$$(D_f g)_j = e^{-v\,\Delta_j}(D_b g)_{j+1}. \tag{25}$$

Summation by parts. An important result is the summation by parts. The sum of equalities (18) and (19) combined with equalities (10) and (11) provide the exact finite differences summation by parts results,

$$\sum_{j=n}^{m} \chi_2(v,j) g_{j+1}(D_b h)_{j+1} + \sum_{j=n}^{m} \chi_1(v,j) h_j(D_f g)_j = g_{m+1}h_{m+1} - g_n h_n, \tag{26}$$

where $1 \le j < N$, and

$$\sum_{j=n}^{m} \chi_2(v,j-1) g_j(D_b h)_j + \sum_{j=n}^{m} \chi_1(v,j-1) h_{j-1}(D_f g)_{j-1} = g_m h_m - g_{n-1}h_{n-1}, \tag{27}$$

where $1 < j \le N$.

The integration by parts theorem of continuous functions is the basis that allows to define adjoint, symmetric and self-adjoint operations for continuous variables [8, 9]. Therefore, the

summation by parts results can be used in the finding of an appropriate momentum operator for discrete quantum systems. The summation by parts relates two operators between themselves and with boundary conditions on the functions.

4. The matrix associated to the exact finite differences derivative

It is advantageous to use a matrix to represent the finite differences derivative on the whole interval so that we can consider the whole set of derivatives on the partition at once. Let us consider the backward and forward exact finite differences derivative matrices $\mathbf{D}_{b,f}$ given by

$$
\mathbf{D}_b := \begin{pmatrix}
\frac{-1}{\chi_1(v,1)} & \frac{1}{\chi_1(v,1)} & 0 & 0 & \cdots & 0 & 0 & 0 \\
\frac{-1}{\chi_2(v,1)} & \frac{1}{\chi_2(v,1)} & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & \frac{-1}{\chi_2(v,2)} & \frac{1}{\chi_2(v,2)} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \frac{-1}{\chi_2(v,3)} & \frac{1}{\chi_2(v,3)} & \cdots & 0 & 0 & 0 \\
\vdots & & & & & & & \\
0 & 0 & 0 & 0 & \cdots & \frac{-1}{\chi_2(v,N-2)} & \frac{1}{\chi_2(v,N-2)} & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & \frac{-1}{\chi_2(v,N-1)} & \frac{1}{\chi_2(v,N-1)}
\end{pmatrix},
\tag{28}
$$

and

$$
\mathbf{D}_f := \begin{pmatrix}
\frac{-1}{\chi_1(v,1)} & \frac{1}{\chi_1(v,1)} & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & \frac{-1}{\chi_1(v,2)} & \frac{1}{\chi_1(v,2)} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \frac{-1}{\chi_1(v,3)} & \frac{1}{\chi_1(v,3)} & \cdots & 0 & 0 & 0 \\
\vdots & & & & & & & \\
0 & 0 & 0 & 0 & \cdots & \frac{-1}{\chi_1(v,N-2)} & \frac{1}{\chi_1(v,N-2)} & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & \frac{-1}{\chi_1(v,N-1)} & \frac{1}{\chi_1(v,N-1)} \\
0 & 0 & 0 & 0 & \cdots & 0 & \frac{-1}{\chi_2(v,N-1)} & \frac{1}{\chi_2(v,N-1)}
\end{pmatrix}.
\tag{29}
$$

We have used the definition for the backward derivative $(D_b g)_j$ for all the rows of the backward derivative matrix D_b but not for the first line in which we have instead used the forward derivative $(D_f g)_1$. A similar thing was done for the forward derivative matrix D_f. These matrices act on bounded vectors $\mathbf{g} = (g_1, g_2, \cdots, g_N)^T \in \mathbb{C}^N$.

The matrix formulation of the derivative operators allows the derivation of some useful results for the derivative itself.

4.1. Higher order derivatives

Many properties can be obtained with the help of the derivative matrices $\mathbf{D}_{b,f}$. Expressions for the exact second finite differences derivative associated to the exponential function are obtained through the square of the derivative matrices $\mathbf{D}_{b,f}$. These expressions are

$$\left(D_b^2 g\right)_1 = v\frac{g_2 - g_1}{\chi_1(v,1)} = v\left(D_f g\right)_1, \tag{30}$$

$$\left(D_b^2 g\right)_2 = v\frac{g_2 - g_1}{\chi_2(v,1)} = v\left(D_b g\right)_2, \tag{31}$$

$$\left(D_b^2 g\right)_j = \frac{1}{\chi_2(v,j-1)}\left(\frac{g_j - g_{j-1}}{\chi_2(v,j-1)} - \frac{g_{j-1} - g_{j-2}}{\chi_2(v,j-2)}\right) = \frac{\left(D_f g\right)_j - \left(D_f g\right)_{j-1}}{\chi_2(v,j-1)}, \quad j = 3, \cdots, N. \tag{32}$$

These expressions have the exponential function $e^{v\,x}$ as one of their eigenfunctions with eigenvalue v^2, as is also the case of the continuous variable derivative. Higher order derivatives can be obtained in an analogous way.

The derivative matrices are singular, which means that they do not have an inverse matrix, but, at a local level, the inverse operator to the derivative is the summation, as we have already shown in a previous section.

4.2. Eigenfunctions and eigenvectors of $D_{b,f}$

Now that we have the matrices $D_{b,f}$ representing the backward and forward derivatives, we are interested in finding their eigenvalues $\lambda \in \mathbb{C}$ and its corresponding eigenvectors e_λ. Therefore, we begin by finding the values of λ for which the matrices $D_{b,f} - \lambda\,I$ are not invertible, that is, when they are singular.

On one hand, for the backward finite difference matrix D_b, the characteristic polynomial is

$$|D_b - \lambda\,I| = \lambda\left(\lambda + \frac{1}{\chi_1(v,1)} - \frac{1}{\chi_2(v,1)}\right)\left(\frac{1}{\chi_2(v,2)} - \lambda\right)\left(\frac{1}{\chi_2(v,3)} - \lambda\right)\cdots\left(\frac{1}{\chi_2(v,N-1)} - \lambda\right) = 0, \tag{33}$$

whose roots are $\lambda_0 = 0$, $\lambda_v = -1/\chi_1(v,1) + 1/\chi_2(v,1) = v$ and $\lambda_j = 1/\chi_2(v,j)$, $2 \leq j \leq N-1$. Let us denote by $e_\lambda = (e_{\lambda,1}, e_{\lambda,2}, \cdots, e_{\lambda,N})^T$ to the eigenvector corresponding to the eigenvalue λ. The system of equations for the components of the eigenvectors is

$$-\frac{e_{\lambda,k}}{\chi_2(v,k)} + \left(\frac{1}{\chi_2(v,k)} - \lambda\right)e_{\lambda,k+1} = 0, \tag{34}$$

with $k = 1, \cdots, N-1$. Then, the eigenvectors are

$$e_0 = C\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad e_v = C\begin{pmatrix} e^{v\,x_1} \\ e^{v\,x_2} \\ \vdots \\ e^{v\,x_N} \end{pmatrix}, \quad e_j = C\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ y_{j+1} \\ \vdots \\ y_N \end{pmatrix}, \tag{35}$$

where C is the normalization constant, and

$$y_m = \prod_{k=m}^{N-1} \left(1 - \frac{\chi_2(v,k)}{\chi_2(v,j)} \right), \tag{36}$$

where $2 \leq j < m \leq N$. The quantities y_m usually are very small.

On the other hand, for the forward finite difference matrix, $\mathbf{D}_f$, the characteristic polynomial is

$$|\mathbf{D}_f - \lambda\,\mathbf{I}| = (-1)^{N-1} \lambda (v - \lambda) \left(\frac{1}{\chi_1(v,1)} + \lambda \right) \left(\frac{1}{\chi_1(v,2)} + \lambda \right) \cdots \left(\frac{1}{\chi_1(v,N-2)} + \lambda \right) = 0, \tag{37}$$

Thus, the eigenvalues for the forward derivative are $\lambda_0 = 0$, $\lambda_v = v$ and $\lambda_j = -1/\chi_1(v,j)$, $1 \leq j \leq N - 2$, and the corresponding eigenvectors are

$$e_0 = C \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad e_v = C \begin{pmatrix} e^{v\,x_1} \\ e^{v\,x_2} \\ \vdots \\ e^{v\,x_N} \end{pmatrix}, \quad e_j = C \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_j \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{38}$$

where

$$w_m = \prod_{k=1}^{m-1} \left(1 - \frac{\chi_1(v,k)}{\chi_1(v,j)} \right) \tag{39}$$

and $1 \leq m < j \leq N - 2$. The quantities w_m are also very small; in fact, they vanish for the equally spaced partition.

The matrices, $\mathbf{D}_{b,f}$, have the same eigenvalues λ_0 and λ_v, and eigenvectors which are the discretization of the function $g_v(x) = C\,e^{v\,x}$ on the partition $\{x_1, x_2, \cdots, x_N\}$ (the eigenvector $(1, 1, \cdots, 1)^T$ correspond to the eigenvalue $v=0$). This is the same eigenfunction that is found in the continuous variable case because the exponential function is indeed an eigenfunction of the continuous derivative. We note that the local derivatives $(D_{b,f}\,g)_j$ have the same eigenfunctions as the matrices $\mathbf{D}_{b,f}$ which are global objects. The other eigenvectors are fluctuations around the null vector, which is the trivial eigenvector of the derivative.

4.3. The commutator between coordinate and derivative

Since the following equality holds:

$$(D_b\,x)_j = \frac{x_j - x_{j-1}}{\chi_2(v,j-1)} = \frac{\Delta_{j-1}}{\chi_2(v,j-1)} = 1 + \frac{v}{2}\Delta_{j-1} + \mathcal{O}\left(\Delta_{j-1}^2\right), \tag{40}$$

from a local point of view, we have

$$(D_b \, xg)_j = x_j (D_b \, g)_j + g_{j-1} (D_b \, x)_j = x_j (D_b \, g)_j + g_{j-1} \frac{\Delta_{j-1}}{\chi_2(v, j-1)}, \tag{41}$$

and then, the commutator between x and D_b, acting on g, is given by

$$([D_b, x]g)_j = g_{j-1} \left(1 + \frac{v}{2} \Delta_{j-1} + \mathcal{O}\left(\Delta_{j-1}^2\right) \right).$$

Thus, the commutator between D_b and x becomes one in the limit of small Δ_j, or large N, because it also happens that $g_{j-1} \rightarrow g_j$.

We now consider the commutator between the coordinate matrix $\mathbf{Q} := \mathrm{diag}(x_1, x_2, \cdots, x_N)$, and the forward derivative matrix $\mathbf{D}_f$. That commutator is

$$[\mathbf{D}_f, \mathbf{Q}] = \begin{pmatrix} 0 & \frac{\Delta_1}{\chi_1(v,1)} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \frac{\Delta_2}{\chi_1(v,2)} & \cdots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \cdots & 0 & \frac{\Delta_{N-2}}{\chi_1(v,N-2)} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{\Delta_{N-1}}{\chi_1(v,N-1)} \\ 0 & 0 & 0 & \cdots & 0 & \frac{\Delta_{N-1}}{\chi_2(v,N-1)} & 0 \end{pmatrix}, \tag{42}$$

The small Δ_j ($N \rightarrow \infty$) approximation of this commutator is just

$$[\mathbf{D}_f, \mathbf{Q}] \underset{\Delta_j \rightarrow 0}{\longrightarrow} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}. \tag{43}$$

There is coincidence with the local calculation; as expected, this matrix approaches the identity matrix in the small Δ_j limit. Note that this matrix is composed of *backward translations* of the first $N-1$ points and a *forward translation* of the point $N-1$ without periodicity; the value of the first point is lost.

4.4. Translations

It is well known that the derivative is the generator of the translations of its domain [8]. Therefore, here we investigate briefly how translations are carried out by means of the derivative matrices $\mathbf{D}_{b,f}$ used as their generators. We will focus on the translation of the common eigenvector $\boldsymbol{e}_v = (e^{v \, x_1}, e^{v \, x_2}, \cdots, e^{v \, x_N})^T$ of both matrices.

Let the linear transformation represented by the matrix formed by means of the standard definition of a translation operator and of the exponential operator, given by

$$e^{s\,\mathbf{D}_{b,f}} = \sum_{k=0}^{\infty} \frac{\left(s\,\mathbf{D}_{b,f}\right)^k}{k!}, \tag{44}$$

where $s \in \mathbb{R}$. Since e_v is an eigenvector of $\mathbf{D}_{b,f}$ with eigenvalue v (see Eqs. (35) and (38)), it follows that $\mathbf{D}_{b,f}^k e_v = v^k\,e_v$, $k = 1, 2, \cdots$, and then,

$$e^{s\,\mathbf{D}_{b,f}} e_v = \sum_{k=0}^{\infty} \frac{\left(s\,v\right)^k}{k!}\,e_v = e^{s\,v} e_v = C \begin{pmatrix} e^{v\,(s+x_1)} \\ e^{v\,(s+x_2)} \\ \vdots \\ e^{v\,(s+x_N)} \end{pmatrix}, \tag{45}$$

that is, $e^{s\,v}$ is an eigenvalue of $e^{s\,\mathbf{D}_{b,f}}$ with corresponding eigenvector e_v, but the right-hand side of this equality is also a translation by the amount s of the domain of the derivative operators. We point out that s is arbitrary and then the vector $e'_v = e^{s\,\mathbf{D}_{b,f}} e_v$ is the function $e^{v\,x}$ evaluated at the points of the translated partition $P' = \{x_1 + s, x_2 + s, \cdots, x_N + s\}$. Thus, we can perform not only discrete translations but continuous translations as well.

The usual periodic, discrete translation found in the papers of other authors [6, 7] is obtained when the separation between the partition points is the same (denoted by Δ, a constant) and with periodic boundary conditions $e_{v,1} = e_{v,N}$.

4.5. Fourier transforms between coordinate and derivative representations

In this section, we define continuous and discrete Fourier transforms and establish some of their properties regarding the Fourier transform of continuous and discrete derivatives. The derivative eigenvalue $-ip$ should be understood, and we will omit it from the formulae below for the sake of simplicity of notation.

Given a function $g(p)$ in the L^1-space and a non-uniform partition $P = \{x_{-N}, x_{-N+1}, \cdots, x_N\}$, with $x_{-N} = -x_N$, the function.

$$(Fg)(x_j) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ix_j p} g(p)\,dp, \tag{46}$$

is the continuous Fourier transform of $g(p)$ at x_j. Having introduced the summation with weights $\chi_1(v, j)$ of Eq. (10), here we define two discrete Fourier transforms at p as

$$(\mathcal{F}_b g)(p) := \frac{p}{2\,\sin(px_N)} \sum_{j=-N}^{N} \chi_2(\Delta_j) e^{-ix_{j+1}p} g_{j+1}. \tag{47}$$

$$(\mathcal{F}_f g)(p) := \frac{p}{2\,\sin(px_N)} \sum_{j=-N}^{N} \chi_1(\Delta_j) e^{-ix_j p} g_j \tag{48}$$

Now, the discrete derivative of the product $e^{-ixp}g$ at x_j, with derivative eigenvalue $-ip$, is readily computed to give (see Eq. (18)).

$$\left(D_f e^{-ixp}g\right)_j = -ip\, g_{j+1}\left(e^{-ixp}\right)_j + e^{-ix_jp}\left(D_f g\right)_j. \tag{49}$$

The summation of this equality, with weights $\chi_1(-ip,j)$, results in

$$\sum_{j=-N}^{N-1} \chi_1(j)\left(D_f e^{-ixp}g\right)_j = -ip \sum_{j=-N}^{N-1} \chi_1(j)g_{j+1}e^{-ix_jp} + \sum_{j=-N}^{N-1} \chi_1(j)e^{-ix_jp}\left(D_f g\right)_{j'} \tag{50}$$

or

$$\sum_{j=-N}^{N-1} \chi_1(j)e^{-ix_jp}\left(-iD_f g\right)_j = p \sum_{j=-N}^{N-1} \chi_2(j)e^{-ix_{j+1}p}g_{j+1} + \sum_{j=-N}^{N-1} \chi_1(j)\left(-iD_f e^{-ixp}g\right)_j. \tag{51}$$

According to Eqs. (10), (24), (47) and (48), this equality can be rewritten in terms of discrete Fourier transforms.

$$\left(\mathcal{F}_f\left(-iD_f g\right)\right)(p) = p\,\left(\mathcal{F}_b g\right)(p) - i\,p\,\frac{e^{-ix_N p}g_N - e^{-ix_{-N}p}g_{-N}}{2\sin\left(px_N\right)}. \tag{52}$$

Another expression for the finite differences of the derivative of a function is obtained as follows. Considering the relationship (see Eq. (18), the second expression with $g = e^{-ixp}$)

$$\left(D_f e^{-ixp}g\right)_j = e^{i\Delta_j p}e^{-ix_{j+1}p}\left(D_b g\right)_{j+1} + g_j\left(D_f e^{-ixp}\right)_j. \tag{53}$$

The summation of this equality, with weights $\chi_1(j)$, results in

$$\sum_{j=-N}^{N-1} \chi_2(j)e^{-ix_{j+1}p}\left(-iD_b g\right)_{j+1} = p \sum_{j=-N}^{N-1} \chi_1(j)e^{-ix_jp}g_j + \sum_{j=-N}^{N-1} \chi_1(j)\left(-iD_f e^{-ixp}g\right)_{j'} \tag{54}$$

and, according to Eq. (10), this equality can be rewritten as the discrete Fourier transform

$$\left(\mathcal{F}_b\left(-iD_b g\right)\right)(p) = p\,\left(\mathcal{F}_f g\right)(p) - i\,p\,\frac{e^{-ix_N p}g_N - e^{-ix_{-N}p}g_{-N}}{2\sin\left(px_N\right)}. \tag{55}$$

These are the equivalent to the well-known identities found in continuous variables theory. Thus, the multiplication by p in forward p-space corresponds to the backward finite differences derivative in coordinate space. Additionally, the multiplication by p in backward p-space corresponds to the forward finite differences derivative in coordinate space, when choosing vanishing or periodic boundary conditions.

The integration by parts of the simple relationship

$$\frac{d\, e^{ix_j p}}{dp} = i\, x_j e^{ix_j p} \tag{56}$$

results in

$$i\, x_j \int_{-\infty}^{\infty} dp\, e^{ix_j p} h(p) = -\int_{-\infty}^{\infty} dp\, e^{ix_j p} \frac{d\, h(p)}{dp} + e^{ix_j p} h(p) \big]_{p=-\infty}^{\infty} \tag{57}$$

or in terms of continuous Fourier transforms,

$$x_j (Fh)_j = \left(F\, i\frac{d\, h}{dp} \right)_j - \frac{i\hbar}{\sqrt{2\pi}}\, e^{ix_j p} h(p) \bigg|_{p=-\infty}^{\infty}. \tag{58}$$

These equalities are like the usual properties between the spaces related by the Fourier transform.

5. Quantum mechanical momentum and time operators

We can apply the results of previous sections to discrete Quantum Mechanics theory. Let us rewrite Eq. (26) in terms of complex wave functions $\psi, \phi \in \ell^2(P, [a, b])$ defined on the partition $P = \{x_1, x_2, \cdots, x_N\}$ of $[a, b]$. We obtain

$$\sum_{j=1}^{N-1} \chi_2(v, j) \psi_{j+1}^* (-i\hbar D_b \phi)_{j+1} - \sum_{j=1}^{N-1} \chi_1^*(v, j) \phi_j (-i\hbar D_f \psi)_j^* = -i\hbar \big(\psi_N^* \phi_N - \psi_1^* \phi_1 \big). \tag{59}$$

This equality is rewritten as

$$\left(\psi | \widehat{P}_b \phi \right)_b - \left(\widehat{P}_f \psi | \phi \right)_f = -i\hbar \big(\psi_N^* \phi_N - \psi_1^* \phi_1 \big), \tag{60}$$

where the momentum-like operators $\widehat{P}_b$ and $\widehat{P}_f$ are defined as

$$\widehat{P}_b := -i\hbar D_b, \quad \widehat{P}_f := -i\hbar D_f, \tag{61}$$

and the bilinear forms $(\psi | \phi)_b$ and $(\psi | \phi)_f$ are defined as

$$(\psi | \phi)_b := \sum_{j=1}^{N-1} \chi_2(v, j) \psi_{j+1}^* \phi_{j+1}, \tag{62}$$

$$(\psi | \phi)_f := \sum_{j=1}^{N-1} \chi_1^*(v, j) \psi_j^* \phi_j. \tag{63}$$

We recognize Eqs. (60) and (61) as the finite differences versions of the equation that is used to define the adjoint operator and the symmetry of an operator in continuous Quantum

Mechanics. Thus, we propose that the momentum-like operators $\widehat{P}_b$ and $\widehat{P}_f$ are the "adjoint" of each other, on a finite interval $[a, b]$, when

$$\left(\psi|\widehat{P}_b\phi\right)_b = \left(\widehat{P}_f\psi|\phi\right)_{f'} \tag{64}$$

together with the boundary condition on the wave functions ψ and ϕ,

$$\psi_N = e^{i\theta}\psi_1, \quad \phi_N = e^{i\theta}\phi_1, \tag{65}$$

where $\theta \in [0, 2\pi)$ is an arbitrary phase. This gets rid of boundary terms.

With these definitions, we are closer to have a finite differences version of a self-adjoint momentum operator on an interval [12, 13] for use in discrete Quantum Mechanics. We believe that our results will lead to a sound definition of a discrete momentum operator and to the finding of a time operator in Quantum Mechanics [10–13].

6. The particle in a linear potential

As an application of the ideas presented in this chapter, we consider the particle under the influence of the linear potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ c\,x, & x > 0, \end{cases} \tag{66}$$

where $c > 0$. The eigenfunction corresponding to this potential is

$$\psi_E(x) = d\,\mathrm{Ai}\left[\sqrt[3]{\frac{2mc}{\hbar^2}}\left(x - \frac{E}{c}\right)\right], \tag{67}$$

where Ai denotes the Airy function and d is the normalization factor, m is the mass of the quantum particle and $\hbar$ is Planck's constant divided by 2π. The boundary condition $\psi_E(x = 0) = 0$ provides an expression for the energy eigenvalues E, which is

$$E_n = -\sqrt[3]{\frac{\hbar^2 c^2}{2m}}\,\alpha_{n+1}, \quad n = 0, 1, \cdots \tag{68}$$

where $\{\alpha_n\}$ are the roots of the Airy function, which are negative quantities.

In this case, the energy values are discrete and non-uniformly spaced, and the operator conjugate to the Hamiltonian would be a time-type operator with a discrete derivative $\widehat{T} = -i\hbar D_{b,f}$. The eigenfunctions of this time-type operator are calculated as in Eq. (38)

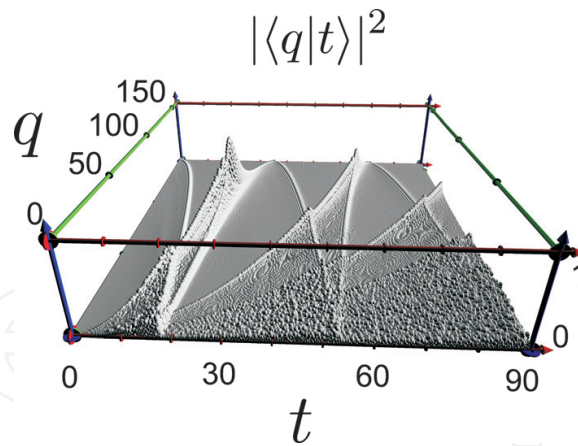$$\langle x|t\rangle = \sum_{n=0}^{M} e^{-i\,t\,E_n}\psi_n(x), \tag{69}$$

Figure 3. Three-dimensional plot of the squared modulus $|\langle q|t\rangle|^2$ of the time eigenstates for the wall-linear potential in coordinate representation, using 600 energy eigenfunctions. Dimensionless units.

where $\psi_n(x)$ is the eigenfunction of the Hamiltonian with energy E_n, Eq. (67). A plot of these time-type eigenstates, with $M = 600$, is found in **Figure 3**. We can identify the classical trajectories with initial conditions $(x_0, p_0) = \left(\frac{E_n}{c}, 0\right)$ in that figure; they are the regions in which the probability is higher. We can also identify the interference pattern between them.

In conclusion, we can have an exact derivative without the need of many terms, and this allows for the definition of adjoint operators related to the derivative on a mesh of points.

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