Annals of Physics 480 (2025) 170126

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Hidden $sl(2)$-symmetry of the generalized Landau–Zener vibronic model

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ARTICLE INFO

Keywords:
Vibronic model
Two-level system
Exceptional energy
Fourth-order differential equation
Hidden *sl*(2) symmetry

ABSTRACT

The one-dimensional harmonic vibronic model, which is a generalization of the so-called linear Landau–Zener model and appears in the form of coupled Schrödinger equations, is revisited. After decoupling the components, the resulting fourth-order equation is shown to have a hidden $sl(2)$ algebra. The so-called exceptional part of the spectrum is then expressed in a rather simple way. For completeness, the eigenfunctions are obtained via the Bethe ansatz approach directly in position space.

1. Introduction

The term *vibronic*, which is a combination of the words vibrational and electronic terms, includes spin and nuclear Hamiltonians as well as their interaction [1–6] . Vibronic models are present in many areas of physics and their interface with modern technologies, including quantum computing [7], quantum optics [8], quantum cellular automata [9], molecular dimers [10], chemical physics [11], Rydberg atoms [12], molecule magnets [13], and quantum advantage [14] .

However, from the point of view of mathematical physics, this is a difficult problem that cannot be solved simply analytically, even in apparently simple cases. This is because we have a system of coupled spinor components. In particular, for the simple case of a one-dimensional problem in Cartesian coordinates, which will be considered in the next section, the problem appears in the form of a fourth-order differential equation in position space. The classification of fourth-order linear differential equations with variable coefficients, which may appear in quantum physics, is something that goes beyond the scope of this article and requires a rather exhaustive analysis. However, in summary, we can say that these problems have not been considered in depth in the analytical field due to the large number of technical problems they present.

In this work we aim to use the powerful tool of Lie symmetries to partially address this problem. The main thrust of our work comes from the novel idea of Zhang [15–17], which extends to the fourth-order case the standard idea of quasi-exact solvability in a class of second-order differential equations, originally proposed in the works of Turbiner, Ushveridze, Kamran, González-López and Olver [18–22].

The structure of the present work is as follows. In Section 2 we first review the main equation of the one-dimensional vibronic model which contains the harmonic oscillator plus a linear interaction [4] and which can be considered as a generalized Landau–Zener problem. Then, using some transformations, the problem becomes a fourth-order differential equation after decoupling the components. In Section 3 w then review, in a fairly compact manner, the main idea of quasi-exact solvability for the unfamiliar reader and for the sake of continuity. It is then shown that the problem has a hidden structure by which the exceptional part of the

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https://doi.org/10.1016/j.aop.2025.170126
Received 28 February 2025; Accepted 7 June 2025

Available online 23 June 2025

exceptional energy can be derived in a simple, conceptually brief manner and without a lengthy calculations. In Section 4 we also derive the eigenfunctions of the problem using the Bethe ansatz approach. The paper ends in Section 5 with final comments and possible ideas for future research.

2. Vibronic model

In their pioneering work [1] Fulton and Gouterman proved that the vibronic coupling in molecules and the exciton coupling of dimers can be included in a 2×2 matrix Hamiltonian in the nuclear coordinates. They started from the Hamiltonian

$$\hat{H} = T_n + T_e + V(q, Q), \tag{1}$$

where, as the indices indicate, T_n and T_e represent the nuclear and electronic kinetic energy, respectively, and $V(q, Q)$ stands for the potential energy which depends on the electronic and nuclear coordinates respectively denoted by q and Q. In (1), some simplifications have been made including neglecting the uniform motion of the center of mass and the rotation of the molecule. It is also obvious that a spin-dependent term is not included. Working on the basis of the adiabatic approximation, the equations in a two-state linear curve crossing model appear in the form (see [1] for a detailed derivation)

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + \left(V_{11}(x) - E\right)\psi_1 &= -V_{12}(x)\psi_2, \\ -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + \left(V_{22}(x) - E\right)\psi_2 &= -V_{21}(x)\psi_1, \end{aligned} \tag{2}$$

where m is the particle mass, the coordinate x is defined in the full line, E stands for the energy, and ψ_1 and ψ_2 are the two components of the wave function. Here, we consider the frequently used model where the two diagonal components are considered to be linear plus harmonic, and the off-diagonal ones are considered to be constants (denoted below by V). Therefore, we start from the main equations [4–6]

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + \left(\frac{m\Omega^2 x^2}{2} - F_1 x\right)\psi_1 + V\psi_2 &= E\psi_1, \\ -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + \left(\frac{m\Omega^2 x^2}{2} - F_2 x\right)\psi_2 + V\psi_1 &= E\psi_2. \end{aligned} \tag{3}$$

The latter, via $x = X + \frac{F_2}{m\Omega^2}$, is rewritten as

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dX^2} + \left(\frac{m\Omega^2}{2}X^2 + (F_2 - F_1)X\right)\psi_1 + V\psi_2 &= \left(E - \frac{F_2^2}{2m\Omega^2} + \frac{F_1 F_2}{m\Omega^2}\right)\psi_1, \\ -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dX^2} + \left(\frac{m\Omega^2}{2}X^2\right)\psi_2 + V\psi_1 &= \left(E + \frac{F_2^2}{2m\Omega^2}\right)\psi_2. \end{aligned} \tag{4}$$

Applying the change of variable

$$X = \left(\frac{\hbar}{m\Omega}\right)^{1/2} z, \tag{5}$$

the two Eqs. (4) become

$$\begin{aligned} -\frac{1}{2}\frac{d^2\psi_1}{dz^2} + \left(\frac{1}{2}z^2 + (F_2 - F_1)\left(\frac{1}{\hbar m\Omega^3}\right)^{1/2} z\right)\psi_1 + \frac{V}{\hbar\Omega}\psi_2 &= \frac{1}{\hbar\Omega}\left(E - \frac{F_2^2}{2m\Omega^2} + \frac{F_1 F_2}{m\Omega^2}\right)\psi_1, \\ -\frac{1}{2}\frac{d^2\psi_2}{dz^2} + \frac{1}{2}z^2\psi_2 + \frac{V}{\hbar\Omega}\psi_1 &= \frac{1}{\hbar\Omega}\left(E + \frac{F_2^2}{2m\Omega^2}\right)\psi_2. \end{aligned} \tag{6}$$

Using the transformations

$$\psi_{1,2}(z) = e^{-z^2/2}\ y_{1,2}(z), \tag{7}$$

the two Eqs. (6) take the form

$$\begin{aligned} \frac{1}{2}\frac{d^2 y_1}{dz^2} - z\frac{dy_1}{dz} - \frac{V}{\hbar\Omega}y_2 + \left(\left(F_2 - F_1\right)\left(\frac{1}{\hbar m\Omega^3}\right)^{1/2} z + \frac{1}{\hbar\Omega}\left(E - \frac{F_2^2}{2m\Omega^2} + \frac{F_1 F_2}{m\Omega^2}\right) - \frac{1}{2}\right)y_1 &= 0, \\ \frac{1}{2}\frac{d^2 y_2}{dz^2} - z\frac{dy_2}{dz} - \frac{V}{\hbar\Omega}y_1 + \left(\frac{1}{\hbar\Omega}\left(E + \frac{F_2^2}{2m\Omega^2}\right) - \frac{1}{2}\right)y_2 &= 0. \end{aligned} \tag{8}$$

We can decouple these two equations by solving for y_2 in the first one and replacing it in the second, so that we arrive at

$$\begin{aligned} \hat{H}_4\, y_1 = {} & \frac{1}{4}\frac{d^4 y_1}{dz^4} - z\frac{d^3 y_1}{dz^3} + \left[z^2 + \frac{F}{2}z + \left(\frac{E_1}{2} + \frac{E_2}{2} - 1\right)\right]\frac{d^2 y_1}{dz^2} \\ & + \left[-Fz^2 + z(1 - E_2 - E_1)\right]\frac{dy_1}{dz} + \left[FE_2 z + (E_1 E_2 - v^2)\right]y_1 = 0, \end{aligned} \tag{9}$$

where the explicit form of the fourth-order differential operator $\widehat{H}_4$, which can be considered a kind of "Hamiltonian" for this problem, is clear, and where we have used the abbreviations

$$F=\left(F_2-F_1\right)\left(\frac{1}{\hbar m\Omega^3}\right)^{1/2}, \qquad E_1=\frac{1}{\hbar\Omega}\left(E-\frac{F_2^2}{2m\Omega^2}+\frac{F_1F_2}{m\Omega^2}\right)-\frac{1}{2},$$
$$E_2=\frac{1}{\hbar\Omega}\left(E+\frac{F_2^2}{2m\Omega^2}\right)-\frac{1}{2}, \qquad \upsilon=\frac{V}{\hbar\Omega}. \tag{10}$$

Eq. (9) is an ordinary fourth-order differential equation with variable coefficients. To our best knowledge, this equation has not been reported as a generalized special function of mathematical physics, nor has been recognized as a named equation. It should be noted that papers on fourth-order differential equations in physics are really scarce, although there are important cases of such forms. One might think that the problem can be solved simply by numerical techniques, but no one can deny the merits of analytical techniques, including their deep insight into the physics of the system as well as their pedagogical importance. We can comment on the need for analytical approaches for a variety of other reasons, but this is beyond the scope of the present paper and we hope to return to it in a subsequent study.

3. The hidden $sl(2)$ symmetry and the spectrum

To obtain the energy spectrum of the system, let us first review the basic idea of the Lie algebraic approach, or quasi-exact solvability, in a summarized manner. The term quasi-exact solvability comes from the fact that only part of the spectrum, and not all states, can be derived in this way. Let us first review the idea as it is used for second-order differential equations and then generalize it to the fourth-order case.

3.1. Lie algebraic approach for second-order differential equations

The most general form of the second-order quasi-exactly solvable differential operator which can be expressed as an $sl(2)$ algebra is [18,19,21,22]

$$\widehat{H}_{QES}=C_{++}J_n^+J_n^++C_{+0}J_n^+J_n^0+C_{+-}J_n^+J_n^-+C_{0-}J_n^0J_n^-+C_{--}J_n^-J_n^-+C_+J_n^++C_0J_n^0+C_-J_n^-+C, \tag{11}$$

in which

$$J_n^+=z^2\frac{d}{dz}-n\,z, \qquad J_n^0=z\frac{d}{dz}-\frac{n}{2}, \qquad J_n^-=\frac{d}{dz}, \tag{12}$$

where the nonunique generators satisfy

$$[J_n^+,J_n^-]=-2J_n^0, \qquad [J_n^\pm,J_n^0]=\mp J_n^\pm. \tag{13}$$

Using (12), the operator $\widehat{H}_{QES}$ can be written as

$$\widehat{H}_{QES}=P_4(z)\frac{d^2}{dz^2}+P_3(z)\frac{d}{dz}+P_2(z), \tag{14}$$

where

$$\begin{aligned}
P_4(z)&=C_{++}z^4+C_{+0}z^3+C_{+-}z^2+C_{0-}z+C_{--},\\
P_3(z)&=C_{++}(2-2n)z^3+\left(C_++C_{+0}\left(1-\frac{3n}{2}\right)\right)z^2+\left(C_0-nC_{+-}\right)z+\left(C_--\frac{n}{2}C_{0-}\right),\\
P_2(z)&=C_{++}n(n-1)z^2+\left(\frac{n^2}{2}C_{+0}-nC_+\right)z+\left(C-\frac{n}{2}C_0\right).
\end{aligned} \tag{15}$$

For the sake of simplicity, we write (15) as

$$P_4(z)=\sum_{k=0}^{4}a_kz^k, \qquad P_3(z)=\sum_{k=0}^{3}b_kz^k, \qquad P_2(z)=\sum_{k=0}^{2}c_kz^k. \tag{16}$$

As a result, it can be shown that $\widehat{H}_{QES}$ preserves the finite-dimensional space of polynomials of the form

$$y_n(z)=\sum_{m=0}^{n}c_mz^m. \tag{17}$$

Having reviewed the most essential background of the quasi-exact solvability, we see in the next section that our fourth-order differential equation can be related to the idea via proper identities.

3.2. Hidden $sl(2)$ symmetry for fourth-order differential equations

Based on the proof of Zhang [17], the problem has a hidden $sl(2)$-algebraization if and only if

$$b_3 = -2(n-1)a_4, \qquad c_2 = n(n-1)a_4, \qquad c_1 = -n\left[(n-1)a_3 + b_2\right]. \tag{18}$$

Now, following the identity [17]

$$z\frac{d^3}{dz^3} = J^0\,(J^-)^2 + \frac{n}{2}\frac{d^2}{dz^2}, \tag{19}$$

the "Hamiltonian" $\hat{H}_4$ in (9) can be written in the form

$$\begin{aligned}\hat{H}_4\, y_1 = {} & \left[\frac{1}{4}(J^-)^4 - J^0\,(J^-)^2\right] y_1 + \left[z^2 + \frac{F}{2}z + \left(-\frac{n}{2} + \frac{E_1}{2} + \frac{E_2}{2} - 1\right)\right]\frac{d^2 y_1}{dz^2} \\ & + \left[-Fz^2 + z\left(1 - E_2 - E_1\right)\right]\frac{dy_1}{dz} + \left[FE_2 z + (E_1E_2 - v^2)\right] y_1 = 0,\end{aligned} \tag{20}$$

where we have intentionally kept the equivalent second order part of $\hat{H}_4\, y_1$ in differential form to comment on the hidden symmetry of the system. It is seen that the n-dependent term in (24) has affected the second order part of the fourth-order differential equation. The energy relation from the third equation in (18), i.e. $c_1 = -n\left[(n-1)a_3 + b_2\right] = -nb_2$, is found as $E_2 = n$, or, from (10), more explicitly in the form

$$\frac{1}{\hbar\Omega}\left(E + \frac{F_2^2}{2m\Omega^2}\right) - \frac{1}{2} = n. \tag{21}$$

To make a comparison with [4], noting that in their notation

$$b = \frac{F_2}{(m\hbar\Omega^3)^{1/2}}, \qquad \epsilon = \frac{E}{\hbar\Omega} + \frac{1}{2}, \tag{22}$$

Eq. (21) can be written as

$$\frac{E}{\hbar\Omega} + \frac{1}{2} = \epsilon = (n+1) - \frac{b^2}{2} = k - \frac{b^2}{2}, \tag{23}$$

which is the same result obtained in [4] and possesses the familiar linear form of the harmonic oscillator in terms of the quantum number. Also, doing the shift transformation on the upper equation in (3), one may obtain the other half of the quasi-exact spectrum with the same behavior of the other component.

4. The Bethe ansatz approach and eigenfunctions: a generalization to the fourth-order case

Although the main purpose of the present work was demonstrating the hidden $sl(2)$-symmetry of the vibronic model in its fourth-order form and directly in position space, by which the exceptional part of the spectrum was reported, it is interesting to comment on the eigenfunctions as well. To this aim, we make use of the Bethe ansatz method similar to what is done in [15,16] . The idea in a nutshell is that an ansatz solution is proposed to the equation, and after manipulations, a meromorphic equation is obtained. Based on comparison of different powers on both sides of the arising equation, required material to obtain the spectrum and the eigenfunctions of the system is obtained. There are two main references which are strongly recommended for the unfamiliar reader before starting this section. The first is [15] in which the idea is applied to second-order ordinary differential equations and the basic formalism is obtained. The second is [16] which generalizes the primary idea to a fourth-order ordinary differential equation, the two-photon and two-mode Rabi model in Bargmann space in this case. The generalization to the fourth-order case can be done, rather straightforwardly, using proper series identities and careful use of residue calculus. The basic formulae used there include the identities

$$\begin{aligned}&\sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{1}{z_i - z_j} = 0, && \sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{z_i}{z_i - z_j} = \frac{1}{2}n(n-1),\\ &\sum_{i=1}^{n}\sum_{l\neq j\neq i}^{n}\frac{1}{(z_i - z_l)(z_i - z_j)} = 0, && \sum_{i=1}^{n}\sum_{l\neq j\neq i}^{n}\frac{z_i}{(z_i - z_l)(z_i - z_j)} = 0,\\ &\sum_{i=1}^{n}\sum_{p\neq l\neq j\neq i}^{n}\frac{1}{(z_i - z_p)(z_i - z_l)(z_i - z_j)} = 0, && \sum_{i=1}^{n}\sum_{p\neq l\neq j\neq i}^{n}\frac{z_i}{(z_i - z_p)(z_i - z_l)(z_i - z_j)} = 0.\end{aligned} \tag{24}$$

Let us first review the basic idea from [15] which works for Fuchsian-type equations. In other words, it works for (15) where the coefficients of the eigenfunction and its derivatives do not have a repeated root. If we propose a solution of the form

$$y(z) = \prod_{i=1}^{n}(z - z_i), \quad n = 1, 2, \dots, \tag{25}$$

for the second-order Hamiltonian (14), it can be found that [15]

$$
\begin{aligned}
&-c_0-\sum_{i=1}^{n}\mathrm{Res}\left[\frac{\widehat{H}_{QES}\,y}{y},z=z_i\right]=\left[n(n-1)a_4+nb_3+c_2\right]z^2\\
&+\left[\left(2(n-1)a_4+b_3\right)\sum_{i=1}^{n}z_i+n(n-1)a_3+nb_2+c_1\right]z\\
&+\left(2(n-1)a_4+b_3\right)\sum_{i=1}^{n}z_i^2+2a_4\sum_{i<j}^{n}z_iz_j+\left(2(n-1)a_3+b_2\right)\sum_{i=1}^{n}z_i+n(n-1)a_2+nb_1,
\end{aligned}
\tag{26}
$$

where $\mathrm{Res}[f(z),z=z_i]$ indicates the residue of $f(z)$ at $z=z_i$. In fact, we have a constant term on the left-hand side, and a meromorphic function on the right-hand side, from which the required data to report the solution is provided. In more precise words, the residue term, which must be vanishing, gives the z_i. The coefficients of z^2 and z on the right-hand side normally determine the spectrum of the system and both should vanish to assure that the equality holds. The remaining constant terms on both sides, can be interpreted as a restriction among the parameters, which is the price ought to be paid to obtain an analytical solution. Using [16], which has to be read to carefully to understand the details of calculations, the idea is generalized to the fourth-order case.

Having reviewed the basic idea of the approach, we now propose a solution of the form (25) for $y_1(z)$ in (9), which yields for the quotient $\frac{1}{y_1}\widehat{H}_4\,y_1$:

$$
\begin{aligned}
0=&\,E_1E_2-v^2+\frac{1}{4}\sum_{i=1}^{n}\frac{1}{z-z_i}\sum_{p\neq l\neq j\neq i}^{n}\frac{4}{(z_i-z_p)(z_i-z_l)(z_i-z_j)}-z\sum_{i=1}^{n}\frac{1}{z-z_i}\sum_{l\neq j\neq i}^{n}\frac{3}{(z_i-z_l)(z_i-z_j)}\\
&+\left[z^2+\frac{F}{2}z+\left(\frac{E_1}{2}+\frac{E_2}{2}-1\right)\right]\sum_{i=1}^{n}\frac{1}{z-z_i}\sum_{j\neq i}^{n}\frac{2}{(z_i-z_j)}\\
&+\left[-Fz^2+z\left(1-E_2-E_1\right)\right]\sum_{i=1}^{n}\frac{1}{z-z_i}+FE_2z.
\end{aligned}
\tag{27}
$$

From here we can easily evaluate the following residues

$$
\begin{aligned}
\mathrm{Res}\left[\frac{\widehat{H}_4\,y_1}{y_1},z=z_i\right]=&\frac{1}{4}\sum_{p\neq l\neq j\neq i}^{n}\frac{4}{(z_i-z_p)(z_i-z_l)(z_i-z_j)}-z_i\sum_{l\neq j\neq i}^{n}\frac{3}{(z_i-z_l)(z_i-z_j)}\\
&+\left[z_i^2+\frac{F}{2}z_i+\left(\frac{E_1}{2}+\frac{E_2}{2}-1\right)\right]\sum_{j\neq i}^{n}\frac{2}{(z_i-z_j)}+\left[-Fz_i^2+z_i\left(1-E_2-E_1\right)\right],
\end{aligned}
\tag{28}
$$

which determines the z_i in the ansatz proposed in (25). For example, for the first state, i.e. $z_i=z_1$, we have $-Fz_i^2+z_i\left(1-E_2-E_1\right)=0$ as all other terms vanish (here $E_{1,2}$ are in fact linear functions of the exceptional energy E_n as indicated in (10) and thus vary for different n). A systematic process can be done for higher states. However, as can be seen, the higher the state, the more complicated the calculations. Nevertheless, the approach is quite systematic and can be carried out.

Let us now go back to the arising meromorphic Eq. (26). In fact, this equation can be used here in the fourth-order case recalling that the effect of third- and fourth-order terms are already included in the z_i and the residue at each z_i. As a result, we may conclude that in our case, i.e. for (9):

- The first term on the right-hand side of (26), i.e. the coefficient of z^2, yields nothing since $a_4=b_3=c_2=0$ as follows by comparing (9) with (16).
- The second term on the right-hand side of (26) gives $nb_2+c_1=0$, i.e. the coefficient of z, yields the exceptional energy already obtained in (21). This is because $a_3=0$ as follows by comparing (9) with (16).
- Taking into account that, comparing (9) with (16), we also get that $a_2=1$, $b_1=1-E_2-E_1$ and $b_2=-F$, the constant terms on both sides of (26) yield

$$
-c_0=v^2-E_1E_2=-F\sum_{i=1}^{n}z_i+n(n-1)+n\left(1-E_2-E_1\right),
\tag{29}
$$

  which can be considered as a restriction among the parameters. More explicit form of this restriction can be easily obtained using the value of z_i, from (28), and $E_{1,2}$ from (10) and (21) for each level/state.

5. Conclusion

A two-state vibronic model was considered in one spatial dimension with a harmonic plus linear interaction for the diagonal scattering matrix element and constant terms for the off-diagonal ones. We worked directly in the position space instead of transforming the problem into other spaces or using integral transforms. It was shown that the problem, via proper transformations and identities, has a hidden $sl(2)$ symmetry which gives the exceptional part of the spectrum in a simple manner. This is of particular interest due to various complexities and challenges of the other approaches. In particular, the present problem, which of great importance from both research and pedagogical points of view, was solved by first transforming the equation into $p-$ representation space and then working on the arising Heun-like equation in the transformed space [4]. Here, however, the exceptional part of the spectrum was derived from quite basic ideas of quasi-exactly solvable models and elements of group theory.

Although the main purpose of this work was recognizing and introducing the hidden symmetry of the problem, the eigenfunctions were also obtained via the Bethe ansatz approach in a systematic manner. The latter has its own limitations and complexity and is certainly rather lengthy. Nevertheless, when compared to the other parallel approaches, it might still look more economical.

The idea might be generalized to other classes of vibronic models, on which we are working. We hope the present work renews the interest in the analytical structure of the other vibronic and two- and/or multi-level models, which have not been extensively explored for many realistic terms mainly due to their higher-order structure. It is also an interesting survey to consider the idea in different fields and in particular within the so-called Generalized Uncertainty Principle (GUP) formalism where we have to deal with higher-order wave equations, and in particular, the fourth and sixth order Schödinger equations for a frequently used form of GUP originating from the interface of quantum physics and gravity. Work in this direction is also in progress.

CRediT authorship contribution statement

L.M. Nieto: Writing – review & editing, Validation, Supervision, Software, Resources, Project administration, Funding acquisition, Formal analysis, Data curation. **S. Zarrinkamar:** Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Both authors, L.M. Nieto and S. Zarrinkamar, report financial support provided by European Union, by Government of Castile and Leon and by the Ministry of Science, Innovation and Universities of Spain. They declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This research was supported by the Q-CAYLE project, funded by the European Union-Next Generation UE/MICIU/Plan de Recuperacion, Transformacion *y* Resiliencia/Junta de Castilla *y* Leon (PRTRC17.11), and also by project PID2023-148409NB-I00, funded by MICIU/AEI/10.13039/501100011033. Financial support of the Department of Education of the Junta de Castilla *y* Leon and FEDER Funds is also gratefully acknowledged (Reference: CLU-2023-1-05).

Data availability

No data was used for the research described in the article.

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