

REVISTA DE LA REAL ACADEMIA DE CIENCIAS

REVISTA
DE LA
REAL ACADEMIA
DE CIENCIAS
Exactas
Físicas
Químicas y
Naturales
DE
ZARAGOZA



Serie 2.^a
Volumen 74

2019

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Exactas, Físicas, Químicas y Naturales

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2019

Revista de la Real Academia de Ciencias Exactas, Físicas, Químicas y Naturales de Zaragoza es una revista anual, editada por la Real Academia de Ciencias Exactas, Físicas, Químicas y Naturales de Zaragoza, y editada y distribuida a través de Prensas de la Universidad de Zaragoza. Calle Pedro Cerbuna, 12. 50009 Zaragoza (España). Tel +34 976761330 puz@unizar.es <http://puz.unizar.es/>

Este número se publica con la financiación del Vicerrectorado de Política Científica de la Universidad de Zaragoza.

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Depósito legal: Z 218-1960

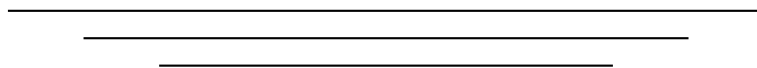
ISSN: 0370-3207

Edita: Prensas de la Universidad de Zaragoza

Imprime: Servicio de Publicaciones. Universidad de Zaragoza

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Positivity, accuracy, optimality and applications

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Abstract

This paper surveys some recent advances relating positivity, accuracy and optimal bases. In particular, high relative accuracy computations for some structured classes of matrices adequately parametrized are considered. Some applications of these classes of matrices are commented.

1 Introduction

In many mathematical models, positivity is one of the fundamental underlying hypotheses because the involved variables only have meaning when they are nonnegative. This also implies that nonnegative matrices also play a crucial role in many mathematical models dealing with problems of the real world or arising in other scientific or technical fields. Spectral properties of nonnegative matrices are also remarkable because, by the Perron–Frobenius theorem (cf. [12]), the nonnegativity is inherited by an eigenvalue of the matrix with maximum absolute value and by a corresponding eigenvector, properties that also play a key role in many mathematical models. For instance, in the Leontief input–output model, very important in Economy (cf. [12]). More recent applications of positivity are related with the advantages of positivity in

*This work was partially supported through the Spanish research grant PGC2018-096321-B-I00 (MCIU/AEI), by Gobierno de Aragón (E41-17R) and Feder 2014-2020 “Construyendo Europa desde Aragón”.

the context of numerical computations in floating point arithmetic, as explained in Section 2. In this sense, we mention two main sources of such applications. On the one hand, applications related to the factorization of a nonnegative sparse matrix as a product of two nonnegative matrices, which are natural applications in the context of Big Data (cf. [114, 82]). On the other hand, applications related to the search of numerical methods adapted to the structure of the classes of matrices and leading to computations with high relative accuracy. This will be one of the topics surveyed in this paper. In spaces of nonnegative functions arise optimal bases under different viewpoints. This problem was first studied in the context of Total Positivity and later extended to a more general framework, and it is another topic considered in this paper.

The paper is organized as follows. Section 2 presents some basic concepts about the errors obtained when computing with floating point arithmetic. The classical error analysis involves concept such as growth factor and conditioning. This leads to present some optimal bases and to recall that, in some problems related with positivity, it is possible to find a parametrization of the data and an algorithm leading to small roundoff errors in spite of a bad conditioning with its initial parametrization. Section 3 is devoted to optimal bases for several properties in the context of Total Positivity and more general contexts. In particular, we point out some optimal properties of the Bernstein basis of the space of polynomials.

Up to now, methods with high relative accuracy for algebraic computations (such as the eigenvalues, singular values or inverses) independently of the conditioning have been found mainly for classes of matrices related with positivity and coming from one of the two following sources: generalizations of diagonally dominant matrices (considered in Section 4) and subclasses of totally positive matrices (considered in Section 5). In both cases, we comment the parameterizations of the matrices leading to the computations with high relative accuracy as well as some applications. These parameterizations lead to some matrix factorizations that are used by algorithms with high relative accuracy: rank revealing decompositions, obtained for classes of matrices generalizing diagonal dominance, and bidiagonal factorization, obtained for nonsingular totally positive matrices. In Section 5 we provide some details of the accurate computations and bidiagonal factorizations of matrices of matrices related to the following five subclasses of nonsingular totally positive matrices: Pascal matrices, rational Bernstein-Vandermonde matrices, Jacobi-Stirling matrices, Laguerre matrices and Bessel matrices.

2 Error analysis, optimal bases and high relative accuracy

When we apply an algorithm and perform the computations with floating point arithmetic, since we do not know the exact error performed with our computations, it is convenient to try to derive upper bounds of this error, usually known as *forward* error bounds. However, it is usually very difficult to get directly such bounds. An alternative approach that has been very successful in the field of Numerical Linear Algebra, and later in other fields, bounds the forward error through the backward error. If we consider that our computed solution is the exact solution of a perturbed problem, the *backward* error measures the distance between the perturbed problem and the initial problem. The backward error depends on the numerical method that we have used and it is well known that the growth factor of an algorithm is an indicator of its backward stability (cf. [68], [71]). Let us recall that the *growth factor* of a numerical algorithm is usually defined as the quotient between the maximal absolute value of all the elements that occur during the performance of the algorithm and the maximal absolute value of all the initial data. The optimal growth factor for a numerical method is 1. Hence optimal methods under this viewpoint are methods with growth factor 1 (cf. [106, 108, 27]).

The *conditioning* of the problem measures the effect of data perturbations on the solution of the problem. In general, when we have defined the corresponding forward error, backward error and the condition number for a given problem, one tries to prove the relation:

$$\text{forward error} \leq \text{condition number} \times \text{backward error},$$

which allows us to obtain a forward error bound through the backward error. Although the computed solution has a small backward error, it can be amplified by the condition number leading to a large forward error. So, in contrast to the backward error, which depends of the used method, the conditioning can become an intrinsic cause to get a large forward error bound. In conclusion, under this approach, in order to get a small forward error we need a small conditioning and using a method with small backward error.

In the problem of evaluating a real function of a finite dimensional vector space of functions, the conditioning depends on the basis that we use. The problem of finding bases with minimal condition number has been analyzed in the context of bases of nonnegative functions, which play an important role in many problems of

approximation theory or computer aided geometric design (cf. [53]). The optimal bases in this context for the evaluation of a function are bases b of nonnegative functions that cannot be expressed, up to permutation and positive scaling, in the form vK , where v is another basis of nonnegative functions and K is a nonnegative matrix (see [25, 105, 106]). Examples of these optimal bases are the Bernstein basis [52] for the space of polynomials on a compact interval, the B-spline basis [101] or the bases of spaces of real multivariate functions given in [84]. Let us recall that the *Bernstein basis* $(b_0^n(t), \dots, b_n^n(t))$ of the space P_n of polynomials of degree at most n on $[0, 1]$ is given by

$$(1) \quad b_i^n(t) = \binom{n}{i} t^i (1-t)^{n-i}, \quad t \in [0, 1], \quad i = 0, 1, \dots, n.$$

and it is the polynomial basis most used in computer aided geometric design. In the next section, we consider again this basis and other optimal properties that it satisfies. The conditioning for the representations associated to polynomial interpolation problems (depending on the nodes distribution and ordering) and to least squares approximations have been analyzed recently (see [16, 17, 18, 19]). Coming back to the problem of evaluating a function, in addition to bases with minimal condition number, backward stable methods are also required in order to obtain small forward errors. These backward stable methods and their corresponding error analysis can be seen in [85, 109, 110, 8, 9, 34, 36, 10, 38, 42].

We now comment an alternative approach to assure small forward errors and that can be applied in fields where positivity plays a key role. In some problems it is possible to find a parametrization of the data and an algorithm leading to small forward error bounds in spite of a bad conditioning with its initial parametrization. The desired goal is to guarantee *high relative accuracy* (HRA). We say that we have performed an algorithm with HRA if the following formula holds: relative forward error $\leq Ku$, for some constant K , where u is the unit roundoff. It is not always possible to guarantee HRA for a given problem. An example of a simple problem for which an HRA algorithm cannot be found is provided by the sum of three real numbers $x + y + z$ (see [44]). For some structured classes of matrices, HRA algorithms can be found, as we shall recall in this paper. However, there are classes of structured matrices for which we again have that these algorithms cannot be found. For instance, accurate linear algebra for the problem of calculating determinants or minors is impossible on the class of Toeplitz matrices (see corollaries 3.43 and 3.45 of

[44]). Let us recall that a Toeplitz matrix B has the following simple structure:

$$B = \begin{pmatrix} a_0 & a_1 & \cdots & a_{n-2} & a_{n-1} \\ a_{-1} & a_0 & \ddots & & a_{n-2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ a_{-n+2} & & \ddots & \ddots & a_1 \\ a_{-n+1} & a_{-n+2} & \cdots & a_{-1} & a_0 \end{pmatrix}.$$

There exists a sufficient condition to assure the HRA of an algorithm that we now recall. Given an algorithm using only additions of numbers of the same sign, multiplications and divisions, and assuming that each initial real datum is known to HRA, then it is well known that the output of the algorithm can be computed to HRA (cf. [45, p. 52]). Moreover, in (well implemented) floating point arithmetic, HRA is also preserved even when we perform true subtractions when the operands are original (and so, exact) data (cf. p. 53 of [45]). So, the sufficient condition to assure the HRA of an algorithm is called “no inaccurate cancellation” (NIC) and it is satisfied if it only uses additions of numbers of the same sign, multiplications, divisions and subtractions (additions of numbers of different sign) of the initial data. In order to find algorithms with HRA for some classes of matrices, it is usually necessary to reparameterize the matrices belonging to these classes, since HRA will be satisfied independently of the conditioning of the matrices. Up to now, the main classes of matrices for which algorithms with HRA have been found are closely related with positivity and the corresponding algorithms are in fact NIC algorithms. We show many examples of these classes of matrices in sections 4 and 5.

3 Optimal bases

In the previous section, we have mentioned the bases of nonnegative functions that are optimal, with respect to the corresponding condition number, for the problem of evaluating a real function of a finite dimensional vector space of functions. Let us now recall this condition number. Given a basis $u = (u_0, \dots, u_n)$ of a real vector space \mathcal{U} of real functions defined on a subset S of \mathbf{R}^m ($m \geq 1$) and a function $f \in \mathcal{U}$, we can write $f(x) = \sum_{i=0}^n c_i u_i(x)$ for all $x \in S$, where $c_i \in \mathbf{R}$ for all $i = 0, \dots, n$. The stability of the basis U with respect to the evaluation at a point is measured by the function $C_u : \mathcal{U} \times I \rightarrow \mathbf{R}_+$ given by

$$(2) \quad C_u(f, x) := \sum_{i=0}^n |c_i u_i(x)|.$$

Given two bases of nonnegative functions u, v , let A the matrix of change of basis such that $v = uA$. The following result compares the conditioning of the bases by means of the nonnegativity of K . The result can be proved with the adaptation to the condition number (2) of the proof of Lemma 3.1 of [84], which proves a similar result for a relative condition number derived from the previous one.

Lemma 3.1 *Let \mathcal{U} be a finite dimensional vector space of functions defined on a subset S of \mathbf{R}^m . Let u, v be two bases of nonnegative functions of \mathcal{U} . Then*

$$(3) \quad C_u(f, x) \leq C_v(f, x), \quad \forall f \in \mathcal{U}, \quad \forall x \in S$$

if and only if the matrix A such that $v = uA$ is nonnegative.

In the case of the space P_n of polynomials of degree at most n on an interval $[0, 1]$, Theorem 3 of [52] leads to the optimality result of the Bernstein basis given by (1).

Theorem 3.2 *Let $b = (b_0^n, \dots, b_n^n)$ be the Bernstein basis. Then there does not exist (up to reordering and positive scaling) another basis $u = (u_0, \dots, u_n)$ of nonnegative functions in P_n such that $C_u(p, t) \leq C_b(p, t)$ for all $t \in [0, 1]$ and $p \in P_n$.*

Similar results to the previous one are satisfied, for instance, by the B-spline basis [101] or by the bases of spaces of real multivariate functions given in [84] (see also [105]).

Now we shall focus on optimal bases for shape preservation in Computer Aided Geometric Design (CAGD). We shall see that they are closely related with the optimal bases for the evaluation commented previously. We start with the definition of collocation matrix of a system of functions, which will be used later to introduce special bases. Given a system of functions $U = (u_0, \dots, u_n)$ defined on $I \subseteq \mathbf{R}$, the *collocation matrix* of U at $t_0 < \dots < t_m$ in I is given by

$$(4) \quad M \begin{pmatrix} u_0, \dots, u_n \\ t_0, \dots, t_m \end{pmatrix} := (u_j(t_i))_{i=0, \dots, m; j=0, \dots, n}.$$

We now recall some concepts of CAGD. Given a sequence of functions (u_0, \dots, u_n) on $I = [a, b]$, and a sequence of points (C_0, \dots, C_n) in \mathbf{R}^k , we may define a parametric curve

$$\gamma(t) = \sum_{i=0}^n C_i u_i(t), \quad t \in [a, b].$$

The points $C_i, i = 0, \dots, n$, are called *control points*. The *control polygon* of the curve γ is the polygonal arc with vertices C_0, \dots, C_n . In CAGD, it is usually required that

the functions $u_i, i = 0, \dots, n$, are nonnegative and $\sum_{i=0}^n u_i(t) = 1$ for all $t \in I$ (i.e., the system $u = (u_0, \dots, u_n)$ is *normalized*, or equivalently, the functions form a partition of unity). A normalized system of nonnegative functions is called a *blending* system. An important property for curve design is the *convex hull property*: for any control polygon, the curve lies always in the convex hull of the control polygon. The convex hull property holds if and only if the system of functions is blending. These geometric properties correspond to some properties of the collocation matrices of the system of functions. Observe that u is blending if and only if all its collocation matrices are stochastic (that is, nonnegative and such that the sum of the entries of each row is one).

More shape preserving properties of the systems of functions require in turn additional properties to their corresponding collocation matrices. In interactive design we also desire that the shape of a parametrically defined polynomial curve mimics the shape of its control polygon in order to predict or manipulate the shape of the curve by suitably choosing or changing the control polygon. This leads to the concept of totally positive systems and totally positive matrices, due to the variation diminishing property of these matrices. A matrix is *totally positive* (TP) if all its minors are nonnegative and a system of functions is totally positive (TP) if all its collocation matrices (4) are totally positive. If all minors of a matrix are positive, then the matrix is called *strictly totally positive* (STP) matrix. TP and STP matrices have been also called in the literature as totally nonnegative and totally positive, respectively. If a system u is normalized totally positive (NTP) then the curve γ inherits many shape properties of the control polygon. Let us mention that, in addition to the space of polynomials on a compact interval and polynomial spline spaces, many other spaces containing algebraic, trigonometric and hyperbolic polynomials also possess NTP bases (cf. [90, 86, 20, 87, 88, 21, 22]).

Now we consider the problem of comparing two NTP systems of the same space. Given two NTP bases (p_0, \dots, p_n) and (b_0, \dots, b_n) of a space of functions \mathcal{U} , let K be the nonsingular matrix given by

$$(p_0, \dots, p_n) = (b_0, \dots, b_n)K.$$

Since both bases are normalized we conclude that each row of K has sum 1. If we now assume that the matrix K of change of basis is TP, then it is a stochastic nonsingular TP matrix. The following properties of the control polygons $B_0 \cdots B_n$ (with respect to (b_0, \dots, b_n)) and $P_0 \cdots P_n$ (with respect to (p_0, \dots, p_n)) can be obtained (see [65])

and [67]):

1. If $P_0 \cdots P_n$ is convex, then so are $B_0 \cdots B_n$ and the curve γ , and $B_0 \cdots B_n$ lies between $P_0 \cdots P_n$ and γ .
2. $\text{Length } \gamma \leq \text{length } B_0 \cdots B_n \leq \text{length } P_0 \cdots P_n$.
3. If $P_0 \cdots P_n$ turns through an angle $< \pi$, then $I(\gamma) \leq I(B_0 \cdots B_n) \leq I(P_0 \cdots P_n)$, where $I(\beta)$ denotes the number of inflexions of a curve β .
4. $\theta(\gamma) \leq \theta(B_0 \cdots B_n) \leq \theta(P_0 \cdots P_n)$, where $\theta(\beta)$ denotes the angular variation of a curve β .

Therefore, the curve γ imitates better the form of the control polygon $B_0 \cdots B_n$ than the form of the control polygon $P_0 \cdots P_n$. This motivates that an NTP basis with optimal shape preserving properties satisfies the following definition.

Definition 3.3 *Let (u_0, \dots, u_n) be a TP basis of a space \mathcal{U} . Then (u_0, \dots, u_n) is a B-basis if for any other TP basis (v_0, \dots, v_n) of \mathcal{U} the matrix K of change of basis*

$$(v_0, \dots, v_n) = (u_0, \dots, u_n)K$$

is TP.

By the previous reasoning, a normalized B-basis has *optimal shape preserving properties*. A space with an NTP basis has a unique normalized B-basis (see [24]). Example of normalized B-bases are the Bernstein basis (1) and the B-spline basis (see [23, 24]).

Another optimal property of normalized B-basis is related to the *progressive iteration approximation* property (see [35]), which is satisfied by NTP bases. Given a sequence of points $(P_i)_{i=0}^n$ such that the i th point is assigned to a parameter value t_i for $i = 0, 1, \dots, n$ and a basis (u_0, \dots, u_n) , we construct a starting curve $\gamma^0(t) = \sum_{i=0}^n P_i^0 u_i(t)$ with $P_i^0 = P_i$ for all $i \in \{0, 1, \dots, n\}$. Then, computing the adjusting vector $\Delta_i^0 = P_i - \gamma^0(t_i)$ we can take $P_i^1 = P_i^0 + \Delta_i^0$, for $i = 0, 1, \dots, n$, and construct a new curve as $\gamma^1(t) = \sum_{i=0}^n P_i^1 u_i(t)$. Iterating this process we can get a sequence of curves $\{\gamma^k\}_{k=0}^\infty$. The progressive iteration approximation property holds when this curve sequence converges to the polynomial curve interpolating the given initial sequence of points. This property holds for NTP bases and we proved in Theorem 4 of [35] the optimal convergence speed of the normalized B-basis.

Theorem 3.4 *The normalized B-basis of a space \mathcal{U} with an NTP basis provides a progressive iterative approximation with the fastest convergence rate among all NTP bases of \mathcal{U} .*

Other optimal properties of normalized B-bases can be found in [25, 102].

Now, we finish this section presenting the optimal conditioning of the collocation matrices of the Bernstein basis. Given a nonsingular matrix $A = (a_{ij})_{1 \leq i, j \leq n}$, let us consider the classical condition number

$$\kappa_\infty(A) := \|A\|_\infty \|A^{-1}\|_\infty.$$

Denoting by $|A|$ the matrix whose (i, j) -entry is $|a_{ij}|$, the Skeel condition number of a nonsingular matrix A is defined as

$$\text{Cond}(A) := \||A^{-1}|\| |A|\|_\infty.$$

The following result corresponds to Theorem 2.1 of [37]. It shows that the collocation matrices of the Bernstein basis are the best conditioned among all the corresponding collocation matrices of NTP bases of the space P_n of polynomials of degree at most n on $[0, 1]$, and a similar result using the Skeel condition number of the transposes of the collocation matrices.

Theorem 3.5 *Let (b_0^n, \dots, b_n^n) be the Bernstein basis, let (v_0, \dots, v_n) be another NTP basis of P_n on $[0, 1]$, let $0 \leq t_0 < t_1 < \dots < t_n \leq 1$ and $V := M \begin{pmatrix} v_0, \dots, v_n \\ t_0, \dots, t_n \end{pmatrix}$ and $B := M \begin{pmatrix} b_0^n, \dots, b_n^n \\ t_0, \dots, t_n \end{pmatrix}$. Then:*

$$\kappa_\infty(B) \leq \kappa_\infty(V), \quad \text{Cond}(B^T) \leq \text{Cond}(V^T).$$

The previous result deals with the conditioning of certain totally positive matrices, In Section 5 we shall show some subclasses of totally positive matrices for which many algebraic computations can be performed with high relative accuracy (HRA).

4 Generalizing diagonal dominance: computations with HRA and applications

For some classes of matrices closely related with diagonal dominance, some algebraic calculations can be performed with HRA: singular values, inverses, the solution of some linear system and, in some cases, even the eigenvalues. An adequate

parametrization of the matrices has been needed. Let us first recall some related classes of matrices. A square real matrix is called a *P-matrix* if all its principal minors are positive (the principal minors use the same rows and columns). Examples of subclasses of *P*-matrices with many applications are the nonsingular TP matrices (considered in the next section) and the nonsingular *M*-matrices. A real matrix with nonpositive off-diagonal entries is called a *Z-matrix*. A matrix $A = (a_{ij})_{1 \leq i, j \leq n}$ is (*row*) *diagonally dominant* (resp., *strictly (row) diagonally dominant*) if, for each $i = 1, \dots, n$, $|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|$ (reps., $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$). If A^T is row diagonally dominant, then we say that A is column diagonally dominant. Given a matrix $M = (m_{ij})_{1 \leq i, j \leq n}$, its *comparison matrix* $\tilde{M} = (\tilde{m}_{ij})_{1 \leq i, j \leq n}$ is the *Z*-matrix defined by $\tilde{m}_{ii} := |m_{ii}|$ and $\tilde{m}_{ij} := -|m_{ij}|$ if $i \neq j$, $1 \leq i, j \leq n$. Let us recall (cf. [12]) that if a *Z*-matrix A can be expressed as $A = sI - B$, with $B \geq 0$ and $s \geq \rho(B)$ (where $\rho(B)$ is the spectral radius of B), then it is called an *M-matrix*. A *Z*-matrix A is a nonsingular *M*-matrix if and only if A^{-1} is nonnegative (cf. [12]). Nonsingular *M*-matrices have important applications, for instance, in iterative methods in numerical analysis, in the analysis of dynamical systems, in economics and in mathematical programming (see [12]). Finally, we say that a matrix is an *H-matrix* if its comparison matrix is a nonsingular *M*-matrix. A is a nonsingular *H*-matrix if and only if there exists a diagonal matrix D such that AD is strictly diagonally dominant, and so these matrices are also called generalized diagonally dominant matrices.

An important concept related with the construction of algorithms with HRA for the computation of the singular values of a matrix is the rank revealing decomposition. A *rank revealing decomposition* of a matrix A is defined in [45] as a decomposition $A = XDY^T$, where X, Y are well conditioned and D is a diagonal matrix. In [45] it was proved that the singular value decomposition can be computed with HRA and efficiently for matrices possessing rank revealing decompositions with HRA. We have mentioned previously the need to reparametrize matrices in order to obtain accurate computations. In the class of diagonally dominant *M*-matrices, the natural parameters that permit obtaining efficient algorithms with HRA are the off-diagonal entries and the row sums (or the column sums): see [2] and [3]. These parameters can even have a meaningful interpretation when such matrices arise in the field of digital electrical circuits: the column sums are given by the quotient between the conductance and capacitance of each node (see [2]). For $n \times n$ diagonally dominant *M*-matrices, an algorithm of [3] computes to HRA the *LDU* factorization if the off-diagonal entries and the row sums are given. It modifies Gaussian elimination to

compute the off-diagonal entries and the row sums of each Schur complement without performing subtractions.

In order to obtain, rank revealing decompositions, pivoting strategies were later used. For a diagonally dominant M -matrix A , a symmetric pivoting leading to an LDU -decomposition of A is equivalent to the following factorization of A : $PAP^T = LDU$, where P is the permutation matrix associated to the pivoting strategy. Symmetric complete pivoting was used in [46] to compute well conditioned L and U factors because U is row diagonally dominant and the off-diagonal entries of L have absolute value less than 1. This factorization is a special case of a rank revealing decomposition. To implement symmetric complete pivoting, the algorithm in [46] calculates all the diagonal entries and all Schur complements and this increases the cost in $\mathcal{O}(n^3)$ flops with respect to standard Gaussian elimination. In [107] another symmetric pivoting strategy (called diagonally dominant pivoting) was used, also with a subtraction-free implementation and a similar computational cost, but improving the conditioning of L because it leads to both triangular matrices L and U column and row diagonally dominant, respectively. In [6], an accurate algorithm for the same LDU -decomposition of [107], but requiring $\mathcal{O}(n^2)$ elementary operations beyond the cost of Gaussian elimination (instead of $\mathcal{O}(n^3)$), was presented. This method can also be applied for diagonally dominant matrices satisfying certain sign patterns: with off-diagonal entries of the same sign or satisfying a chessboard pattern. The problem of computing an accurate LDU decomposition of diagonally dominant matrices from adequate parameters has been solved by Ye in [117], although in this case it is not used a subtraction-free algorithm. Diagonally dominant matrices with arbitrary sign patterns were also considered in [48]. For a class of $n \times n$ nonsingular almost row diagonally dominant Z -matrices, and given adequate parameters, an efficient method to compute its LDU decomposition with HRA is provided in [7]. It adds an additional cost of $\mathcal{O}(n^2)$ elementary operations over the computational cost of Gaussian elimination. In all these cases, we can later apply the method of [45] to calculate all the singular values with HRA.

Let us now recall another class of matrices generalizing diagonally dominant. Let us start by defining the concept of a Nekrasov matrix (see [115]). We can define recursively for a complex matrix $A = (a_{ij})_{1 \leq i, j \leq n}$ with $a_{ii} \neq 0$, for all $i = 1, \dots, n$,

$$(5) \quad h_1(A) := \sum_{j \neq 1} |a_{1j}|, \quad h_i(A) := \sum_{j=1}^{i-1} |a_{ij}| \frac{h_j(A)}{|a_{jj}|} + \sum_{j=i+1}^n |a_{ij}|, \quad i = 2, \dots, n.$$

We say that A is a *Nekrasov matrix* if $|a_{ii}| > h_i(A)$ for all $i = 1, \dots, n$. A Nekrasov matrix is a nonsingular H -matrix [115]. Therefore, a Nekrasov Z -matrix with positive diagonal entries is a nonsingular M -matrix. In [98], computations with HRA for the class of Nekrasov Z -matrices were studied. The proposed n^2 parameters used for an $n \times n$ Nekrasov Z -matrix $A = (a_{ij})_{1 \leq i, j \leq n}$ with positive diagonal are:

$$(6) \quad \begin{cases} a_{ij}, & i \neq j \\ \Delta_j(A) := a_{jj} - h_j(A), & j \in N \end{cases}$$

A is a Nekrasov Z -matrix with positive diagonal if and only if the first $n^2 - n$ parameters are nonpositive and the last n parameters $\Delta_j(A)$ ($j = 1, \dots, n$) are positive. In [98], this parametrization was used to compute the inverse of a Nekrasov Z -matrix with positive diagonal with HRA.

Let us now focus on some applications of the tools and classes of matrices considered in this section. For instance, the graph Laplacian matrices (see [95]) are positive semidefinite symmetric diagonally dominant M -matrices with zero row sums and zero column sums. Let us recall that these matrices and their spectral properties have important applications to chemistry, mathematical biology, information theory, quantum graphs or pattern recognition problems.

Diagonal dominance is closely related with the obtention of results for localizing the eigenvalues of a matrix. It is well known that the nonsingularity of a strictly diagonally dominant matrix is equivalent to the first part of the Gerschgorin circles Theorem for the localization of the eigenvalues of a matrix. More general nonsingularity conditions than diagonal dominance lead to sharper localization regions of the eigenvalues. On the other hand, it is also well known that a strictly diagonally dominant matrix with positive diagonal entries has positive determinant. In [15], it was proved that a matrix with positive row sums and all its off-diagonal elements bounded above by their corresponding row means has also positive determinant. This condition was used in [103] for the localization of the real eigenvalues of real matrices, which complement the information provided by the Gerschgorin circles. Sharper conditions were obtained in [104, 28, 29].

The next application corresponds to the field of optimization. Let us recall the linear complementarity (LC) problem. The LC problem consists of finding vectors $x \in \mathbf{R}^n$ satisfying

$$(7) \quad Mx + q \geq 0, \quad x \geq 0, \quad x^T(Mx + q) = 0,$$

where M is an $n \times n$ real matrix and $q \in \mathbf{R}^n$. We denote this problem by $\text{LCP}(M, q)$ and its solutions by x^* . A linear complementarity problem has always a unique solution if and only if the associate matrix M is a P -matrix. Many problems can be posed in the form (7): problems in linear and quadratic programming, the problem of finding a Nash equilibrium point of a bimatrix game or some free boundary problems of fluid mechanics (see Chapter 10 of [12], [94] and [30], and references therein). It is well-known that an H -matrix with positive diagonals is a P -matrix (see, for instance, Theorem 2.3 of Chapter 6 of [12]) and that a strictly diagonally dominant matrix is an H -matrix. In [94], error bounds for $\|x - x^*\|$ were derived when M in (1.1) is a P -matrix. When M in (7) is an H -matrix with positive diagonals, sharper error bounds were obtained in [26]. Sharper bounds can be obtained for particular subclasses of H -matrices or P -matrices: see, for instance, [56, 59], [57, 99] for Nekrasov matrices, or [58] for B_π^R -matrices. The class of B_π^R -matrices (introduced in [97]) has also been extended in [100] to define a new class of tensors. Tensors (also called hypermatrices) provide, joint with the Kronecker product of matrices, a very useful tool for the treatment of Big Data (see also [81, 111]).

5 Totally positive matrices: computations with HRA and applications

Let us recall that totally positive (TP) matrices are matrices whose minors are all nonnegative (see Section 3, where STP matrices are also defined). These matrices present important applications (see [72], [55], [5], [60], [51], [112]) in many fields such as Approximation Theory, Biology, Economics, Combinatorics, Statistics, Differential Equations, Mechanics or Computer Aided Geometric Design (CAGD). TP and STP matrices satisfy some remarkable properties, such as the variation diminishing property (see Section 5 of [5]), which is fundamental in their applications. They also satisfy nice spectral properties (see Section 6 of [5]), for instance the nonnegativity of the eigenvalues of TP matrices or the positivity of the eigenvalues of STP matrices

The parametrization of TP matrices leading to HRA algorithms is provided by their bidiagonal factorizations, which are in turn closely related to an elimination procedure known as Neville elimination. In some papers by M. Gasca and G. Mühlbach ([61], for example) on the relationship between interpolation formulas and elimination techniques, it became clear that what they called *Neville elimination* had special interest for TP matrices. It is a procedure to make zeros in a column of a matrix by

adding to each row an appropriate multiple of the previous one and had been already used in some of the first papers on TP matrices. However, in later papers such as [62] and [63], a better knowledge of the properties of Neville elimination was developed and permitted to improve many previous results on those matrices. Given a nonsingular matrix $A = (a_{ij})_{1 \leq i, j \leq n}$, the *Neville elimination* (NE) procedure consists of $n - 1$ steps and leads to the following sequence of matrices:

$$(8) \quad A =: A^{(1)} \rightarrow \tilde{A}^{(1)} \rightarrow A^{(2)} \rightarrow \tilde{A}^{(2)} \rightarrow \dots \rightarrow A^{(n)} = \tilde{A}^{(n)} = U,$$

where U is an upper triangular matrix. The matrix $\tilde{A}^{(k)} = (\tilde{a}_{ij}^{(k)})_{1 \leq i, j \leq n}$ is obtained from the matrix $A^{(k)} = (a_{ij}^{(k)})_{1 \leq i, j \leq n}$ by a row permutation that moves to the bottom the rows with a zero entry in column k below the main diagonal. For nonsingular TP matrices, it is always possible to perform NE without row exchanges (see [62]). If a row permutation is not necessary at the k -th step, we have that $\tilde{A}^{(k)} = A^{(k)}$. The entries of $A^{(k+1)} = (a_{ij}^{(k+1)})_{1 \leq i, j \leq n}$ can be obtained from $\tilde{A}^{(k)} = (\tilde{a}_{ij}^{(k)})_{1 \leq i, j \leq n}$ using the formula:

$$(9) \quad a_{ij}^{(k+1)} = \begin{cases} \tilde{a}_{ij}^{(k)} - \frac{\tilde{a}_{ik}^{(k)}}{\tilde{a}_{i-1,k}^{(k)}} \tilde{a}_{i-1,j}^{(k)}, & \text{if } k \leq j < i \leq n \text{ and } \tilde{a}_{i-1,k}^{(k)} \neq 0, \\ \tilde{a}_{ij}^{(k)}, & \text{otherwise,} \end{cases}$$

for $k = 1, \dots, n - 1$. The (i, j) *pivot* of the NE of A is given by

$$p_{ij} = \tilde{a}_{ij}^{(j)}, \quad 1 \leq j \leq i \leq n.$$

If $i = j$ we say that p_{ii} is a *diagonal pivot*. The (i, j) *multiplier* of the NE of A , with $1 \leq j \leq i \leq n$, is defined as

$$m_{ij} = \begin{cases} \frac{\tilde{a}_{ij}^{(j)}}{\tilde{a}_{i-1,j}^{(j)}} = \frac{p_{ij}}{p_{i-1,j}}, & \text{if } \tilde{a}_{i-1,j}^{(j)} \neq 0, \\ 0, & \text{if } \tilde{a}_{i-1,j}^{(j)} = 0. \end{cases}$$

The multipliers satisfy that

$$m_{ij} = 0 \Rightarrow m_{hj} = 0 \quad \forall h > i.$$

Pivots and multipliers of the NE of A and A^T characterize nonsingular TP and STP matrices, as the following result shows. It follows from theorems 4.1 and 4.2 of [63] and p. 116 of [63].

Theorem 5.1 *A matrix A is nonsingular TP (STP, respectively) if and only if the NE of A and A^T can be performed without row exchanges, all the multipliers of the NE of A and A^T are nonnegative (positive, respectively) and all the diagonal pivots of the NE of A are positive.*

for all $i \in \{1, \dots, n-1\}$. If, in addition, the entries m_{ij} and \tilde{m}_{ij} satisfy

$$(13) \quad \begin{aligned} m_{ij} = 0 &\Rightarrow m_{hj} = 0 \quad \forall h > i, \\ \tilde{m}_{ij} = 0 &\Rightarrow \tilde{m}_{hj} = 0 \quad \forall h > i, \end{aligned}$$

then the decomposition is unique.

In the bidiagonal decomposition given by (10), (11) and (12), the entries m_{ij} and p_{ii} are the multipliers and diagonal pivots, respectively, corresponding to the NE of A (see Theorem 4.2 of [63] and the comment below it) and the entries \tilde{m}_{ij} are the multipliers of the NE of A^T (see p. 116 of [63]). In [76] the following matrix notation $\mathcal{BD}(A)$ was introduced to represent the bidiagonal decomposition of a nonsingular TP matrix

$$(14) \quad (\mathcal{BD}(A))_{ij} = \begin{cases} m_{ij}, & \text{if } i > j, \\ \tilde{m}_{ji}, & \text{if } i < j, \\ p_{ii}, & \text{if } i = j. \end{cases}$$

In the particular case that the nonsingular $n \times n$ TP matrix A is also stochastic (the entries of every row sum up to 1), the bidiagonal factorization of A can be transformed into a bidiagonal factorization of $n-1$ lower triangular bidiagonal stochastic matrices and $n-1$ upper triangular bidiagonal stochastic matrices. This idea had been used in important applications of several fields. For instance, through this factorization Frydman and Singer ([54], Theorem 1) showed that the class of transition matrices for the finite state time-inhomogeneous birth and death processes coincides with the class of nonsingular stochastic TP matrices. The fact that those transition matrices for birth and death processes are all stochastic TP had already been pointed out in by Karlin and Mc Gregor (see [73] and [74]) with probabilistic arguments. All these results have been surveyed in 1986 by G. Goodman [64], who extended them to compound matrices, that is, matrices whose elements are the values of the minors of a certain order m of a given matrix A . On the other hand, factorizations of stochastic TP matrices as product of bidiagonal stochastic TP matrices are also important in the field of Computer Aided Geometric Design (CAGD). In fact, the main family of algorithms used in this field, called corner cutting algorithms, can be represented in this way. In [66], Goodman and Micchelli showed, again through the mentioned factorization of stochastic TP matrices, that the existence of a corner cutting algorithm transforming a control polygon of a curve into another one with the same number of

vertices was equivalent to the fact that both polygons were related by a nonsingular stochastic TP matrix.

More recently, the bidiagonal factorization has been used to compute accurately with these matrices (see [75, 76]). In fact, if we have the $\mathcal{BD}(A)$ of a nonsingular TP matrix with HRA, then we can perform many computations of A with HRA, such as computing its inverse or computing its eigenvalues or its singular values (cf. [76, 77]). There are some subclasses of nonsingular TP matrices for which this factorization can be obtained to HRA, and so, the computations mentioned previously can be also performed with HRA. For instance, for Vandermonde positive matrices [47], for Cauchy-Vandermonde positive matrices [93], arising in rational interpolation and that include the famous example of ill-conditioned matrices given by Hilbert matrices, or for Schoenmakers-Coffey matrices [33], arising in Finance. From now on, we shall illustrate other subclasses of TP matrices for which the $\mathcal{BD}(A)$ can be computed with HRA or for which we can perform computations with HRA.

5.1 Bidiagonal decomposition and HRA with Pascal matrices

A *Pascal matrix* of order n is the symmetric matrix

$$(15) \quad P = (p_{ij})_{1 \leq i, j \leq n}; \quad p_{ij} := \binom{i+j-2}{j-1}.$$

Pascal matrices have a long history (cf. [1, 49, 83]) and arise in important applications in filter design and image and signal processing (cf. [49]), as well as in probability, combinatorics, numerical analysis and electrical engineering (cf. [13]), among other fields.

Conditioning and the bidiagonal factorization of Pascal matrices was analyzed in [4] (see also [76]). The $\mathcal{BD}(P)$ can be obviously computed with HRA because it is extremely simple:

$$\mathcal{BD}(P) = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & \cdots & 1 \end{pmatrix}.$$

5.2 Bidiagonal decomposition and HRA with rational Bernstein-Vandermonde and related matrices

A collocation matrix of the Bernstein basis (1) is called a *Bernstein-Vandermonde matrix*. The bidiagonal factorization and computations with HRA of Bernstein-

Vandermonde matrices were obtained in [91]. The Said-Ball basis is another interesting basis used in CAGD and their collocation matrices are called Said-Ball-Vandermonde matrices. Their bidiagonal factorization and computations with HRA were obtained in [92]. Now we shall consider the corresponding rational bases and matrices, whose bidiagonal factorizations and computations with HRA were considered in [39].

Given a basis $u = (u_0^n, \dots, u_n^n)$ of nonnegative functions on $[a, b]$ and a sequence of strictly positive weights $(w_i)_{i=0}^n$, we can construct a rational basis $r = (r_0^n, \dots, r_n^n)$ defined by

$$(16) \quad r_i^n(t) = \frac{w_i u_i^n(t)}{W(t)}, \quad t \in [a, b], \quad i \in \{0, 1, \dots, n\},$$

where $W(t) = \sum_{j=0}^n w_j u_j^n(t)$. If the initial basis u is the Bernstein basis, then the corresponding rational basis r is called the *rational Bernstein basis*. In CAGD, the usual representation of a polynomial curve is the so called Bernstein-Bézier form, that is, these curves are expressed in terms of the Bernstein basis (1). The Bernstein basis is a rational Bernstein basis with all weights equal to 1: $w_i = 1$ for all $i = 0, \dots, n$. Bidiagonal decompositions and computations with HRA have been also obtained for other bases used in CAGD and closely related with the Bernstein basis. For instance, for the q -Bernstein basis [41], for the Lupaş basis [43] or the Bernstein-like bases (which are normalized B-bases, see Section 3) of the spaces mixing algebraic, trigonometric and hyperbolic polynomials [89].

The corresponding square collocation matrices of the rational Bernstein basis at a sequence of parameters $0 < t_0 < t_1 < \dots < t_n < 1$, given by $(r_j^n(t_i))_{0 \leq i, j \leq n}$, where functions r_i^n are given by (16) with $u_i^n = b_i^n$ for $i = 0, 1, \dots, n$, will be called *rational Bernstein-Vandermonde* (RBV) matrices.

In [39], the HRA calculations with RBV matrices through their bidiagonal decompositions and those of their inverses in terms of the diagonal pivots and multipliers of their Neville elimination and the multipliers of the Neville elimination of their transposes were obtained. We now recall the bidiagonal decomposition of a RBV matrix.

Theorem 5.3 *Let $A = (w_j b_j^n(t_i)/W(t_i))_{0 \leq i, j \leq n}$ be a RBV matrix whose nodes satisfy $0 < t_0 < t_1 < \dots < t_n < 1$. Then A admits a factorization of the form*

$$(17) \quad A = \bar{F}_n \bar{F}_{n-1} \cdots \bar{F}_1 D \bar{G}_1 \cdots \bar{G}_n,$$

following recurrence relation

$$(22) \quad JS_n^{(j)}(z) = JS_{n-1}^{(j-1)}(z) + j(j+z)JS_{n-1}^{(j)}(z) \quad (n, j \geq 1),$$

$$(23) \quad JS_n^{(0)}(z) = JS_0^{(j)}(z) = 0, \quad JS_0^{(0)}(z) = 1.$$

Again, the Jacobi-Stirling numbers $Jc_n^{(j)}(z)$ of the first kind only depend on the parameter $z = \alpha + \beta + 1$ and satisfy the following recurrence relation

$$(24) \quad Jc_n^{(j)}(z) = Jc_{n-1}^{(j-1)}(z) + (n-1)(n-1+z)Jc_{n-1}^{(j)}(z) \quad (n, j \geq 1),$$

$$(25) \quad Jc_n^{(0)}(z) = Jc_0^{(j)}(z) = 0, \quad Jc_0^{(0)}(z) = 1.$$

The Jacobi-Stirling numbers $Jc_n^{(j)}(z)$ of the first kind are a generalization of the Legendre-Stirling numbers because for $z = 1$ we obtain the Legendre-Stirling numbers.

In Theorem 4.2 of [96] the Jacobi-Stirling numbers of the second kind $JS_n^{(j)}$ were defined via the following expansion of the n -th composite power of $I_{\alpha,\beta}[y](t)$:

$$(1-t)^\alpha(1+t)^\beta I_{\alpha,\beta}[y](t) = \sum_{j=0}^n (-1)^j (JS_n^{(j)}(\alpha + \beta + 1)(1-t)^{\alpha+j}(1+t)^{\beta+j} y^{(j)}(t))^{(k)},$$

where $I_{\alpha,\beta}[y](t)$ is the Jacobi differential operator (21).

The Jacobi-Stirling numbers $JS_n^{(j)}(z)$ of the second kind satisfy

$$x^n = \sum_{j=0}^n JS_n^{(j)}(z) \langle x \rangle_j(z) \quad (n \in \mathbf{N}),$$

where

$$\langle x \rangle_j(z) := \prod_{i=0}^{j-1} (x - i(i+z))$$

for all $j \geq 1$ and $\langle x \rangle_0(z) := 1$. The (unsigned) Jacobi-Stirling numbers of the first kind $Jc_n^{(j)}(z)$ are defined via

$$\langle x \rangle_n(z) = \sum_{j=0}^n (-1)^{n+j} Jc_n^{(j)}(z) x^j \quad (n \in \mathbf{N}).$$

Here we consider the infinite matrices $JS(z) = (JS_i^{(j)}(z))_{i,j \geq 0}$ and $Jc(z) = (Jc_i^{(j)}(z))_{i,j \geq 0}$ and their corresponding truncated matrices given by the formulas $JS_n(z) = (JS_i^{(j)}(z))_{0 \leq i,j \leq n-1}$ and $Jc_n(z) = (Jc_i^{(j)}(z))_{0 \leq i,j \leq n-1}$ formed by the Jacobi-Stirling numbers of the first and second kind, respectively. In [40], the HRA calculation of singular values and inverses of the matrices $JS_n(z)$ and $Jc_n(z)$ was presented through their bidiagonal decomposition.

The following result is a consequence of Proposition 4 of [96] and states the bidiagonal decomposition of the matrices $JS_n(z)$.

Theorem 5.4 *The Jacobi-Stirling matrix $JS_n(z)$, $n \in \mathbf{N}$, admits a factorization of the form*

$$(26) \quad JS_n(z) = \overline{G}_1^2 \cdots \overline{G}_{n-1}^2,$$

where \overline{G}_i^2 , $i \in \{1, \dots, n-1\}$, are the $n \times n$ upper bidiagonal triangular matrices given by

$$(27) \quad \overline{G}_i^2 = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ & \ddots & \ddots & & & & & & \vdots \\ & & 1 & 0 & & & & & \vdots \\ & & & 1 & m_{i+1,1} & & & & \vdots \\ & & & & 1 & m_{i+2,2} & & & \vdots \\ & & & & & \ddots & \ddots & & 0 \\ & & & & & & & 1 & m_{n,n-i} \\ & & & & & & & & 1 \end{pmatrix},$$

where $m_{ij} = j(z+j)$ for $1 \leq j < i \leq n$.

The next result is also a consequence of Proposition 4 of [96] and provides the bidiagonal decomposition of the matrices $Jc_n(z)$.

Theorem 5.5 *The Jacobi-Stirling matrix $Jc_n(z)$, $n \in \mathbf{N}$, admits a factorization of the form*

$$(28) \quad Jc_n(z) = \overline{G}_1^1 \cdots \overline{G}_{n-1}^1,$$

where \overline{G}_i^1 , $i \in \{1, \dots, n-1\}$, are the $n \times n$ upper bidiagonal triangular matrices given by

$$(29) \quad \overline{G}_i^1 = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ & \ddots & \ddots & & & & & & \vdots \\ & & 1 & 0 & & & & & \vdots \\ & & & 1 & \overline{m}_{i+1,1} & & & & \vdots \\ & & & & 1 & \overline{m}_{i+2,2} & & & \vdots \\ & & & & & \ddots & \ddots & & 0 \\ & & & & & & & 1 & \overline{m}_{n,n-i} \\ & & & & & & & & 1 \end{pmatrix},$$

where $\overline{m}_{ij} = (i-j)(z+i-j)$ for all $1 \leq j < i \leq n$.

5.4 HRA with Laguerre matrices and Lah numbers

Laguerre polynomials form a classical family of orthogonal polynomials (cf. [11]) and present many applications. For instance, they are used for Gaussian quadrature to numerically compute integrals. The larger family of generalized Laguerre polynomials presents important applications in quantum mechanics (see [78]). For $\alpha > -1$, the generalized Laguerre polynomials are given by

$$(30) \quad L_n^{(\alpha)}(t) = \sum_{k=0}^n (-1)^k \binom{n+\alpha}{n-k} \frac{t^k}{k!}, \quad n = 0, 1, 2, \dots$$

and they are orthogonal polynomials on $[0, \infty)$ with respect to the weight function $x^\alpha e^{-x}$.

Given a real number x and a positive integer k , let us denote the corresponding *falling factorial* by

$$x^{(k)} := x(x-1)(x-2) \cdots (x-k+1).$$

Let us also denote $x^{(0)} := 1$. Let $M := \left(L_{j-1}^{(\alpha)}(t_{i-1}) \right)_{1 \leq i, j \leq n+1}$ be the collocation matrix of the generalized Laguerre polynomials at $(0 >) t_0 > t_1 > \dots > t_n$, let P_U be the $(n+1) \times (n+1)$ upper triangular Pascal matrix with $\binom{j-1}{i-1}$ as its (i, j) -entry for $j \geq i$ and let S_α and J be the $(n+1) \times (n+1)$ diagonal matrices:

$$(31) \quad S_\alpha := \text{diag} \left((\alpha + i)^i \right)_{0 \leq i \leq n}, \quad J := \text{diag} \left((-1)^i \right)_{0 \leq i \leq n}.$$

The following result, corresponding to Theorem 2 of [31], assures that, given the parameters $(0 >) t_0 > t_1 > \dots > t_n$, many algebraic computations with these collocation matrices M can be performed with HRA, as well as the strict total positivity and a particular factorization of these matrices.

Theorem 5.6 *Let $M := \left(L_{j-1}^{(\alpha)}(t_{i-1}) \right)_{1 \leq i, j \leq n+1}$ for $(0 >) t_0 > t_1 > \dots > t_n$ with $\alpha > -1$, let P_U be the $(n+1) \times (n+1)$ upper triangular Pascal matrix, let S_α and J be the $(n+1) \times (n+1)$ diagonal matrices given by (31) and let $V := \left(t_{i-1}^{j-1} \right)_{1 \leq i, j \leq n+1}$. Then $M = VJS_\alpha^{-1}P_US_0^{-1}S_\alpha$ is an STP matrix and, given the parametrization t_i ($0 \leq i \leq n$), the following computations can be performed with HRA: all the eigenvalues, all the singular values and the inverse of M , as well as the solution of the linear systems $Mx = b$, where $b = (b_0, \dots, b_n)^T$ has alternating signs.*

The particular case $\alpha = 0$ corresponds to the classical Laguerre polynomials. Extending (30) to the case $\alpha = -1$, it was obtained in [31] an analogous result to

Theorem 5.6 for the particular set of polynomials:

$$L_0^{(-1)}(t) = 1, \quad L_n^{(-1)}(t) = \sum_{k=1}^n (-1)^k \binom{n-1}{n-k} \frac{t^k}{k!}, \quad n = 1, 2, \dots,$$

The interest of these polynomials arises from the close relationship between their coefficients and the unsigned Lah numbers (cf. [14]), and which will be described below:

$$L_n^{(-1)}(t) = \frac{1}{n!} \sum_{k=1}^n (-1)^k L(n, k) t^k \text{ for } n \geq 1$$

with $L(n, k) := \binom{n-1}{k-1} \frac{n!}{k!}, k \leq n.$

The unsigned Lah numbers $L(n, k)$ are included as the sequence A105278 in the Online Encyclopedia of Integer Sequences (OEIS). The Lah numbers were introduced by Ivo Lah in 1955 (see [80]) and arise in applications such as combinatorics and analysis (see pages 44–45 of [113]).

5.5 HRA with Bessel matrices

Bessel polynomials arise in many fields such as partial differential equations, number theory, algebra and statistics (see [69]). They form an orthogonal sequence of polynomials and are related to the modified Bessel function of the second kind (cf. pp. 7 and 34 of [69]). They are also closely related to the reverse Bessel polynomials, with many applications in Electrical Engineering, in network analysis of electrical circuits (cf page 145 of [69]). The coefficients of the reverse Bessel polynomials are also known, in Combinatorics, as signless Bessel numbers of the first kind. The Bessel numbers are also closely related to the Stirling numbers [70, 116]. Bessel polynomials also occur naturally in the theory of traveling spherical waves (cf. [79]) and are very important for some problems of static potentials, signal processing and electronics. The zeros of Bessel polynomials and generalized Bessel polynomials also play a crucial role in applications in Electrical Engineering and are related with the length of the parameter domain where cycloidal spaces admit shape preserving representations ([22]).

Let us recall that the *Bessel polynomials* are defined by

$$(32) \quad B_n(x) = \sum_{k=0}^n \frac{(n+k)!}{2^k (n-k)! k!} x^k, \quad n = 0, 1, 2, \dots$$

Given a real positive integer n , let us define the corresponding *semifactorial* by

$$n!! = \prod_{k=0}^{\lfloor n/2 \rfloor - 1} (n - 2k).$$

Let $A = (a_{ij})_{1 \leq i, j \leq n}$ be the lower triangular matrix such that

$$(33) \quad (B_0(x), B_1(x), \dots, B_{n-1}(x))^T = A(1, x, \dots, x^{n-1})^T,$$

that is, the lower triangular matrix A is defined by

$$(34) \quad a_{ij} := \begin{cases} \frac{(i+j-2)!}{2^{j-1}(i-j)!(j-1)!} = \frac{(2j-2)!}{2^{j-1}(j-1)!} \binom{i+j-2}{i-j}, & \text{if } i \geq j, \\ 0, & \text{if } i < j. \end{cases}$$

We now recall Theorem 3 of [32], which proves the total positivity of A , and provides $\mathcal{BD}(A)$.

Theorem 5.7 *Let $A = (a_{ij})_{1 \leq i, j \leq n}$ be the lower triangular matrix in (33) defined by (34). Then we have that*

(i) *the pivots of the NE of A are given by*

$$(35) \quad p_{ij} = \frac{1}{2^{j-1}} \frac{(i-1)!}{(i-j)!} \prod_{r=1}^{j-1} \frac{(2i-r-1)}{(i-j+r)}, \quad 1 \leq j \leq i \leq n,$$

and the multipliers by

$$(36) \quad m_{ij} = \frac{(2i-2)(2i-3)}{(2i-j-1)(2i-j-2)}, \quad 1 \leq j < i \leq n,$$

(ii) *A is a nonsingular TP matrix*

(iii) *and the bidiagonal factorization of A is given by*

$$(37) \quad \mathcal{BD}(A)_{ij} = \begin{cases} \frac{(2i-2)(2i-3)}{(2i-j-1)(2i-j-2)}, & \text{if } i > j, \\ 1, & \text{if } i = j = 1, \\ (2i-3)!!, & \text{if } i = j > 1, \\ 0, & \text{if } i < j, \end{cases}$$

and can be computed to HRA.

Let us now introduce the collocation matrices of the Bessel polynomials. Given a sequence of parameters $0 < t_0 < t_1 < \dots < t_{n-1}$, we call the collocation matrix of the Bessel polynomials (B_0, \dots, B_{n-1}) at this sequence of parameters,

$$M = M \begin{pmatrix} B_0, \dots, B_{n-1} \\ t_0, \dots, t_{n-1} \end{pmatrix} = (B_{j-1}(t_{i-1}))_{1 \leq i, j \leq n},$$

a *Bessel matrix*.

The following result corresponds to Theorem 4 of [32] and shows that the Bessel matrices are STP and that some usual algebraic problems with these matrices can be solved to HRA.

Theorem 5.8 *Given a sequence of parameters $0 < t_0 < t_1 < \dots < t_{n-1}$, the corresponding Bessel matrix M is an STP matrix and given the parametrization t_i ($0 \leq i \leq n-1$), the following computations can be performed with HRA: all the eigenvalues, all the singular values, the inverse of the Bessel matrix M , and the solution of the linear systems $Mx = b$, where $b = (b_1, \dots, b_n)^T$ has alternating signs.*

By reversing the order of the coefficients of $B_n(x)$ in (32), we can introduce the reverse Bessel polynomials:

$$(38) \quad B_n^r(x) = \sum_{k=0}^n \frac{(n+k)!}{2^k(n-k)!k!} x^{n-k}, \quad n = 0, 1, 2, \dots,$$

Given a sequence of parameters $0 < t_0 < t_1 < \dots < t_{n-1}$ we call the collocation matrix of the reverse Bessel polynomials $(B_0^r, \dots, B_{n-1}^r)$ at that sequence,

$$M_r = M \begin{pmatrix} B_0^r, \dots, B_{n-1}^r \\ t_0, \dots, t_{n-1} \end{pmatrix} = (B_{j-1}^r(t_{i-1}))_{1 \leq i, j \leq n}$$

a reverse Bessel matrix.

The following result, which corresponds to Theorem 6 of [32], shows that the reverse Bessel matrices are STP and that some usual algebraic problems with these matrices can be solved to HRA.

Theorem 5.9 *Given a sequence of parameters $0 < t_0 < t_1 < \dots < t_{n-1}$, the corresponding reverse Bessel matrix M_r is an STP matrix and given the parametrization t_i ($0 \leq i \leq n-1$), the following computations can be performed with HRA: all the eigenvalues, all the singular values, the inverse of the reverse Bessel matrix M_r , and the solution of the linear systems $M_r x = b$, where $b = (b_1, \dots, b_n)^T$ has alternating signs.*

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Light-matter interaction in the nonperturbative regime: a lecture

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Abstract

Quantum electrodynamics (QED) is the understanding of how light and matter interact. In this lecture, I give an overview of the non-relativistic limit of the theory, which is the foundation of quantum optics. I introduce cavity and waveguide QED and explain its role in the construction of a quantum computer. Finally, I review the many-body physics emerging when light and matter interact beyond the perturbative regime. The lecture is focused on the theoretical tools typically used.

1 Introduction

Because of its extreme complexity, most physicists will be glad to see the end of QED.

P. A. M. Dirac, 1937.

Light and matter interact. Attracted by the Earth's magnetic field, charged particles pass through the atmosphere, ionising it and triggering the emission of visible light. This form the auroras and it is beautiful consequence of that interaction. Other examples are lasers, the scattering of an electron and positron in two muons, the functioning of a quantum computer or, in a healthy eye, the photodetection that allows to read this manuscript. These dissimilar phenomena are understood within the theory of quantum electrodynamics and is *perhaps the best fundamental physical theory that we have*¹.

¹Here, I steal the words of Peskin and Schroeder in their popular book *An Introduction to Quantum Field Theory*.

In this manuscript, I will review the theory and its nonrelativistic limit, which is the basis of quantum optics. Then, I will discuss selected topics on quantum optics and the many-body phenomena occurring because of this interaction. I will spend some time to explain different theoretical tools used to do the calculations. To fit the lecture in a reasonable extension, I will focus on the strongly correlated phenomena occurring when the interaction enters into the nonperturbative regime.

1.1 The interaction (in a tiny nutshell)

Here, I will follow the excellent explanations of Nolting & Ramakanth [50, Sects. 2.2 and 2.3] and Snoko [74, Sect. 10.9] and the standard treatises of Peskin & Schroeder [54] and Tong [71].

In the modern viewpoint, *gauge invariance* is promoted to a general principle [28]. A gauge transformation is:

$$(1) \quad A'_\mu(x) = A_\mu(x) - \frac{1}{e} \partial_\mu \lambda(x),$$

for the potential vector, $A_\mu = (\phi, \mathbf{A})$. Here, $\partial_\mu = (\frac{1}{c} \partial_t, \nabla)$ and $x_\mu = (ct, -\mathbf{x})$, e is the charge of an electron and c is the speed of light in vacuum. Besides, the wave function transforms as,

$$(2) \quad \psi'(x) = \psi(x) \exp[ie\lambda/\hbar c]$$

It turns out that the transformations (1) and (2) fix the interaction between light and matter. In particular, the *Dirac equation* for an electron, of mass m_e interacting with the electromagnetic field is

$$(3) \quad (i\hbar \not{D} - m_e c) \psi(x) = 0$$

Here, we use the field theoretical notation $\not{D} \equiv \partial_\mu + ieA_\mu(x)$, which makes explicit the gauge invariance of the Dirac equation. Notice that $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ is a four-component spinor. The Dirac equation is really famous. It was invented to provide a relativistic version of the *Schrödinger equation*. It comes with the appearance of negative energy solutions which form the Dirac sea. In the non-relativistic limit, $v \ll c$ with v the the

particle velocity, two components of the solutions for (3) are small enough so the theory is effectively a two-component one. In this limit, the theory reduces to the *Pauli Hamiltonian*:

$$(4) \quad H = \frac{1}{2m_e}(\mathbf{p} + e\mathbf{A})^2 - e\phi + \frac{\mu_B}{\hbar}\boldsymbol{\sigma} \cdot \mathbf{B} .$$

Here, we have introduced the Bohr magneton $\mu_B = e\hbar/2m_e$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices² and $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic field. It is difficult to exaggerate the importance of the Hamiltonian (4). It is the starting point of every quantum optics book. It is *the* light-matter Hamiltonian. Due to its relevance, it deserves to appreciate the way it was found. Notice that only gauge and Lorentz invariance (Dirac equation) and the nonrelativistic limit was used. Grounded in such a general laws, in its validity we trust.

1.2 Light Quantization

The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.

Sidney Coleman.

Gauge invariance fixes the interaction form [cf. Eqs. (3) and (4)] and introduces a redundancy. The piece of reality that emerges from gauge invariance is that the phase space is enlarged, foliated by gauge orbits. Every point in the orbit must be reached by a gauge transform. Then, in our calculation, we pick one point from each orbit. Obviously, the output of the calculation must be independent of this choice. Picking a point in each orbit means to fix the gauge. Important examples are the Lorentz, Coulomb or dipole gauges. In particular, here we are interested in quantizing the EM field in (4). In this way we treat on equal footing both matter and light. In the quantization, it is convenient to choose the Coulomb gauge,

$$\nabla \cdot \mathbf{A} = 0 .$$

²The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In doing so, we have only the transversal component of the field.

The details of quantization would occupy a regular sized book, so I will just sketch the idea and I will argue how the result is reasonable. In other words, I am going to summarise the Cohen-Tannoudji, Dupont-Roc and Gryberg book [12] in a single paragraph. In these books the quantization is rigorously done by identifying the action in terms of the fields (at the classical level). Then, the canonical variables are found. Finally, they tackle the quantization program. Here, however, I will take a non-rigorous shortcut and quantize arguing why the electromagnetic field is a collection of harmonic oscillators (photons) and that \mathbf{A} (and \mathbf{B} and \mathbf{E}) are linear combinations of creation-annihilation operators. In the Coulomb gauge, the equation for \mathbf{A} is the wave equation $\partial_\mu \partial^\mu \mathbf{A} = 0$, which is solved via separation of variables with the *ansatz*, $\mathbf{A} = \sum_l q_l(t) \mathbf{u}_l(\mathbf{r})$ with $\mathbf{u}_l(\mathbf{r})$ orthogonal functions (in free space they are Fourier series). Using the Maxwell equations, $\mathbf{E} = -\partial_t \mathbf{A}$ and $\mathbf{B} = \nabla \times \mathbf{A}$ we express the electromagnetic (EM) fields in terms of dimensionless time-functions q_k, \dot{q}_k . Introducing these expressions in the EM-energy, $U_{\text{EM}} = \int dV \epsilon_0 \mathbf{E}^2(\mathbf{r})/2 + \mu_0 \mathbf{B}^2(\mathbf{r})/2$, we arrive to [64]

$$(5) \quad U_{\text{EM}} = \hbar \sum_k \frac{1}{2} \dot{q}_k^2 + \frac{1}{2} \omega_k^2 q_k^2,$$

where $\omega_k = c|\mathbf{k}_k|$ is the solution of the Helmholtz equation $-\nabla^2 \mathbf{u}_k = \mathbf{k}_k^2 \mathbf{u}_k$. Identifying $\dot{q}_k \sim p_k$ (p_k is the momentum) the above is nothing but the Hamiltonian of uncoupled harmonic oscillators. Introducing the creation operator $a_k^\dagger = \frac{1}{\sqrt{2\hbar\omega_k}}(\omega_k q_k + ip_k)$ and the Hermitean conjugate annihilation operators, a_k , we arrive to the quantum Hamiltonian for the EM:

$$(6) \quad H_{\text{EM}} = \sum_l \omega_k a_k^\dagger a_k,$$

and the corresponding expressions for the fields \mathbf{A} , \mathbf{B} and \mathbf{E} :

$$(7) \quad \mathbf{A} = \sum_l \sqrt{\frac{\hbar}{2\epsilon_0 V_k \omega_k}} \mathbf{u}_k (a_k + a_k^\dagger),$$

$$(8) \quad \mathbf{B} = \sum_k \sqrt{\frac{\hbar}{2\epsilon_0 V_k \omega_k}} \nabla \times \mathbf{u}_k (a_k + a_k^\dagger),$$

$$(9) \quad \mathbf{E} = \sum_k \sqrt{\frac{\hbar \omega_k}{2\epsilon_0 V_k \omega_k}} \mathbf{u}_k i(a_k - a_k^\dagger).$$

A final word of caution. The quantum operators have been derived in the *Coulomb gauge*. Therefore, the quantum version of (4) with (7) must be named with the surname *in the Coulomb gauge*. Obviously, we can always change of gauge by the corresponding unitary transformation. We will come to this point later. For a general discussion see [12, Chap. IV].

1.3 What is Quantum Optics?

The quantum vacuum is not empty
Anonymous.

Quantum optics deal with the simplest objects: few level systems and photons. In particular, quantum optics *is* the entanglement of light and matter. The most basic phenomenon, the emission of light (with is certainly important for life and electrical companies) is a manifestation of entanglement and, in addition, an elementary example of particle creation from a field theoretical point of view. In simple words, light emission occurs when an atom changes from one state to another and, then, emits a photon. Let me describe the experimental fact and we will see how the light-matter entanglement builds up in the emission.

Consider a spinless neutral atom, e.g. strontium or helium. Therefore, the Zeeman coupling, the last term in (4), does not play any role. For further convenience, we write the rest of the Hamiltonian in the dipole gauge. This is done with the Power–Zienau–Woolley unitary transformation yielding [12]

$$(10) \quad H^{(D)} = H_{\text{EM}} + H_{\text{atom}} + i\mathbf{d} \sum_l \sqrt{\frac{\hbar \omega_k}{2\epsilon_0}} u_k(\mathbf{r}_0) a_k^\dagger + \text{h.c.} .$$

Here \mathbf{d} is the atom dipole. Besides, to make our life even simpler I consider that only two states of the atom are relevant in the dynamics. Thus, the atom is projected in a two level system (2LS) with energy difference Δ and a space spanned in the basis $\{|0\rangle, |1\rangle\}$ ³. Typically, the atomic states have a well defined parity. Since the dipole operator \mathbf{d} is an odd operator, its matrix elements are thus $\langle 0|\mathbf{d}|0\rangle = \langle 1|\mathbf{d}|1\rangle = 0$ and $\langle 0|\mathbf{d}|1\rangle = \langle 1|\mathbf{d}|0\rangle \equiv d$. So (10) can be rewritten (after the two level projection) as (from now on I will set $\hbar = 1$)

$$(11) \quad \mathcal{H}^{(D)} = \frac{\Delta}{2}\sigma^z + \sum_l \omega_l a_l^\dagger a_l + \sigma^x \sum_l c_l (a_l^\dagger + a_l) .$$

with $c_k = d\sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}u_k(\mathbf{r}_0)$, cf. Eq. (10). This is an important and familiar model for the coupling of a two level system (or qubit) with the electromagnetic field. It is also well known beyond the quantum optics community. It models impurity models in condensed matter and it is the paradigmatic model in open systems [41, 72].

Consider now that, driven via an external field, the atom is excited from the ground state,

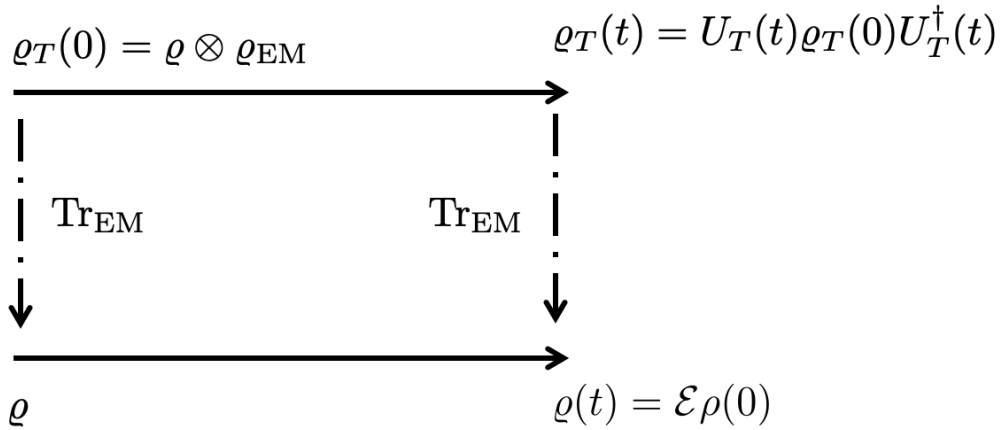


Figure 1: **Light-matter entanglement.** Given the state at $t = 0$ the system can be evolved with the total unitary operator $U_T = e^{-i\mathcal{H}^{(D)}t}$. If the observables act on the 2LS only trace over the EM-field is taken. Alternatively, we can take the trace at the beginning and find the non-unitary map \mathcal{E} .

$|0\rangle$, to the excited state $|1\rangle$ and that this driving is sufficiently fast to avoid correlations

³Through the rest of the manuscript I will restrict the discussion that the atoms can be model with two level systems (2LS). In the modern terminology they are named as qubits.

between the atom and field. Then, the density matrix at time t_0 can be written as $\varrho_T = |1\rangle\langle 1| \otimes \varrho_{\text{EM}}(t_0)$. $\varrho_{\text{EM}}(t_0)$ is the equilibrium density matrix for the electromagnetic field at a given temperature T . I will consider the case $T = 0$ ⁴. This initial density matrix may be evolved with the total Hamiltonian (11). Then, the time evolution of $P_e = \langle \sigma^+ \sigma^- \rangle$ can be computed. This way of computing is represented in the upper path in figure 1. Because P_e is a 2LS observable, an alternative is to find the map for the reduced density matrix $\varrho(t) = \mathcal{E}\varrho(0)$ in the space spanned by the two atomic relevant states $\{|0\rangle, |1\rangle\}$. This is the lower path indicated in the figure 1. During the time evolution some light-matter entanglement is built up, $\varrho(t)$ becomes a mixed state and the map cannot be unitary⁵. Let me sketch a simpler way of finding \mathcal{E} . I restrict myself to linear operators [24]. Adding an imaginary term in the energy, $P_e = e^{-i(\Delta - i\Gamma)t}$, is a phenomenological way of introducing dissipation. However, the corresponding equation $\dot{\varrho} = -i[\Delta/2\sigma^z, \varrho] - \{\Gamma/2\sigma^z, \varrho\} = -i[\Delta\sigma^+\sigma^-, \varrho] - \{\Gamma\sigma^+\sigma^-, \varrho\}$ does not conserve the trace, $\frac{d}{dt}\text{Tr}(\varrho) = -\Gamma\varrho_{11}$. This is unacceptable. Then, we realize that, apart from dissipation, fluctuations should be introduced (fluctuation-dissipation theorem). These are jumps that transform $|1\rangle \rightarrow |0\rangle$ with some rate Γ' . They are conveniently written as the transformation for ϱ : $\Gamma'\sigma^-\varrho\sigma^+$. It turns out that imposing $\text{Tr}(\dot{\varrho}) = 0$ yields $\Gamma' = \frac{1}{2}\Gamma$. Therefore, the differential form for the map \mathcal{E} is

$$(12) \quad \dot{\varrho} = -i[\Delta\sigma^+\sigma^-, \varrho] + \frac{\Gamma}{2}(\sigma^-\varrho\sigma^+ - \{\sigma^+\sigma^-, \varrho\})$$

This is a Lindblad-type master equation⁶. I argued that it provides a *bona fide* evolution, it was built ensuring all the density matrix properties. The only free parameter is the value for the spontaneous rate Γ . It is computed using the spin-boson model (11). Using

⁴Finite temperature can be done in a similar way.

⁵The exponential decay means that $\varrho_{11} = \exp(-\Gamma t)$ and $\varrho_{00} = 1 - \exp(-\Gamma t)$. Then, the purity ($\equiv \text{Tr}(\varrho^2)$) equals to $1 + 2\exp(-2\Gamma t) - 2\exp(-\Gamma t) < 1$.

⁶The equation was found independently by Lindblad and Kossakowski, Gorini and Sudarshan in 1976. However, following the well know rule that regardless of what most physicists do there is always a Russian paper which “did it first”. In 1969, Belavin, Zel’dovich, Perelomov and Popov found the Lindblad equation before Lindblad. Though unfair, I will use the standard notation and I will refer to (12) as the Lindblad equation.

perturbation theory the Fermi's golden rule is obtained:

$$(13) \quad \frac{\Gamma}{\Delta} = \frac{\Delta^2 d^2}{3\pi\epsilon_0 \hbar c^3} = \frac{4\alpha}{3} \frac{\Delta^2 r^2}{c^2} .$$

In the second equality I have introduced the fine-structure constant $\alpha = e^2/4\pi\epsilon_0\hbar c \cong 1/137$. The latter is a dimensionless combination of fundamental constants including the electron charge. It accounts for the coupling strength in electrodynamics. Besides, I have replaced the dipole $d = er$, with r being the inter-atomic distance. We can make $r \sim 10^{-10}m$ while the optical wavelength is of the order 10^7cm^{-1} , so $\Gamma/\Delta \sim 10^{-8}$. This is a rather small number saying that atoms and photons in free space are weakly coupled.

I have just sketched the most fundamental phenomenon in quantum optics. Let me enumerate another important examples that can be computed from (11) or more generally from (10) . In the interaction Hamiltonian the leading terms are $\sigma^- a_k + \text{h.c.}$, *i.e.* a one photon transition, thus 2LS are single photon emitters. Another, paradigmatic example is the amplification of the emission when a collection of atoms emit coherently. Consider N atoms place at the same point ⁷. In this case, the coupling is through the total spin operator, $\sum \sigma^x = \sqrt{N}J_x$. Thus, in the second part of Eq. (12) σ^\pm is replaced by $\sqrt{N}J^\pm$ and $\Gamma \rightarrow N\Gamma$, *i.e.* the emission is N -*enhanced*, this is nothing but *superradiance*. Finally, there is the Mollow triplet that occurs when an atom is driven with a sufficiently large intensity and the atom is dressed by the EM-field. For all of them, the ultimate responsibility is the light-matter entanglement.

2 Cavity and waveguide QED

In the early 1980's, reaching this situation, now called the strong coupling regime of cavity QED, became our Holy Grail.

Serge Haroche, 2012 (Nobel Prize lecture)

⁷This is a good approximation when the atom separations are smaller than the emitted light-wavelength

2.1 Cavity QED

In free space, when a photon is emitted it does so in an irreversible way. Eq. (12) generates an irreversible time evolution⁸. Therefore it is not possible to generate interactions in a *coherent* way, *i.e.* exchanging light and matter in a periodic fashion. The solution to both problems is to trap photons in a cavity. Naively speaking, the photon would travel back and forward inside the cavity enlarging the effective atomic cross section. Besides, if the atom is excited and emits a photon, this cannot escape and eventually is re-absorbed obtaining the desired periodic (or coherent) coupling. The setup of atoms interacting with cavity photons is known as cavity QED. The leaders of the first two groups that measured this coherent interaction, Haroche and Wineland, were awarded with the Nobel prize in 2012. In the following few lines I will explain the model for cavity QED and its main consequences.

A cavity is a box where the walls are made of mirrors. The finite volume of the cavity fixes the extension of the photon selecting its allowed wavelengths. You can think in a one cylindrical cavity with radial symmetry, see figure 2a). Then, the stationary waves have the frequencies $\omega_n = c\pi n/L$. The lowest frequency mode has $\omega_c = c\pi/L$ (it is named as the fundamental mode). It fits half of the wavelength, thus it is also known as the $\lambda/2$ -mode. If an atom is placed inside the cavity the light-matter coupling is given by (11) where the EM-frequencies are restricted to ω_n . The difference between two consecutive normal modes is $\omega_{n+1} - \omega_n = \omega_0$. Since the light-matter coupling is sufficiently weak, the 2LS is mainly coupled to the mode which is closest to the atom level spacing Δ . Therefore, we can single out one mode from (11) *e.g.* ω_0 , yielding the third Hamiltonian of this lecture, also quite important,

$$(14) \quad \mathcal{H}_{\text{qR}} = \frac{\Delta}{2}\sigma^z + \omega_c a^\dagger a + g\sigma^x(a + a^\dagger)$$

This equation is known as the quantum Rabi model. Here, the key parameter is the single photon-atom coupling $g/(\omega_c + \Delta)$. It determines how fast light and matter exchange excitations. Its importance in the physics of cavity QED deserves to estimate its value. In the single-mode approximation, the electric field inside the cavity can be written as $\mathbf{E}(\mathbf{r}) = \mathcal{E}(\mathbf{r})(a^\dagger + a)$, see Eq. (9). Therefore, $g = \mathbf{d} \cdot \mathcal{E}(\mathbf{r})$. Besides, $\langle \mathbf{0} | \mathbf{E}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) | \mathbf{0} \rangle = |\mathcal{E}(\mathbf{r})|^2$,

⁸Recall that it was built by adding two terms, one of them is an anti-hermitean operator, see the discussion above Eq. (12).

and the vacuum EM energy is $\langle \mathbf{0} | \int dV \epsilon_0 \mathbf{E}^2(\mathbf{r})/2 + \mu_0 \mathbf{B}^2(\mathbf{r})/2 | \mathbf{0} \rangle = \frac{1}{2} \hbar \omega_c$. To give numbers, like in the previous section, I assume a cylindrical cavity with radius R . The volume of integration is $V = \pi R^2 \lambda/2$, with λ the wavelength of the fundamental mode. Putting all together an upper bound for the coupling is found,

$$(15) \quad \frac{g}{\omega_c} \leq \frac{r}{R} \frac{2\alpha}{\pi}.$$

As in the spontaneous emission calculation (13), I took the dipole: $d = er$. Again, the interaction strength is bounded by the fine structure and the ratio between two magnitudes, the interatomic one r and the radial dimension of the cavity R . This bound is reasonable. The photon occupies the whole cavity so the interaction must depends on this ratio between lengths. Up to 2004, experiments confirmed that the coupling was rather small ($2c$). In this case, the Hamiltonian can be approximated by the so called Jaynes-Cummings model, obtained in perturbation theory up to terms $(g/\omega_c)^2$,

$$(16) \quad \mathcal{H}_{\text{qR}} \cong \mathcal{H}_{\text{JC}} = \frac{\Delta}{2} \sigma^z + \omega_c a^\dagger a + g(\sigma^+ a + \sigma^- a^\dagger).$$

In \mathcal{H}_{JC} there are not the counterrotating terms $\sigma^+ a^\dagger + \sigma^- a$, both of them create (annihilate) one photon and one atom excitation at the same time and they are irrelevant when $g/\omega_c \ll 1$. \mathcal{H}_{JC} is simpler to solve than \mathcal{H}_{qR} because $[\mathcal{H}_{\text{JC}}, N] = 0$, with $N = a^\dagger a + \sigma^+ \sigma^-$ being the number of excitations. The diagonalization is done in subspaces with fixed N . They are two dimensional: $\{|n0\rangle, |n-1, 1\rangle\}$, with $a^\dagger a |n\rangle = n |n\rangle$. Recall that $|0\rangle$ and $|1\rangle$ are the fundamental and first excited state of the 2LS respectively. Besides, the ground state is the trivial vacuum $|GS\rangle = |0; 0\rangle$. In particular, at resonance $\Delta = \omega_c$, the eigenvectors, conveniently labelled by the number of excitations are

$$(17) \quad |\psi_{n,\pm}\rangle = \frac{1}{\sqrt{2}} \left(|n1;\rangle \pm |n-1, 0\rangle \right),$$

with energies

$$(18) \quad E_{n,\pm} = n\omega_c \pm \sqrt{n}g.$$

Notice that these states are light-matter entangled states. In the literature they are called *polaritons*. Knowing the spectrum, the dynamics can be easily obtained. Consider as initial

condition that the atom is excited, $|\psi(0)\rangle = |0; 1\rangle$ then (this state overlaps equally with $|\psi_{1,\pm}\rangle$)

$$(19) \quad P_e = \text{Tr}_c(|1\rangle\langle 1| |\psi(t)\rangle\langle\psi(t)|) = \cos(2gt) .$$

These are the quantum Rabi oscillations. The frequency of the oscillations is given by $2g$.

Why was it so difficult to observe these oscillations? (the first experimental observation was achieved in 1992). The reason is that the cavity is not perfect and it has some leakage. In addition, the two level system can decay in other channels apart from the cavity photons. Both the leakage and the non-radiative channels can be modelled as a coupling to a continuum set of modes, see Appendix A and Eq. (12). The full dynamics, including these dissipative channels, is governed by a master equation of the form

$$(20) \quad \dot{\rho} = -i[\mathcal{H}_{\text{JC}}, \rho] - \kappa(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}) - \gamma(\sigma^- \rho \sigma^- - \frac{1}{2}\{\sigma^+ \sigma^-, \rho\}) ,$$

with κ and γ are decay rates. Solving the master equation, the Rabi oscillations decay on time,

$$(21) \quad P_e = e^{-(\kappa+\gamma)t} \cos\left(2\sqrt{g^2 - (\gamma - \kappa)^2/4}t\right) .$$

Therefore, for resolving the Rabi oscillations g must be greater the losses κ and γ . This is the *strong* coupling regime. Reaching this limit opens the possibility of doing quantum operations at the single photon limit and winning a Nobel prize.

In 2004, in Yale, instead atoms and cavities they used superconducting circuits, see figure 2d) [76] . The cavity used was a superconducting coplanar waveguide (CPW) and the atom was a charge qubit⁹. Circuits mimicking cavity QED are named circuit QED. The coupling measured was $g/\omega_c \sim 10^{-3}$, See 2c). The reason of such a sizeable coupling is that the CPW was essentially one-dimensional (reducing the cavity volume) and that the artificial atom was huge, few microns-size. Thus, lengths in (15) approach each other.

In 2010, in the Walther Meissner Institut, a new milestone occur. A coupling $g/\omega_c \cong 0.1$ was reached by increasing the cross talk between the superconducting circuit (in this case it

⁹Superconductors are used to minimise losses and to use Josephson junctions for having nonlinearities [15]. All of these circuits operate in the microwave regime.

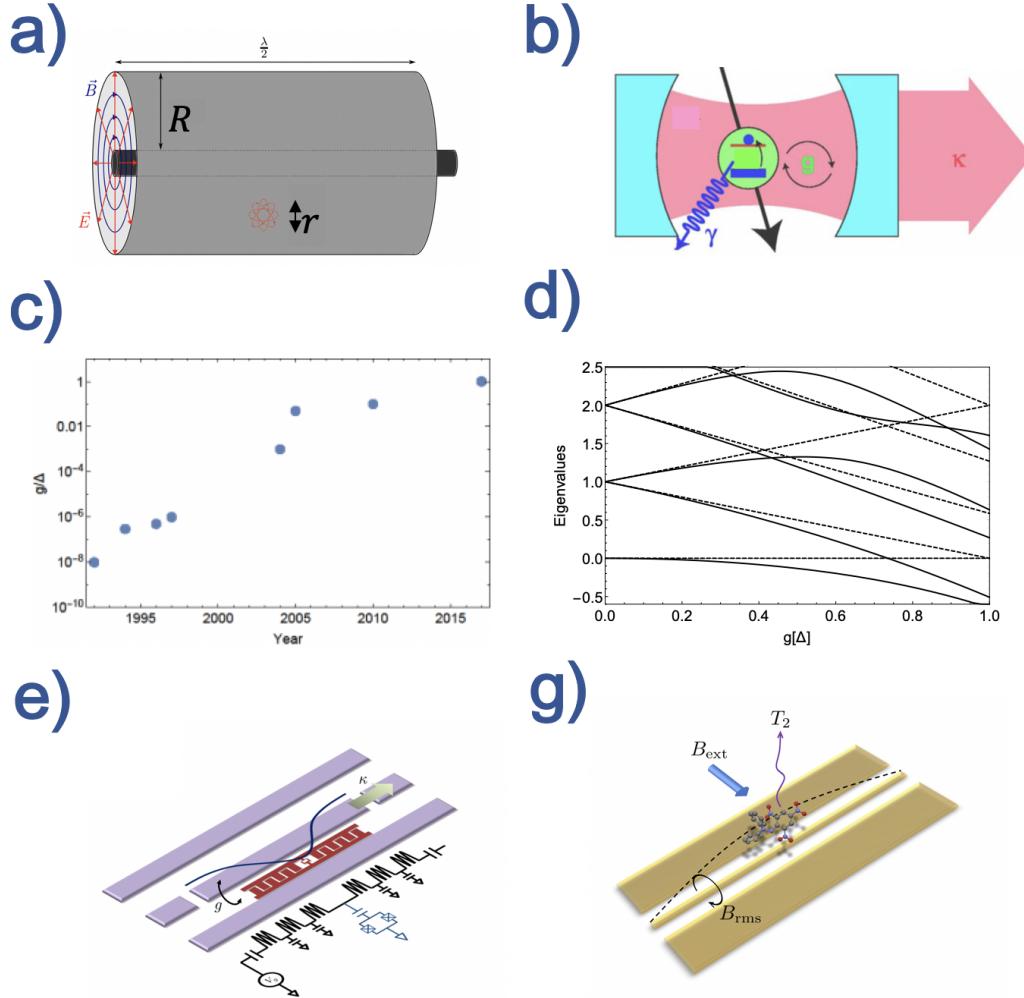


Figure 2: **Cavity QED** a) Cylindrical cavity. b) A generic cavity QED system with the main rates indicated. c) The time evolution for the maximum coupling achieved in the lab between a two level system and a single mode cavity (data taken from [21]). d) Spectrum for the quantum Rabi model (14) [solid lines] and the JC model (16) [shaded lines]. e) A circuit QED sketch (the qubit, in red, is not in scale). g) a magnetic molecule coupled to a superconducting cavity.

was of a flux-type) and the microwave cavity [49]. Apart from this number, the interesting feature is that the experimental results can not be understood within the JC-model \mathcal{H}_{JC} but require the full quantum Rabi model. When this occurs, *i.e.* that the full model is needed, the light-matter is said to be in the ultrastrong coupling regime (USC). In a similar

experiment, in Delft, the USC was also reached using an LC-resonator [22]¹⁰.

Model (14) is known to be integrable since a few years ago [7]. However its solution is not practical, but one can always diagonalize it in a computer. The eigenvalues for the quantum Rabi, compared to the ones of the JC, are shown in figure 2d). Several features need to be discussed. At very large coupling, the eigenstates of H_{qR} are two-fold degenerate. In the limit of large coupling, the full model can be approximated by $\mathcal{H}_{\text{qR}} \cong \omega_c a^\dagger a + g\sigma^z(a^\dagger + a)$, *i.e.* a displaced harmonic oscillator. This displacement can be positive or negative depend on the eigenvalues of σ^z . The energy do not depend on the sign of the displacement, explaining the degeneracy. Besides, the ground state is not longer the trivial but $|gs\rangle = \sum_2 n c_n |2n, 0\rangle + c'_n |2n - 1, 1\rangle$. Notice that this is a sum over states with an even number of excitations. The reason is that the model is parity-conserving, $[\mathcal{H}_{\text{qR}}, P] = 0$, with $P = \sigma^z e^{i\pi a^\dagger a}$. In a more pedestrian way, this symmetry can be appreciated by noticing that the interaction term in (14) creates (destroys) excitations by pairs. Finally, a striking feature in the USC is the subtlety with the gauge principle [14, 16]. In short, the gauge principle must be satisfied (of course). However a problem arises when using the dipole and the Coulomb gauges within the two level approximation as they yield non equivalent Hamiltonians. The solution to the puzzle, is to show that the two level approximation is accurate in the dipole gauge but not in the Coulomb one. Therefore, the two level projection should be done in the latter gauge and transformed to the Coulomb one. The transformation must be projected in the two level subspace. Finally, the correct gauge-invariant Hamiltonian in the Coulomb gauge was found [16]. Due to its importance, let me write the correct quantum Rabi model in the Coulomb gauge

$$(22) \quad \mathcal{H}_{\text{qR}}^{(\text{C})} = \omega_c a^\dagger a + \frac{\Delta}{2} \left(\sigma^z \cos \left[\frac{2g}{\Delta} (a + a^\dagger) \right] + \sigma^y \sin \left[\frac{2g}{\Delta} (a^\dagger + a) \right] \right)$$

Expanding the cosine and sine in powers of g/Δ we recover (14), thus both Coulomb and dipole gauges coincide and the issues disappear. Therefore, the USC also serves for testing the gauge invariance in cavity QED.

¹⁰In this history, I have only discussed circuits because they are exact realisations of the qR model (a two level system coupled to a single mode cavity). Other light-matter systems as exciton polaritons or intersubband polaritons have also reached couplings of $0.1 \omega_c$ and beyond. A full history of the USC regime can be read in two recent reviews [21, 34].

2.2 Waveguide QED

We can still insist in our desire to connect distant atoms through the EM field. Several people do. Propagating photons are the ideal carriers of information. To enhance the atom cross section, the electromagnetic field is confined in one dimensional waveguides [58]. The waveguide QED Hamiltonian in the dipole gauge is given by (11). It turns out that the the spin boson is classified with the spectral density,

$$(23) \quad J(\omega) = 2\pi \sum_k c_k^2 \delta(\omega - \omega_k) .$$

In particular, the spontaneous emission (13) in the line is $\Gamma_{\text{line}} = J(\Delta)$. The factor $\beta = \frac{\Gamma_{\text{line}}}{\Gamma_{\text{line}} + \gamma}$ measures the atom-waveguide coupling compared to another channels of atom dissipation with rate γ . Experiments in waveguide QED are done with superconducting circuits [4, 73, 43, 26], optical waveguides [19] among others [44, 11] with β -factors approaching one. Thus, waveguide QED has an clear application for emitting single photons. Another advantage of being one dimensional is that a single atom can act as a perfect mirror [4] for single photons. This paves the way to control the transport of photons or create atomic cavities. Besides, it is also quantifiable the induced interaction between distant atoms mediated the propagating photons in the waveguide [18, 81]. After tracing out the waveguide modes the the master equation [See App. A] is obtained,

$$(24) \quad \dot{\rho} = -i[\Delta(\sigma_1^z + \sigma_2^z + J_{12}\sigma_i^+ \sigma_j^-, \rho] - \sum_{i,j=1,2} \gamma_{ij}(\sigma_i \rho \sigma_j^\dagger - \frac{1}{2}\{\sigma_i^+ \sigma_j^-, \rho\}) .$$

Two spin-spin interactions are generated. A coherent tight-binding interaction between atoms with strength $J_{ij} = J(\Delta) \cos(\Delta/vd_{12})$ and a cross-dissipation rate given by $\gamma_{12} = J(\Delta) \sin(\Delta/vd_{12})$. Here, v is the light propagation velocity in the waveguide and $\gamma_{11} = \gamma_{22} = J(\Delta)$. Both interactions, the coherent and the dissipative can be qualitatively understood. The former, occurs for $\lambda/4$ distances. The first atom emits a photon. The wavepacket is maximum in the second atom. The latter, however, happens when the atoms are separated $\lambda/2$. In this case, both points are equivalent (except a phase) and the atoms emit collectively [cf. the discussion on enhanced transmission in Section 1.3]. This interaction could be used to generate entanglement or gates. However they are not optimal, since there is always a dissipative term (the last term in (24)). In fact, one can guess that

only 50% of efficiency can be reached at maximum. When one atom emits a photon half of it goes in the *bad* direction (the one which is opposite to the other atom). This can be fixed using mirrors [61] or chiral waveguides [45]. Another alternative is by looking for waveguides supporting bound states [69, 9, 63]. These are dressed light-matter states localized (non propagating) around the qubit. A necessary condition for their existence is the photonic band to be finite. The bound state energies must lie outside the photonic band. See figure 3b). With the help of bound states several spin-like models can be obtained where all the interactions are dissipationless making them an attractive approach for, *e.g.* quantum simulations.

2.3 *The quantum technology*

Quantum information science has put quantum optics into the spotlight of modern physics
Ulf Leonhardt in *Essential Quantum Optics* [42].

While writing this manuscript, newspapers around the world announced that the *quantum supremacy* has been reached. That's it, the demonstration that a computational task that can be done in a quantum computer cannot be made in a classical computer without spending thousands of years. John Martinis and his group in the Google lab were able to generate a random quantum state of 53-qubits and measuring (calculate) the bit distribution [3]. This is extremely hard for a classical computer. This problem may not seem the most interesting one but building a quantum computer of 53 qubits is a remarkable technological milestone. Importantly enough for this manuscript, the functioning of the computer is based on the light-matter-like interaction.

A quantum computer is a set of two level systems that can be coupled and decoupled performing logical gates. Besides, qubit preparation and readout is also needed. In the superconducting prototypes, the qubits are artificial atoms that may interact via cavity photons or directly because of the cross talk between them [5, 31]. The coupling-decoupling is done by tuning on/off resonance the qubits. The readout is done via their coupling to a cavity. In the case of the Google prototype, each qubit is coupled to a cavity mode, see [5]. If the two level system and the cavity mode are conveniently detuned they do not share real but virtual excitations. In this regime, called dispersive, the Hamiltonian (14) is

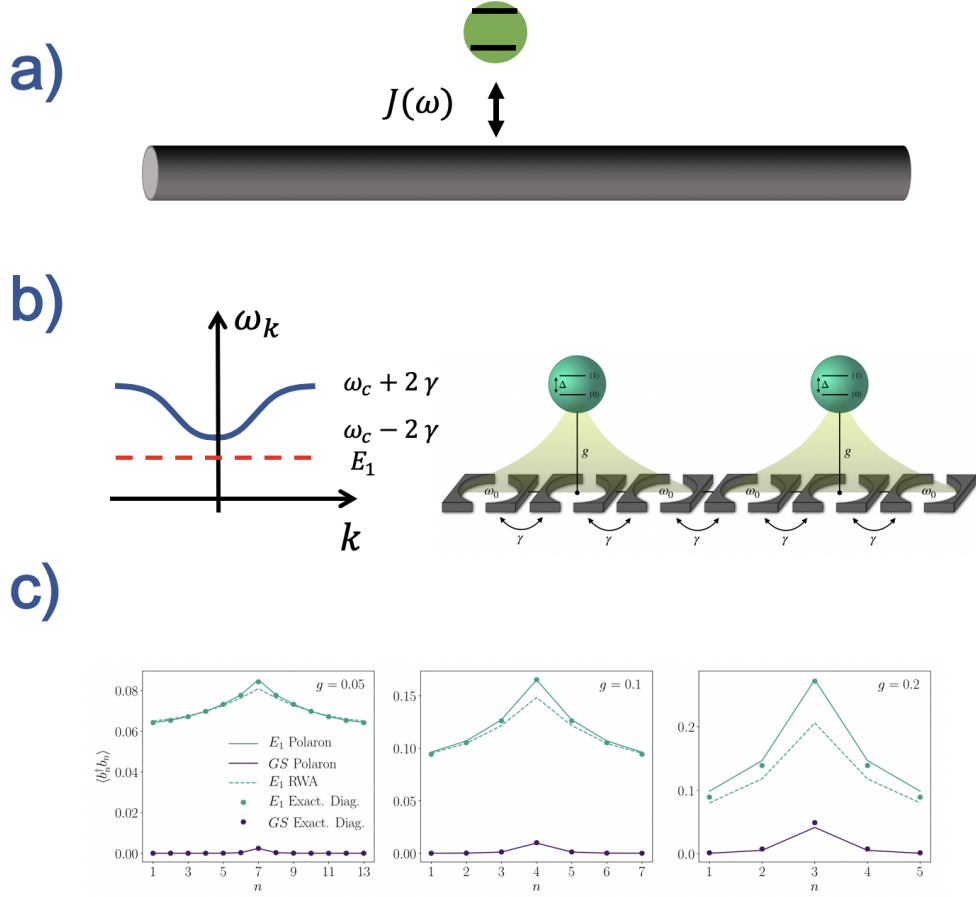


Figure 3: **Waveguide QED** a) Sketech of waveguide QED: an atom (here a two level system) coupled to a one dimensional waveguide. b) Qubits coupled to a cavity array. Each one is coupled to one cavity of the array with strenght g [cf. (14)]. The cavity array has the Hamiltonian $H = \omega_0 \sum_n^N a_n^\dagger a_n - \gamma \sum_n^N (a_n^\dagger a_{n-1} + \text{H.c.})$ that gives the dispersion relation $\omega_k = \omega_c - 2\gamma \cos(k)$. Each two level system coupled to the cavity array contribute to one bound state E_1 . If the qubits are closer enough E_1 lifts its degeneracy and the bound states are coupled. c) Comparison of spatial boson distributions from the PT, the RWA and exact diagonalisation (small chains, here are of 12 sites, can be diagonaized within a classical computer). They correspond to $\Delta = 0.3$, and $g = 0.05$, $g = 0.1$ and $g = 0.2$ respectively from left to right. Solid lines are used to indicate polaron results, dashed lines for RWA results and dots for exact diagonalisation results.

equivalent to [82]

$$(25) \quad \mathcal{H}_{\text{qR}} \cong \frac{\Delta}{2} \sigma^z + \omega_c a^\dagger a + g^2 \left(\frac{1}{\Delta - \omega_c} + \frac{1}{\Delta + \omega_c} \right) \sigma^z a^\dagger a$$

I emphasize that this Hamiltonian is valid provided $g \ll |\Delta - \omega_c|$. Notice that the frequency of the cavity is shifted by $\pm g^2 \left(\frac{1}{\Delta - \omega_c} + \frac{1}{\Delta + \omega_c} \right)$ depending on the state of the qubit. This can be used to do the readout. At the same time, if a second qubit is coupled to the cavity mode and both are in the dispersive regime they couple through a term $\sim J_{ij} \sigma_i^\dagger \sigma_j + \text{h.c.}$ [Cf. Eq. (24)] [82]

$$(26) \quad J_{ij} = g_i g_j \left(\frac{1}{\Delta_i - \omega_c} + \frac{1}{\Delta_j - \omega_c} - \frac{1}{\Delta_i + \omega_c} - \frac{1}{\Delta_j + \omega_c} \right)$$

This has been used to generate interactions between the qubits via the cavity which plays the role of a quantum bus [47]. Therefore, both the interaction and the readout, ingredients of a quantum computer are based on the light-matter Hamiltonian (14). In this manuscript, I have focused on the superconducting circuit architecture. Other quantum computers are based on the ion-trap technology. In that case, the functioning is based on the coupling between ions and light [78].

3 Many-body quantum optics in the non perturbative regime

I: Mom, how do I know that the water is boiling?

Mom: You will.

My mom, giving the best explanation of a phase transition the day I introduced myself in the fine art of cooking an egg.

There are many works doing quantum many-body physics with light-matter systems [27, 2, 40]. In this section, I focus on the strongly correlated phenomena occurring because the coupling between light and matter enters into the nonperturbative or USC regime.

3.1 Many body cavity QED

A two level system coupled to a single mode cavity is not a many-body system. A quantum many-body system can be build by coupling N 2LS to a single mode cavity. The Dicke model is the generalisation of (14) to N -qubits,

$$(27) \quad \mathcal{H}_{\text{Dicke}} = \frac{\Delta}{2} \sum_j^N \sigma_j^z + \omega_C a^\dagger a + g \sum_j^N \sigma_j^x (a + a^\dagger).$$

For simplicity, let me consider equal atoms that are equally coupled to the cavity. It turns out that this model has a phase transition, called superradiant. Understanding this transition is easy. In the mean field approximation (27) $a + a^\dagger \rightarrow \alpha$, with α a real number. The ground state energy is given by $E = \omega\alpha^2 - \frac{N}{2}\sqrt{\Delta^2 + 4g^2\alpha^2}$. Energy minimisation yields that if $g < g_c = \sqrt{\omega_c\Delta}/2\sqrt{N}$ then $\alpha = 0$ while if $g > g_c$, $\alpha \neq 0$. α is the order parameter and this phase transition belongs to the mean-field Ising universality class [33]. This transition has not been observed yet. The reason is that the realization of (27) is not trivial. Model (27) does not account for N independent atoms in single mode cavity. In the dipole gauge it reads however,

$$(28) \quad \mathcal{H}^{(D)} = \mathcal{H}_{\text{Dicke}} + \frac{g^2}{\Delta} \sum \sigma_i^x \sigma_j^x.$$

This term ruins the phase transition. Notice, that pretty much like in the gauge issues discussed in section 2.1, this term is important whenever $g\sqrt{N}$ is large enough. This is the regime where the transition is expected to occur. Currently, there is an enormous interest for searching systems to observe this phase transition [13].

Many-body spin-spin interactions is mediated by the cavity field (remind the previous section) [1, 75, 51]. In the detuned cavity-atoms case the interaction is of the type $\sigma_i^x \sigma_j^x$ with the coupling constants given in (26). Recently, we have found a novel way of obtaining a hybrid spin-spin-boson model [46]. The starting point is again the Dicke model with a parity breaking (second term below) for the spins [Cf. Eq. (14)]

$$(29) \quad \mathcal{H} = \frac{\Delta}{2} \sum \sigma_j^z + \frac{\epsilon}{2} \sum \sigma_j^z + \omega_c a^\dagger a + g(\hat{a} + \hat{a}^\dagger) \sum \sigma_j^x.$$

When $\epsilon \neq 0$, \mathcal{H} can couple states differing by an odd number of excitations. For example, an avoided level crossing, originating from the coupling of the states $\hat{a}^\dagger|0, j, -j\rangle \leftrightarrow \hat{J}_+^2|0, j, -j\rangle$, is expected when the resonance frequency of the cavity $\omega_c \simeq 2\omega_q = 2\sqrt{\Delta^2 + \epsilon^2}$ [23]. We label the states as $|n, j, m\rangle$, where the quantum number n describes the Fock states of the cavity, and $j = N/2$ is the total angular momentum and $m = -j + N_{\text{exc}}$ is the $\sum \sigma_j^z$ eigenstate, where N_{exc} describes the number of excited atoms. Notice that this transition is allowed only if the counter-rotating terms are included. Using perturbation theory [66]

the following effective interaction Hamiltonian can be obtained:

$$(30) \quad \hat{H}_{\text{eff}} = g_{\text{eff}} \left(\hat{a} \hat{J}_+^2 + \hat{a}^\dagger \hat{J}_-^2 \right),$$

where

$$(31) \quad g_{\text{eff}} = -\frac{4g^3 \cos^2 \theta \sin \theta}{3\omega_q^2},$$

with $\sin \theta = \epsilon / \sqrt{\Delta^2 + \epsilon^2}$. This procedure also gives rise to a renormalization of the atomic frequencies, which can be reabsorbed into ω_q . This yields a two-axis twisting like-interaction among the spins which can be used to generate macroscopic spin entanglement [46].

3.2 Many body with spin-boson type models

In the previous section I was considering a single mode cavity. Now, let me discuss the coupling with a collection of modes. This is a more general case. It covers many situations described with the Hamiltonian (11), by choosing different functional forms for $J(\omega)$, Eq. (23). Three examples are drawn in figure 4. The first is a one dimensional waveguide, figure 3a). There, $J(\omega) \sim \omega$ [53]. A second example is the cavity QED considering the leakage of photons, figure 2. In this case, $J(\omega)$ is a Lorentzian-type function peaked in the cavity frequency ω_r . Finally, a cavity array is considered, figure 3b) where the density of states diverge at the band edges [62, 59].

In all its generality, the spin-boson Hamiltonian (11) does not have a known solution. See [72, Chap. 18.1] and [41]. However, if the coupling constant is small enough, the rotating wave approximation (RWA) can be used, by which the interaction term becomes [Cf. Eq. (16)]

$$(32) \quad \sum_k c_k \left(\sigma^- a_k^\dagger + \sigma^+ a_k \right).$$

It is clear now that ground state (GS) is $|GS\rangle = |0; \mathbf{0}\rangle$. In addition, the Hamiltonian preserves the number of excitations N , $[\mathcal{H}, N] = 0$ with $N = \sum_k a_k^\dagger a_k + \sigma^+ \sigma^-$. Owing to these properties, within the RWA, the g.s physics and the single excitation dynamics is trivial. Notice that this is the generalization of the JC-model (16) to the multimode case. In this lecture, however I am interested in the regime where the RWA fails. Different

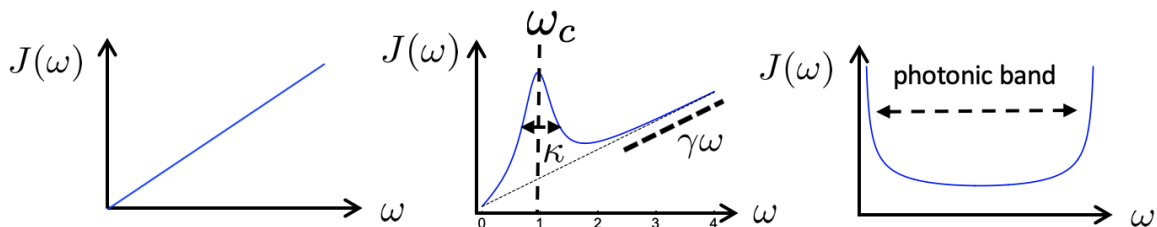


Figure 4: **Spectral density** $J(\omega)$ for different situations. They correspond to coupling to a one dimensional transmission line, Fig. 3a), to a dissipative cavity, Fig 2 and to a cavity array Fig. 3b) respectively from left to right.

numerical techniques have been used to solve (11) beyond the RWA. These are matrix-product state (MPS) [53, 62, 59], density matrix renormalization group (DMRG) [56] or path integral approaches [25, 39]. Analytical treatments are also used. They are based on different variational ansatzs: polaron-like [70, 6, 17, 67, 80, 60] or Gaussian ones [68]. In this overview I will sketch the polaron-like approach that allows to find, in an analytical way, the low energy equilibrium and non-equilibrium dynamics.

In order to understand the motivation behind the polaron *ansatz*, it is convenient to analyse the asymptotic limits where the Hamiltonian is exactly solvable. In the case where $c_k = 0$, the coupling vanishes and the problem splits into a 2LS and a bosonic bath which can both be solved independently. The GS is therefore $|GS\rangle = |0; \mathbf{0}\rangle$, which is clearly localised, in the sense that the spin ket is an eigenstate of σ^z . In the opposite case, $\Delta = 0$, the Hamiltonian becomes that of a set of displaced oscillators. One can choose a state of the form

$$(33) \quad |\psi\rangle = |\pm\rangle \otimes |osc.\rangle,$$

where $|\pm\rangle$ can be either eigenstate of σ^x and $|osc.\rangle$ is an unknown state for the oscillators.

Now it can be seen that

$$(34) \quad H |\psi\rangle = |\pm\rangle \otimes \left(\sum_k \omega_k a_k^\dagger a_k \pm \sum_k c_k (a_k^\dagger + a_k) \right) |osc.\rangle,$$

so the direction of the displacement is determined by the qubit state. By defining new bosonic operators: $A_k = A_k \pm c_k/\omega_k$ and $A_k^\dagger = A_k^\dagger \pm c_k/\omega_k$ with $[A_k, A_k^\dagger] = 1$, one arrives at

$$(35) \quad H |\psi\rangle = |\pm\rangle \otimes \left(\sum_k \omega_k A_k^\dagger A_k - \sum_k \frac{c_k^2}{\omega_k} \right) |osc.\rangle.$$

It is clear now that the GS for this Hamiltonian is $|\pm\rangle, \mathbf{0}$ and the energy is independent on the spin state and equal to $-\sum_k c_k^2/\omega_k$. In this instance the GS is delocalised, as the qubit state can be in either the symmetric or antisymmetric superpositions of the eigenstates of σ^z ¹¹. Here I have introduced the redefined bosonic operators rather *ad hoc*, but they can also be reached by means of the displacement operator, which is presented below in its most general form,

$$(36) \quad D(\alpha) = \exp[\alpha a^\dagger - \alpha^* a].$$

The displacement operator is a unitary transformation, since $D(\alpha)^\dagger \equiv D(-\alpha)$, which justifies that the energy deduced from the transformed Hamiltonian is the same as for the original one. If the operator is tweaked to produce displacements corresponding to the redefined bosonic operators one has

$$(37) \quad D\left(\pm \frac{c_k}{\omega_k}\right) = \exp\left[\sigma^x \sum_k \frac{c_k}{\omega_k} (a_k^\dagger - a_k)\right].$$

The presence of σ^x in the exponent serves to generate the plus or minus sign that determines the direction of displacement, upon acting on the corresponding eigenstate.

¹¹ For those who have a condensed-matter background, the spin-boson is paradigmatical in impurity models. In those formulations that naturally lead to a double-well interpretation of the 2LS, the roles of σ^x and σ^z are switched in the Hamiltonian. In that case, $c_k = 0$ is viewed as the delocalised regime whereas $\Delta = 0$ is viewed as the localised regime.

Therefore, one seeks a unitary transformation that renders the Hamiltonian diagonalisable, with a non-trivial ground state that merges the two asymptotic solutions. Unfortunately, the former condition is not completely satisfied by the polaron transform, but it does produce a quasi-solvable Hamiltonian whose GS can be calculated with the use of a simple *ansatz*. The transformation is

$$(38) \quad U_P = \exp \left[-\sigma^x \sum_k f_k a_k^\dagger - f_k^* a_k \right],$$

and the variational *ansatz* is

$$(39) \quad |GS\rangle = U_P |S; \mathbf{0}\rangle.$$

Where $|S\rangle$ is an unknown spin state and f_k are free parameters to be determined by the application of the variational method. Minimization yields the self-consistent relation

$$(40) \quad f_k = \frac{-c_k/2}{\Delta_r + \omega_k} \quad \text{with} \quad \Delta_r = \Delta e^{-2\sum_k f_k^2}.$$

We have seen that in the polaron picture the GS is trivial, then it is expected that the low energy dynamics consists on single particle excitations over this GS. Exactly, the unitary transformed $H_p = U_p^\dagger H U_p$ reads

$$(41) \quad \begin{aligned} H_p = & \Delta_r \sigma^+ \sigma^- + \sum_{k=1}^N \omega_k a_k^\dagger a_k - 2\Delta_r \left(\sigma^+ \sum_{k=1}^N f_k a_k + \text{H.c.} \right) \\ & - 2\Delta_r \sigma_z \sum_{k,p=1}^N f_k^* f_p a_k^\dagger a_p \\ & + \frac{\Delta}{2} + \sum_{k=1}^N (\omega_k |f_k|^2 - g_k^* f_k - f_k^* g_k) + \text{h.o.t.} \end{aligned}$$

Here, h.o.t. stands for higher-order terms of order $\mathcal{O}(f^3)$ with two and more excitations. Note how the transformed Hamiltonian conserves the number of excitations and can be treated analytically like in the RWA approximation. With this tools at hand, we can overview the main features for the low energy physics of the spin boson model, rather independently of $J(\omega)$, both at equilibrium and non-equilibrium.

Ground state properties.- Notice that due to the coupling to the photons the qubit frequency is renormalized to Δ_r , Cf. (41) and [41]. Besides, from (40), it renormalizes to zero. Rewriting Δ_r in terms of $J(\omega)$

$$(42) \quad \Delta_r = \Delta e^{-1/2 \int_0^{\omega_c} J(\omega)/(\omega+\Delta_r)^2}$$

is obtained. Notice that Δ_r means localised (delocalised) 2LS (see footnote 11). Whether this occurs through a phase transition or not depends only on $J(\omega)$. The most studied cases are $J(\omega) \sim \omega^s$. Depending on the value of s , there exist three distinct cases known as sub-Ohmic ($s < 1$), Ohmic ($s = 1$), and super-Ohmic ($s > 1$) regimes. It has been shown that the transition is of second order in the sub-Ohmic regime and Kosterlitz-Thouless type in the Ohmic regime. In the super-Ohmic regime there is no phase transition [79]. Other $J(\omega)$ are currently been investigated together with their critical properties.

Vacuum emission.- Apart from this phase transition, another interesting phenomena occurring in the spin boson model is its vacuum emission as we recently calculated [60]. The idea is that the ground state (39) depends on f_k . The latter depend on the light-matter coupling strenght. Physically, the ground state photon occupation is different from zero around the qubit, see fig (3)c). Then, by modifying the light-matter interaction non adiabatically the ground state emits light, pretty much like in the Casimir effect [10, 38, 48, 37, 77].

Spontaneous emission.- Within the polaron picture H_p , the model resembles the weak coupling-RWA one. In this case, it is expected that standard perturbative techniques hold here too. In fact, in [80] we have shown that the spontaneous emission is given by

$$(43) \quad \Gamma_{\text{line}} = J(\Delta_r)$$

recovering Fermi's golden rule at the weak-coupling limit and a quenching of the emission at large couplings, which recalls the effective decoupling in the USC regime [21, 34].

Spin-spin interactions in waveguide QED.- Generalising the polaron transformation to several qubits coupled to a one dimensional field, a direct spin-spin interaction of the form, $J\sigma_i^x\sigma_j^x$ emerges. Our calculations with the cavity array, figure 3b) confirm that J decays exponentially with the distance. Therefore, we expect the occurrence of transitions

belonging to the Ising class type (recall our discussion on the superradiance transition) [35]. Finally, in the polaron picture (41), bound states can be also computed. It turns out that the existence of bound states is guaranteed at any coupling strength and that can be computed, see figure 3c). Therefore, non dissipative spin-spin interactions build up also in the USC regime of waveguide QED.

Therefore, the polaron transformation is a convenient tool for discussing the physics of waveguide QED in the USC. This regime is still in its infancy, here I just listed the first calculations but further and more exotic phenomena are currently been investigated [55, 20].

4 Concluding remarks

All right.

Ignatius Farray.

A lot of stuff was not explained here, maybe too much. For example, I did not say anything about magnetic molecules coupled to the cavity field through the last term in (4) [29], see figure 2f). Here, some issues on the gauge principle and/or the superradiance transition may be of relevance. Besides, they are also proposed as prototypes of a quantum computer [30]. I omitted most of the phenomena of quantum optics as the generation of squeezed light, measurement or timely topics as topology and photonics. I have written a naive explanation of a quantum computer. Famous reports on the topic and its relation with the light-matter coupling are Refs. [52, 36]. In addition, I have done an extremely partisan review of the many body physics done with light. As said, I focus on how many body effects emerge due to the entrance in the USC. However, light-matter systems are being used to generate strongly correlated models even without the USC as explained in Refs. [40, 11].

With respect to the topics covered, some of them are still incomplete and need further investigation. Some of them are the occurrence of a localized-delocalized phase transition for $J(\omega)$ besides $J(\omega) \sim \omega^s$, the extension of the polaron technique for finite temperature systems and the study of multimode cavities or going beyond the two level paradigm, for *e.g.* to build quantum simulators for higher spin systems are some examples. Another topic of current interest is to tune the physical and chemical properties of quantum materials inside quantum cavities [65, 32].

Let me say goodbye with a reflection. Quantum mechanics is reaching the level of a technological solution. Apart from the understanding of the fundamental interactions young physicists should acknowledge the big heroes of physics for the existence of job offers where knowing quantum physics is mandatory.

Acknowledgments. I am indebted with so many people that this section would be too large. So, in the spirit of this overview *in a nutshell*, I will do my best to shorten the list. It is an honour to acknowledge the members of the *Real Academia de Ciencias de Zaragoza* for this prize. Thanks to my students. Specially to the QED crew: Fernando Quijandría, Eduardo Sánchez-Burillo, Virginia Ciriano, Juan Román-Roche and Sebas Roca. I learnt a lot from you. To my colleagues-friends. Specially to José Luis García-Palacios, Fernando Luis, Juanjo García-Palacios, Luis Martín-Moreno, Charles Downing, Salvatore Savasta, Franco Nori and Peter Hänggi. It is a pleasure to do physics with you. Finally, I also acknowledge the funding from the Spanish Government, the EU comission and the Aragón regional funds.

A The master equation

Even if one can argue that the Universe follows a Schrödinger-type equation in some limit, it is difficult to defend that practical calculations must include the Hamiltonian for the whole Universe. In fact, most of the physicists are interested in a corner (typically small) of the Universe. This corner interacts with the rest. Denoting it as *the system of interest* and the rest is denoted *the environment* the *total* Hamiltonian is splitted:

$$(44) \quad H_T = H_S + H_E + H_I$$

And the relevant object is the reduced density matrix $\rho \equiv Tr_E(\rho_T)$. I remind you that, for any observable acting on the system ($O_S = O_S \otimes \mathbb{I}_E$), its average is given by $\langle O_S \rangle = Tr(O_S \rho)$. Writen like this, H_S describes an open system and it would be nice to have a dynamical equation for ρ . The latter is a master equation. Below, within the style of this lecture, I will sketch the derivation of a generic master equation with emphasis in its conceptual roots rather than in the algebra.

Notice the *exact* time evolution for the *reduced density matrix* given the H_T in (44) [Cf.

figure 1],

$$(45) \quad \varrho(t) = \text{Tr}_E \left(U_T(t, t_0) \varrho_T(t_0) U_T^\dagger(t, t_0) \right).$$

Consider first the case where both system and environment are in a product state at t_0 (they are not correlated; neither classically nor quantum). Then, $\varrho_T(t_0) = \varrho_S(t_0) \otimes \varrho_B(t_0)$. In this case,

$$(46) \quad \varrho(t) = \sum_{\alpha, \beta} K_{\alpha, \beta}^\dagger(t, t_0) \varrho_S(t_0) K_{\alpha, \beta}(t, t_0) \equiv \mathcal{E}(t, t_0) \varrho(t_0)$$

with $K_{\alpha, \beta}(t, t_0) = \sqrt{\lambda_\alpha} \langle \lambda_\alpha | U(t, t_0) | \lambda_\beta \rangle$. This last formula is rather direct from (45) using the diagonalization for the bath initial density matrix $\varrho_B(t_0) = \sum_\alpha \lambda_\alpha | \lambda_\alpha \rangle \langle \lambda_\alpha |$. The last equivalence is a convenient notation that highlights the fact that this is nothing but a map that transforms a density matrix in another density matrix. We emphasize that this result is exact and that the operators K (so the map \mathcal{E}) are independent of the state. However, it lies in the assumption that at t_0 the density matrix was a product state. This, marks t_0 as an special time. In general, however the state is

$$(47) \quad \varrho_T(t_0) = \rho_S(t_0) \otimes \rho_E(t_0) + \delta_\varrho$$

Here, $\varrho_S = \text{Tr}_E(\varrho_T)$, $\varrho_E = \text{Tr}_S(\varrho_T)$ and $\delta_\varrho = \rho - \rho_S \otimes \rho_E$ wich encapsulates the system-bath correlations. Introducing the latter in (45) the expression for $\varrho(t)$ adds the extra term $\text{Tr}_E \left(U_T(t, t_0) \delta_\varrho U_T^\dagger(t, t_0) \right)$. This term depends on the initial condition δ_ϱ . Therefore, is not always possible to find a Universal dynamical model (this is the standard name) independent on the state of the system density matrix at time t_0 . This is annoying. In general, it is not possible to find a differential operator such that, $\dot{\varrho} = \mathcal{L}[\varrho]$. In other words, we cannot always find a local equation for the evolution of an open system . This is not surprising, the same occurs for classical systems. Thus, an approximation is necessary. I am going to assume that the map (46) is Markovian, wich means that satisfy the composition $(\forall t_2, t_0, t_1)$,

$$(48) \quad \mathcal{E}(t_2, t_0) = \mathcal{E}(t_2, t_1) \mathcal{E}(t_1, t_0)$$

In practice, this means that (46) can be used for any t and t_0 . Obviously this is not true, however let me continue and justify the Markovian approximation at the end. The differential version for (46) can be found noticing that

$$(49) \quad \frac{d\rho}{dt} = \lim_{\epsilon \rightarrow 0} \frac{\mathcal{E}(t + \epsilon, t) - \epsilon}{\epsilon} \rho(t) \equiv \mathcal{L}[\rho].$$

Doing two pages of calculations (not shown here) it is found that

$$(50) \quad \frac{d\rho}{dt} = -i[H_S, \rho] + \sum_{i,j}^{N^2-1} \gamma_{ij} \left(L_i \rho L_j^\dagger - \frac{1}{2} \{L_i^\dagger L_j, \rho\} \right)$$

This is the Lindblad equation discussed in the main text. Here the operators L form an orthogonal basis in the space N^2 and the coefficients are related to the coefficients for the expansion. See [8, Chapter 3] and [57, Chapter 4] for a more detailed discussion.

My final comment on the main approximation used: Eq. (50) has been found under the Markovian condition. This approximation, in practice, neglects the correlated part δ_ρ in (47). This seems to contradict my discussion on the importance of entanglement done in Sect. 1.3. However, it does not. We are *not* neglecting the entanglement, which would mean that ρ_S is a pure state all the time. We are neglecting δ_ρ , a correction to the density matrix that is, at least, of the order of the system-bath coupling. Therefore, Eq. (50) is expected to hold whenever the system and bath are weakly coupled.

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Rev. Real Academia de Ciencias. Zaragoza. **74:** 75–78, (2019).

ISSN: 0370-3207

IN MEMORIAM del Académico Numerario
Víctor Manuel Orera Clemente

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Real Academia de Ciencias de Zaragoza



El martes 28 de enero de 2020 falleció a los 69 años de edad el académico y muy querido compañero de la Real Academia de Ciencias Exactas, Físicas, Químicas y Naturales de Zaragoza Sr. D. Víctor Manuel Orera Clemente, Víctor para todos, profesor “*ad honorem*” del Consejo Superior de Investigaciones Científicas (CSIC) en el Instituto de Ciencia de Materiales de Aragón (ICMA), instituto mixto de la Universidad de Zaragoza y el CSIC.

Nacido en Castellón de la Plana en donde estaban destinados sus padres, funcionarios públicos, a los seis años vino a Zaragoza, ciudad a la que ha estado ligado desde entonces y donde, mayoritariamente, ha ejercido una dilatada y fructífera labor profesional. De raíces

aragonesas y tempranamente seducido por el Pirineo, sentía su tierra en lo más profundo, pero con miras al universo ya que entendía que así debe ser la búsqueda del conocimiento, a la que se dedicó.



Primogénito de una familia de cuatro hermanos, Víctor siempre mantuvo una desbordante vitalidad y optimismo sólo atenuado por un sentido acendrado de su responsabilidad familiar y social y una gran generosidad. Sincero, leal y exigente consigo mismo y con los demás, la montaña y la investigación fueron sus pasiones. Idealista y con gran sensibilidad social pensaba que un científico honesto no podía trabajar sólo para su propio curriculum y prestigio sino que debía de hacerlo en temas de importancia para la sociedad y, coherentemente, así lo hizo.

Bachiller por el colegio Calasancio de los PP Escolapios, cursó con aprovechamiento brillante la Licenciatura en Ciencias Físicas, especialidad de Óptica, en la Facultad de Ciencias de la Universidad de Zaragoza acabando en 1972 con Premio extraordinario de licenciatura y Premio Fin de Carrera “Daza Valdés” de la Sociedad Española de Óptica. Sin pausa alguna, ese mismo año, se inició en las labores de investigación bajo la dirección del Profesor Alcalá Aranda compartiendo esta actividad con docencia en el Colegio Alemán de Zaragoza. En 1973 la obtención de una beca de Formación de Personal Investigador y el nombramiento como Profesor Ayudante de Óptica le permitió dedicarse a tiempo completo a desarrollar su tesis doctoral en Ciencias Físicas “*Estudio de la formación y evolución de grandes agregados de defectos en cristales tipo fluorita*” que defendió en 1976, obteniendo el premio extraordinario de doctorado de la Universidad de Zaragoza.

En épocas en que salir fuera de España era necesario para respirar el aire libre de otra sociedad posible y poder incorporarse rápidamente a la investigación más puntera en su campo, no dudó en realizar, durante el desarrollo de su tesis doctoral, una estancia de diez meses en el “*Atomic Energy Research Establishment, Materials Development Division*” en Harwell, Reino Unido. Posteriormente, en 1978-79, hizo una estancia posdoctoral en la “*Solid State Division*” del Oak Ridge National Laboratory –ORNL– (USA) con el Dr. Yok Chen que en gran grado determinó su evolución científica. Más adelante efectuó otras estancias en el ORNL centro del que fue consultor científico externo durante el bienio 1986-87.

Profesor Adjunto de la Universidad de Zaragoza por oposición en 1978, desarrolló su actividad docente e investigadora en la Facultad de Ciencias hasta que pasó a Investigador Científico del CSIC (1988). Llegó a un ICMA recién creado como centro mixto CSIC-Universidad de Zaragoza, del que fue uno de sus promotores, en un momento de despliegue de la investigación española en Ciencia de Materiales y rápidamente promocionó a Profesor de Investigación (1990).

Primero en la Universidad de Zaragoza y luego en el ICMA y el CSIC, Víctor supo compaginar una investigación de primera línea mundial con tareas de gestor de instituciones de investigación. Fue Vicedecano de la Facultad de Ciencias de la UZ (1984-86) en momentos clave de la transformación democrática de las universidades y las facultades españolas. Fue Director del ICMA (1991-94), Coordinador Científico del Área de Materiales del CSIC (1994-96), Vocal designado del Comité Científico del CSIC (1996-2004), Coordinador institucional del CSIC en Aragón (2005) y posteriormente Vicepresidente de organización y relaciones institucionales del CSIC desde diciembre de 2005 hasta marzo 2006, cuando dimitió por enfermedad. Ya recuperado, fue Representante del CSIC en la European Energy Research Alliance, JP-H2 (2010-14) y Coordinador Institucional del CSIC en Aragón (2011-15).

Magnánimo en su esfuerzo, se implicó activamente en la comunidad científica como: vicepresidente del Grupo Especializado de Física del Estado Sólido-GEFES de la Real Sociedad Española de Física (1984-86), miembro del comité de dirección del proyecto RIS (1997-99), vicepresidente de la Sociedad Española de Materiales, SEMAT (1997-2000) y Miembro del Physical and Engineering Steering Committee of the European Science Foundation (1997-2000). También actuó como evaluador externo del Programa de Materiales del De-

partamento de Energía de los Estados Unidos (desde 2003) y miembro del comité asesor para innovación y transferencia del conocimiento del Ministerio de Ciencia e Innovación (2011–14).

Su actividad fue reconocida con diversas distinciones: “*Fellow*” de la American Physical Society (1993), Premio de la Fundación Domingo Martínez (1999), “*Épsilon de Oro*” de la Sociedad Española de Electrocerámica (2005), “*Patrono de Honor*” de la “Fundación para el Desarrollo de las Tecnologías del Hidrógeno en Aragón” (2008) y “*Fellow*” de la European Ceramic Society (2017).

Víctor, siempre concibió la investigación como una actividad de equipos con habilidades complementarias. El procesado de las cerámicas y las pilas de combustible fueron líneas de investigación que lideró durante años en el Grupo de excelencia del Gobierno de Aragón LPM, *Laser processing of materials* (2003–10) y en el Grupo consolidado, ProCaCEF, *Processing and Characterisation of Structural and functional Ceramics* (2011–16). Es de mencionar sus más recientes trabajos en pigmentos prehistóricos realizados en colaboración con su mujer, la catedrática de Historia e investigadora María Pilar Utrillas.

Elegido por sus méritos y actividades *académico*, el 14 de junio de 2007 leyó su discurso *Los materiales cerámicos y el reto energético*, ingresando con la medalla número 39 en la Sección de Físicas de Real Academia de Ciencias de Zaragoza. En ella ha trabajado, con eficacia y con generosa dedicación de su tiempo y experiencia, hasta su fallecimiento, y le recordaremos por su carácter abierto y disposición a colaborar, y por la precisión y nivel de sus intervenciones fruto de sus amplios conocimientos científicos.

Tuvo una vida plena sabiendo sumar, a un imponente legado científico, una estirpe con sus dos hijas, Alodia e Irene y su nieto Roque. Intuyendo el fin varias veces, la fortaleza que poseía siempre le permitía remontar cual “ave fénix”. Esta vez no hubo opción, consciente de su realidad, Víctor pidió la sedación, cesó la medicación y se dejó llevar. Luchador hasta el final, siempre el primero, descansa en paz amigo y compañero; dejás un hueco irremplazable.

**Actividades de la Real Academia de Ciencias Exactas,
Físicas, Químicas y Naturales
durante el año 2019**

Sesiones y actividades corporativas

La Real Academia de Ciencias Exactas, Físicas, Químicas y Naturales de Zaragoza (en adelante Academia) durante el año 2019 ha celebrado 9 sesiones plenarias, seis de ellas ordinarias y tres extraordinarias. Además, para tareas de programación y coordinación de sus sesiones y actividades, se realizaron cuatro reuniones de la Junta de Gobierno el 11 de marzo 24 de abril, 5 de junio y 17 de septiembre.

Todas las sesiones extraordinarias se celebraron a las 19 horas en la Facultad de Ciencias. En la sesión de 4 de abril tuvo lugar el ingreso del académico Sr. D. Andrés Pocoví Juan, que recibió la medalla número 28. En la de 27 de noviembre, se entregaron los Premios de Investigación 2019 a las propuestas de las secciones de Exactas y de Físicas. Ambas se desarrollaron en la Sala de Grados. En la de 20 de marzo, celebrada en la Sala de Profesores, se aprobó por unanimidad la segunda reforma que se hace al *Reglamento de Régimen interior de la Real Academia de Ciencias de Zaragoza* desde su aprobación en 1916.

Las sesiones ordinarias se desarrollaron en la Sala de Profesores de la Facultad de Ciencias. Las de 20 de febrero, 16 de mayo, 19 de junio, 9 de octubre y 6 de noviembre a las 19:00 horas, y la de 11 de diciembre a las 13:00 horas teniendo lugar después la tradicional comida de hermandad previa a la Navidad.

La Academia, siguiendo el turno rotatorio establecido, organizó la solemne *Apertura de Curso 2019-20 de las Academias de Aragón* que se celebró el 22 de octubre de 2019 en el edificio Paraninfo de la Universidad de Zaragoza a las 19 horas. El académico Sr. D. Juan Cacho Palomar dictó la lección inaugural “*Los misterios del olfato y el aroma del vino*”, contestada por el presidente Sr. D. Antonio Elipe Sánchez. En el acto de apertura además de las autoridades académicas, civiles y militares estuvieron presentes las cuatro academias hermanas:

Real Academia de Medicina de Zaragoza

Real Academia de Nobles y Bellas Artes de San Luis

Academia Aragonesa de Jurisprudencia y Legislación

Academia de Farmacia “Reino de Aragón”.

En sesión de 20 de febrero, la Academia analizó y acordó por unanimidad su adhesión al “*Manifiesto de las Academias del Instituto de España*” elaborado en la Reunión de las Academias asociadas al Instituto de España celebrada en Madrid el 18 diciembre de 2018.

El Manifiesto, dirigido a los Gobiernos de las Comunidades Autónomas, al Ministerio de Administraciones Públicas, a la Casa de S. M. el Rey y a los medios de Comunicación reivindica el papel primordial e insustituible de las Academias en el siglo XXI para la protección, conservación y divulgación de nuestro patrimonio histórico y cultural y establece el firme propósito de renovar las Academias, adaptándolas al tiempo actual. Igualmente, se pide un marco legal y reglamentario adecuado y coherente, y una financiación adecuada de las Academias. Estableciendo un régimen de subvenciones dependientes de la administraciones públicas dignas, justas y suficientes, así como favoreciendo el patronazgo mediante una actualización de la “*ley de Mecenazgo*”.

En la sesión de 19 de junio culminó el proceso cuatrienal de renovación de los cargos de la Academia con elección directa del presidente de la Academia y su junta directiva. Con la posterior elección por las secciones de sus presidentes y cargos, la Junta de Gobierno de la Academia queda formada por:

<i>Presidente:</i>	D. Antonio Elipe Sánchez
<i>Vicepresidente:</i>	D. Fernando José Lahoz Díaz
<i>Académico Editor:</i>	D. Enrique Artal Bartolo
<i>Académico Web:</i>	D. Pablo Alonso Gascón
<i>Académico Tesorero:</i>	D. Miguel Ángel Rebolledo Sanz
<i>Académico Secretario:</i>	D. Rafael Navarro Linares
<i>Presidente Sección Exactas:</i>	D. Mariano Gasca González
<i>Presidente Sección Físicas:</i>	D. Pablo Alonso Gascón
<i>Presidente Sección Químicas:</i>	D. Luis Antonio Oro Giral
<i>Presidente Sección Naturales:</i>	Doña María Victoria Arruga Laviña

Reforma del reglamento y elaboración de protocolos

Los resultados de encuesta realizada en 2018 evidenciaron el problema que supone, para el desarrollo de las actividades de la Academia, el creciente envejecimiento de los académicos de número, problema que no es exclusivo de nuestra Academia como se constató en la Reunión de las Academias asociadas al Instituto de España. La limitación a un total de 40 de académicos, diez por sección, unido al incremento de situaciones de imposibilidad de participar activamente durante largos periodos de tiempo por incidencias de salud, propició la búsqueda de formas de renovación de sus miembros no previstas en el actual Reglamento, redactado hace más de un siglo cuando la esperanza de vida de la población era sensiblemente menor y la dinámica social menos exigente y competitiva.

Se optó por hacer unos cambios mínimos al Reglamento, dejando para más adelante una revisión de mayor profundidad. Con esta condición, en la sesión de 20 de marzo cristalizaron los trabajos previos aprobando una modificación de los artículos 2º, 6º y

27º del Reglamento vigente. Con ella se amplía y explicita la condición de residencia en Aragón para los académicos numerarios y se desarrolla la figura de *Académico Honorario*, que introducida en la primera reforma del Reglamento de 1972 no se había utilizado hasta la fecha. La forma escogida ha sido la ampliación de las condiciones exigidas para la elegibilidad como *Académico Honorífico*, figura que inicialmente estaba restringida a personas ajenas a la Academia de méritos relevantes. Con los nuevos supuestos se ha creído conveniente aumentar los derechos de asistencia y participación de los académicos honorarios a todo tipo de sesiones científicas y de gobierno.

La modificación del Reglamento mantiene las exigencias previas para el nombramiento de profesionales externos como académicos honorarios y abre dos nuevas vías para poder nombrar también a académicos numerarios. Una se dirige a académicos que habiendo tenido una actividad notable en la Academia, no puedan seguir manteniendo la dedicación exigible y así lo solicite el interesado. La otra se extiende a académicos numerarios que, por motivos razonados de situación personal o baja disponibilidad, sean propuestos por la Academia o por las secciones.

Los académicos numerarios, al recibir el nombramiento de *Académico Honorario*, que es de por vida, libran sus plazas de numerarios, devuelven su medalla a la Academia y se les entrega otra de honorario que queda en su propiedad. Siguen siendo académicos honorarios mientras residan en Zaragoza y podrán usar su título, medalla y asistir a las sesiones de la Academia con voz pero sin voto.

Desde la aprobación de la modificación del Reglamento en marzo de este mismo año ya se han producido dos nombramientos de académicos honorarios generando dos vacantes que indudablemente abren nuevas vías de rejuvenecimiento que se espera den fruto.

Otro proceso de mejora de la gestión de la Academia, paralelo a la reforma del Reglamento, ha sido la aprobación en sesión de 16 de mayo de los “*Protocolos de actuación de la Real Academia de Ciencias de Zaragoza*”. El documento, compuesto de tres protocolos y tres procedimientos relacionados, ha recopilado el marco reglamentario, las costumbres no escritas y los acuerdos vigentes para el funcionamiento de los órganos colegiados de la Academia así como para el desarrollo de sus sesiones ordinarias, sesiones extraordinarias y juntas de las secciones.

En la elaboración de estos Protocolos de la Academia se tomó como referencia las normativas de órganos colegiados de corporaciones públicas análogas, homologando a los académicos con los derechos y deberes de sus miembros. Entre otros se han reconocido y regulado los derechos de:

- i) Votación no presencial, con las posibilidades de “*voto anticipado por correo*” para votaciones nominales y secretas y “*voto delegado*” para votaciones no secretas.

- ii)* Inclusión de puntos en el orden del día, estableciendo el procedimiento y los avales necesarios.
- iii)* Expresión de votos particulares e inclusión en las actas.
- iv)* Consulta de las Actas de las sesiones.

Igualmente, se han introducido medidas para mejorar la transparencia de las actuaciones de gobierno tales como explicitar las situaciones de incompatibilidad en las votaciones nominales de académicos, premios . . .

El conjunto se ha completado con la aprobación en la misma sesión de 16 de mayo de la “*Carta de derechos y deberes de los académicos numerarios*”, que es corolario de los Protocolos y recoge en forma escueta un decálogo de los derechos y deberes de los académicos numerarios reconocidos en el Reglamento para facilitar el conocimiento del funcionamiento de la Institución.

Carta de derechos y deberes de los académicos numerarios

DERECHOS:

- 1- Asistir y participar con voz y voto en las sesiones ordinarias y extraordinarias de la Real Academia, así como en las Juntas de su Sección.
- 2- Recibir un Diploma de nombramiento y usar como distintivo una medalla numerada en el reverso y con el título de la Real Academia en el anverso pendiente de un cordón de seda azul que será propiedad de la Academia.
- 3- Hacer valer su condición de Académico en publicaciones, intervenciones y solicitudes a las administraciones públicas y otras Instituciones, y usar públicamente la medalla que le acredita en actos públicos.
- 4- Elegir y ser candidato a los cargos de la Junta de Gobierno de la Real Academia y de su Sección
- 5- Estar puntualmente informado de los acuerdos y debates de la Real Academia y de su Sección, teniendo acceso, mediante los procedimientos que se establezcan, a Actas, propuestas y material utilizado en los debates.
- 6- Formular por escrito voto particular cuando disienta de las decisiones que se tomen en sesiones de la Real Academia o en Juntas de su Sección y que figure en el acta correspondiente.

- 7- Incluir puntos en el orden del día de sesiones ordinarias de la Real Academia o de Juntas de su Sección, siempre que no estén convocadas y cuente con el aval de cuatro académicos para las sesiones y de dos para las Juntas.
- 8- Votar en secreto la aprobación de propuestas o nombramientos de académicos, cargos de la Junta de Gobierno o de su Sección, premios de investigación y modificaciones del Reglamento.
- 9- Votar anticipadamente por correo en todas las votaciones secretas que se realicen en las sesiones ordinarias de la Real Academia o en las Juntas de su Sección.
- 10- Delegar su voto en otro académico para puntos del orden del día de sesiones ordinarias de la Real Academia o de Juntas de su Sección, siempre que proceda.

DEBERES:

- 1- Asistir con asiduidad a las sesiones ordinarias y extraordinarias de la Real Academia, así como a las Juntas de su Sección.
- 2- Abstenerse en debates y votaciones de propuesta y de nombramiento de nuevos académicos o de premiados cuando tenga con ellos parentesco de primer o segundo grado, manifiesta amistad o enemistad.
- 3- Participar activamente en todas las actividades que organice la Real Academia y en especial en las de divulgación y difusión científica.
- 4- Contribuir con sus tareas científicas a los fines de la Real Academia, presentando en su Sección los trabajos que tenga por conveniente.
- 5- Presentar en la Real Academia o en su Sección, los trabajos e informes que por turno le sean encomendados.
- 6- Informar puntualmente a la Real Academia de los temas que tuviera conocimiento y sean de interés para la Corporación, así como de su participación, en condición de académico, en conferencias, actos y actividades públicas.
- 7- Desempeñar con eficacia los cargos que la Real Academia o su Sección le confieran.
- 8- Presentar iniciativas o sugerencias de mejora del funcionamiento de la Real Academia y de su Sección, así como de las distintas actividades que éstas organicen.
- 9- Mantener un comportamiento científico, ético y social acorde con la dignidad de su nombramiento como Académico numerario.
- 10- Residir en la Comunidad Autónoma de Aragón, informando a la Real Academia cuando cambie su lugar de residencia.

Altas y bajas de académicos numerarios y correspondientes

Bajas de académicos numerarios:

Sr. D. Mateo Gutiérrez Elorza de la sección de Naturales, que desde su ingreso en la Real Academia el 21 de mayo de 1988 ostentó la medalla número 8. En sesión de 16 de mayo se acordó darle de baja por incumplimiento reiterado de sus obligaciones de asistencia a las sesiones y actividades de la Academia.

Sr. D. Luis Joaquín Boya Ballet de la sección de Físicas, que desde su ingreso en la Academia el 26 de noviembre de 1996 ocupó la medalla número 18. En sesión de 16 de mayo en consideración a su presente situación y a su destacada actividad fue nombrado *Académico Honorario* por unanimidad. La correspondiente medalla y título le fue entregado en un acto íntimo el 7 de noviembre.

Sr. D. Rafael Núñez-Lagos Roglá de la sección de Físicas, que desde su ingreso en la Academia el 22 enero 1997 ocupó la medalla número 7. En sesión de 9 de octubre, en consideración a su trayectoria y destacada actividad, su solicitud de pasar a ser *Académico Honorario* fue aprobada por unanimidad.

Ingreso de académicos numerarios:

El 4 de abril el académico electo Sr. D. Andrés Pocoví Juan, presentó su discurso de ingreso “*Geología Pirenaica vista desde el Sur*”, recibiendo la medalla número 28 siendo respondido por el académico Sr. D. Juan Pablo Martínez Rica.

Nombramiento de académicos numerarios:

En sesión de 9 de octubre se eligieron tres nuevos académicos de número. La sección de Físicas eligió al Sr. D. Manuel Asorey Carballeira catedrático del Departamento de Física Teórica de la Facultad de Ciencias que, en su caso, recibirá la medalla número 18. La sección de Naturales eligió a la Sra. Doña Gloria Cuenca Bescós y al Sr. D. José Luis Simón Gómez ambos catedráticos del Departamento de Ciencias de la Tierra de la Facultad de Ciencias que, en su caso y respectivamente, recibirán las medallas número 38 y 12.

Firma de convenios

El 26 de noviembre la Academia firmó un convenio de colaboración con el Grupo San Valero en materia docente y científica por el cual se compromete a aportar una dotación económica de 2.000 euros anuales para financiar los dos premios de investigación que la Academia concede cada año. Por su parte, la Academia se compromete a colaborar en

actividades docentes, impartir conferencias y la publicación de artículos científicos en la Revista de la Academia.

Financiación

En virtud del convenio de colaboración firmado con el Grupo San Valero se pudo dotar con 1000 euros cada uno de los dos premios de investigación de la Academia 2019, entregados el 27 de noviembre. Se recupera así la dotación económica de estos premios interrumpida en 2012 por la carencia de fondos propios y la ausencia de convocatorias de financiación específica para el funcionamiento de las Academias reconocidas por el Instituto de España.

En la convocatoria de ayudas de la Universidad de Zaragoza para la edición de publicaciones científicas, se solicitó una subvención para costear la edición y distribución de la Revista de la Academia, obteniendo a tal fin 775 euros.

Durante este año ha seguido sin haber convocatorias para la subvención de los gastos de funcionamiento de las Academias, no se han recibido otra financiación para sufragarlos y los habidos se han cargado a las reducidas reservas de la Academia.

Publicaciones de la Academia

La Academia, como es costumbre, en la Solemne apertura del curso 2019-2020 de las Academias de Aragón de 22 de octubre editó y distribuyó entre los asistentes una publicación con el discurso “*Los misterios del olfato y el aroma del vino*” del académico ponente Sr. D. Juan Cacho Palomar, la intervención del Presidente de nuestra Academia Sr. D. Antonio Elipe Sánchez y el elenco de los académicos de las cinco academias participantes.

Se ha publicado el volumen 73 de la Revista de la Academia de Ciencias de Zaragoza correspondiente a 2018 tanto en papel como en acceso libre en la Web. Igualmente se publicó el discurso de ingreso del Sr. D. Andrés Pocoví Juan y la respuesta al mismo del Sr. D. Juan Pablo Martínez Rica.

Organización de conferencias y eventos

La Academia durante 2019 ha organizado dos ciclos de divulgación científica de tres conferencias cada uno que se desarrollaron en primavera y en otoño en las instalaciones de la Obra social de Ibercaja del Patio de la Infanta, c/ San Ignacio de Loyola 16, a las 19 horas.

Ciclo de conferencias de primavera: “Fronteras de la Física”

Organizado por la Sección de Físicas, el ciclo se desarrolló con los títulos de conferencias y protagonistas siguientes:

7 de marzo, *Fabricando el futuro: de la molécula a la aplicación a través del procesado*, impartida por el Sr. D. Carlos Sánchez Somolinos, investigador del Instituto de Ciencia de Materiales de Aragón (CSIC-Universidad de Zaragoza) y premio investigación 2017 de la Academia. La conferencia fue presentada por el académico Sr. D. Pablo Alonso Gascón, que moderó el turno de preguntas posterior.

14 de marzo, *La aceleración del Universo*, impartida por la Sra. Doña María Pilar Ruiz Lapuente, líder de grupo de investigación en el Instituto de Física Fundamental del Consejo Superior de Investigaciones Científicas (Madrid) y miembro de la Academia Europea. La conferencia fue presentada por el académico Sr. D. Juan Bartolomé Sanjoaquín que moderó el turno de preguntas posterior.

21 de marzo, *Epidemias globales. Uno de los grandes retos actuales de la humanidad*, impartida por el Sr. D. Yamir Moreno Vega, director del Instituto Universitario de Investigación de Biocomputación y Física de Sistemas Complejos de la Universidad de Zaragoza. La conferencia fue presentada por el académico Sr. D. Miguel Ángel Rebolledo Sanz que moderó el turno de preguntas posterior.

Ciclo de conferencias de otoño: “Impacto de las nuevas tecnologías en la evolución biológica”

Organizado por la Sección de Naturales el ciclo se desarrolló con los títulos y protagonistas siguientes:

16 de octubre, *Naturaleza y futuro del “ser humano”*, impartida por el Sr. D. Andrés Moya Simarro, catedrático de Genética en el Instituto de Biología Integrativa de Sistemas, Universidad de Valencia y promotor del Instituto Cavanilles de Biodiversidad y Biología Evolutiva del Centro de Astrobiología (CSIC-INTA). La conferencia fue presentada por la académica Sra. Doña María Victoria Arruga Laviña que moderó el turno de preguntas posterior.

23 de octubre, *Astrobiología, despertando de un sueño milenario*, impartida por el académico Sr. D. Juan Pablo Martínez Rica, Académico Numerario de la Real Academia de Ciencias Exactas, Físicas, Químicas y Naturales de Zaragoza, ha sido Vicepresidente de la Academia, investigador del CSIC y director del Instituto Pirenaico de Ecología. La conferencia fue presentada por el académico Sr. D. Juan Marín Velázquez que moderó el turno de preguntas posterior.

30 de octubre, *Afrontamos la década D de la guerra contra el Cáncer*, impartida por el Sr. D. Alberto Jiménez Schuhmacher, jefe del Grupo de Investigación sobre Oncología Molecular del Instituto de Investigación Sanitaria de Aragón (IIS Aragón), Centro de Investigación Biomédica de Aragón, Hijo Predilecto de la ciudad de Zaragoza y Aragonés del año en 2018. La conferencia fue presentada por la académica Sra. Doña Caridad Sánchez Acedo que moderó el turno de preguntas posterior.

Otras actividades

24 de enero. *Visita a la fabrica de cerveza La Zaragozana* que fue organizada por el Sr. D. Fernando Lahoz Díaz.

25 de junio. *Visita al Parque Nacional de Ordesa* que en 2019 celebró el centenario de su declaración como Parque Nacional y que fue organizada por el Sr. D. Juan Pablo Martínez Rica.

19 de noviembre. *Visita a las instalaciones de la Base Aérea de Zaragoza* (Alas 15 y 31, y GRUNOMAC) organizada por el Sr. D. Antonio Elipe Sánchez.

Premios de investigación de la Academia

Cumplidos los trámites exigidos de entrega de un artículo de su ámbito y especialidad para su publicación en la Revista de la Academia, en la sesión extraordinaria de 27 de noviembre se procedió a la exposición de los trabajos y a la entrega de los Premios de investigación de la Real Academia de 2019 que correspondieron a:

Por la Sección de Exactas: Sr. D. Juan Manuel Peña Ferrández, catedrático de la Universidad de Zaragoza, que presentó su trabajo: “*Positivity, accuracy, optimality and applications*”.

Por la Sección de Físicas: Sr. D. David Zueco Laínez, contratado sénior ARAID en el Instituto de Ciencia de Materiales de Aragón (instituto mixto CSIC-Universidad de Zaragoza) y jefe del departamento “Physics of Materials and Nanosystems”, que presentó su trabajo: “*Light-matter interaction in the non perturbative regime: a lecture*”.

En sesión ordinaria de 11 diciembre, se aprobaron las propuestas de Premios de Investigación de la Academia para el año 2020. Por la Sección de Químicas se ha propuesto al Sr. D. Miguel Baya García y por la Sección de Naturales al Sr. D. Blas Lorenzo Valero Garcés. Ambos aceptaron las propuestas y su concesión definitiva se hará en 2020 cuando cumplan las condiciones exigidas.

Honores, distinciones y nombramientos a académicos

El académico Sr. D. Luis Antonio Oro Giral, ha sido nombrado *doctor honoris causa* por las universidades Complutense de Madrid (22 de mayo) y San Jorge de Zaragoza (30 de Octubre).

El académico Sr. D. Antonio Elipe Sánchez ha sido nombrado *Corresponding Member* por la Section 2 *Engineering Sciences* de la *International Academy of Astronautics*.

El académico Sr. D. Antonio Elipe Sánchez en su condición de Presidente de la Academia fue *miembro del comité de honor* de la XXXVII reunión Bienal de la Real Sociedad Española de Física (RSEF) celebrada en Zaragoza el mes de julio.

El académico Sr. D. Mariano Gasca González el 10 de abril ingresó como académico correspondiente de la Academia de Ciencias de Granada con el discurso: “*Los orígenes del Análisis Numérico en España*”.

El académico Sr. D. Manuel Silva Suárez ha sido Presidente de Honor (*Honorary Chair*) de la 24th IEEE *International Conference on Emerging Technologies and Factory Automation* (ETFAs 2019) celebrada en Zaragoza en septiembre y fue objeto de un acto de homenaje de esta comunidad científica el 12 de este mes.

Participación en la organización de conferencias y congresos

El académico Sr. D. Pablo J Alonso Gascón ha sido miembro del Comité organizador del congreso: *XXXVII Reunión Bienal de la Real Sociedad Española de Física* (RSEF) celebrado en las instalaciones de la Universidad Zaragoza en julio.

El académico Sr. D. Enrique Artal Bartolo ha sido miembro del Comité organizador del congreso: *Geometry in Pyrenees*, celebrado en el mes de septiembre en Pau (Francia) y es miembro del Comité Científico de la *Bienal de la RSME 2021*, a celebrar en Ciudad Real en febrero de 2021.

El académico Sr. D. José F Cariñena Marzo ha sido miembro del Comité científico del congreso: *New challenges in Quantum Mechanics: Integrability and Supersymmetry*, celebrado en Benasque (Huesca) el mes de Septiembre.

El académico Sr. D. Alberto Elduque Palomo ha sido miembro del Comité organizador del congreso: *Workshop on Differential Geometry and Non-associative Algebras*, celebrado en el Centre International de rencontres Mathématiques – CIRM-Luminy, Marsella (Francia) en el mes de noviembre.

El académico Sr. D. José Esteban Galé Gimeno ha sido co-organizador del congreso: XIV EITA *Research Meeting in Approximation Theory 2019*, celebrado en Monzón (Huesca) en el mes de octubre.

El académico Sr. D. Fernando J. Lahoz Díaz ha sido miembro de la Comisión Rectora del congreso: V *Meeting of Italian and Spanish Crystallographic Associations*, MISCA2019, celebrado en Nápoles (Italia) el mes de septiembre.

El académico Sr. D. Juan Marín Velázquez ha sido miembro del Comité científico del congreso: XIII *Reunión de la Sociedad Española de Cultivo In Vitro de Tejidos Vegetales* (SECIVTV): “*Retos del cultivo de tejidos vegetales en la era de la bioeconomía*” celebrada en Vitoria-Gasteiz en septiembre.

La académica Sra. Doña María Luisa Peleato Sánchez ha sido miembro del Comité científico del congreso: II *Congreso Iberoamericano de Cianotoxinas* y VI *Ibérico de Cianotoxinas*, celebrado en las instalaciones de la Universidad de Murcia en julio.

El Académico Sr. D. Miguel Ángel Rebolledo ha sido miembro del Comité Científico del congreso: OPTOEL 2019 (XI *Reunión Española de Optoelectrónica*), celebrado en Zaragoza en el mes de julio.

Conferencias y cursos impartidos por nuestros académicos

La académica Sra. Doña María Victoria Arruga Laviña ha impartido la ponencia: *La huella del ADN en la evolución de la vida*, en la “*Ceremonia de Apertura del Curso 2018-19 de la Universidad de la Experiencia*” celebrada en el Palacio Moncada de Fraga (Huesca) el mes de febrero y en la “*Ceremonia de Clausura del Curso 2018-19 de la Universidad de la Experiencia*” celebrada en el Centro Cultural y Juvenil de Binéfar (Huesca) el mes de mayo.

El académico Sr. D. Juan Cacho Palomar ha impartido la ponencia: *El Vino: Del Neolítico al siglo XXI* en la “*Ceremonia de Apertura del Curso 2018-19 de la Universidad de la Experiencia*”, celebrada en el Salón de Actos del Centro Cultural Juvenil de Binéfar (Huesca) el mes de octubre.

El académico Sr. D. Fernando J. Lahoz Díaz ha impartido la conferencia inaugural: *Ordenando la Ciencia: algunas curiosidades sobre la Tabla Periódica de los Elementos*, de la “*Semana de la Ciencia y la Tecnología del CSIC en Aragón*”, celebrada en Zaragoza el mes de Noviembre.

El académico Sr. D. Manuel Silva Suárez ha impartido las conferencias inaugurales:

- *Formal Methods and Simulation: Cooperation makes strength*, en el marco del congreso “*10th Triennial EUROSIM Congress*” celebrado en Logroño en el mes de julio.
- *Individuals, populations and fluidization: A Petri net based perspective*, en el marco del “*Seminario Internacional sobre Sistemas Discretos e Híbridos*” celebrado en el CINVESTAV (Centro de Investigaciones y Estudios Avanzados) Guadalajara, Jalisco (México) en Octubre.

El académico Sr. D. Enrique Artal Bartolo ha impartido las conferencias plenarias:

- *Cyclotomic Zariski tuples with abelian fundamental group. From the pair to the complement*, en el congreso “*Branched Coverings, Degenerations, and Related Topics*” celebrado en Hiroshima (Japón) el mes de marzo.
- *Cyclic covers of weighted projective planes; applications to weighted-Le-Yomdine singularities*, en el congreso “*Némethi 60: Geometry and Topology of Singularities*” celebrado en Budapest (Hungría) el mes de mayo.
- *Hermitian and Riemannian geometry of plane curves*, en el congreso “*Geometries in Pyrenees*” celebrado en Pau (Francia) el mes de septiembre.
- *Torsion divisors of plane curves and Zariski pairs*, en el congreso “*Workshop on Topological and Analytical Methods in Singularity Theory*” celebrado el mes de noviembre en Guanajuato (México).

El académico Sr. D. José Esteban Galé Gimeno ha impartido la conferencia plenaria: *On domains of functions of Cesàro operators. Poisson equation and discrete Hilbert transform*, en el congreso “*Third Fractional Calculus Meeting*” celebrado en Zaragoza en septiembre

El académico Sr. D. Fernando J. Lahoz Díaz ha impartido la conferencia plenaria: *Highlights of Chemical Research at ISQCH – The Case of Chiral Metal Complexes: Catalysts for Enantioselective Synthesis* en la reunión “*2nd Sino-Spain Research and Innovation Forum*” celebrado en la Universidad de Nanning Tech (Nanjing, China) el mes de Octubre.

El académico Sr. D. Juan Marín Velázquez ha impartido la conferencia magistral: *El cultivo in vitro de plantas: algo más que micropropagación*, en el congreso “*XIII Reunión de la Sociedad Española de Cultivo In Vitro de Tejidos Vegetales (SECIVTV): Retos del cultivo de tejidos vegetales en la era de la bioeconomía*” celebrada en Victoria-Gasteiz en septiembre.

El académico Sr. D. José F Cariñena Marzo ha impartido la conferencia de clausura: *Lie and quasi-Lie systems in Quantum Mechanics*, en el congreso “*New challenges in Quantum Mechanics: Integrability and Supersymmetry*” celebrado en Benasque (Huesca) el mes de Septiembre.

El académico Sr. D. Luis Antonio Oro Giral ha impartido la conferencia plenaria: *From Organometallic Complexes to Homogeneous Catalysis: Forty years of Platinum Group Metal Chemistry*, en el congreso “*UK-SPAIN Organometallic Chemistry Symposium*” celebrado en Alcalá de Henares el mes de septiembre.

El académico Sr. D. Alberto Elduque Palomo ha impartido las conferencias invitadas:

- *Octonions in low characteristics*, en el congreso “*Third Workshop New Trends in Quaternions and Octonions*” celebrado en la Universidad de Coímbra (Portugal) en febrero.
- *Graded-simple algebras and loop algebras*, en el congreso “*II International Workshop on Non-Associative Algebras*” celebrado en la Universidad de Oporto (Portugal) entre abril y mayo.
- *Graded-simple algebras and loop algebras*, en el congreso “*International Workshop on Non-associative Algebras and Geometry*” celebrado en la Bonne Bay Marine Station, Memorial University of Newfoundland (Canadá) en agosto.
- *Clifford algebras as twisted group algebras and the Arf invariant*, en el “*Día de Álgebra, dedicado a Helena Albuquerque, con motivo de su aniversario*” celebrado en la Universidad de Coímbra (Portugal) en el mes de septiembre.
- *Triality*, en el congreso “*Workshop on Differential Geometry and Nonassociative Algebras*” celebrado en CIRM-Luminy, Marsella (Francia) en noviembre.

La académica Sra. Doña María Teresa Lozano Imízcoz ha impartido la conferencia invitada: *About orbifolds and numerical groups* en el congreso “*2019 Interdisciplinary Colloquium in Topology and its Applications*” celebrado en la Universidad de Vigo el mes de junio.

El académico Sr. D. Manuel Silva Suárez ha impartido la conferencia invitada: *Professional organizations in Spanish engineering: Administration bodies; Private associations & Chartered institutes*, en el coloquio “*150 anos da criação da Associação dos Engenheiros Civis Portugueses Ordem dos Engenheiros*” celebrado en Lisboa (Portugal) el mes de diciembre.

El académico Sr. D. Enrique Artal Bartolo ha impartido el curso: *Weighted projective planes and weighted Lê-Yomdine singularities*, en el congreso “*Workshop on Topological and Analytical Methods in Singularity Theory*” celebrado en Guanajuato (México) el mes de noviembre.

El académico Sr. D. Alberto Elduque Palomo ha impartido el seminario: *Codes, Structures, and exceptional Lie algebras*, en el encuentro “*Coloquio del Centro de Matemática de la Universidad de Coímbra*” celebrado en Coímbra (Portugal) el mes de febrero.

El académico Sr. D. Juan Cacho Palomar ha impartido las siguientes conferencias:

- *El Vino: Del Neolítico al Siglo XXI* en la Universidad de la Experiencia en el Salón de Actos del Palacio Ardid de Alcañiz, el mes de febrero de 2019 y en el Salón de Actos del Centro Antonio Fernandez Molina de Alagón (Zaragoza) el mes de marzo.
- *El Aroma del Vino y su Percepción*, en la Jornada Técnica “*Vinos Old-Vidaos*” en EVENA, Olite (Navarra) el mes de mayo.

El académico Miguel Pocoví Mieras ha impartido la conferencia: *La venganza de Moctezuma: El maíz y la pelagra*, en la reunión de la “*Asociación de Amigos del País*” celebrada en Avilés (Asturias) el mes de noviembre.

El académico Sr. D. Luis Antonio Oro Giral ha impartido la conferencia: *Mechanistic Studies on Rhodium and Iridium Homogeneous Catalysts*, en la “*Academia das Ciencias de Lisboa*”, de la que es miembro, el mes de octubre.

El académico Sr. D. José S. Urieta Navarro, como profesor invitado por la Universidad Jaume I de Castellón en el ámbito del Master Interuniversitario de Química Sostenible (curso 2019-2020), ha impartido el curso: *Fotoquímica y Electroquímica Ambiental*, en noviembre.

Otras contribuciones relevantes de nuestros académicos

Los académicos Srs. D. Pablo J. Alonso Gascón y D. Luis A. Oro Giral conjuntamente impartieron la conferencia de divulgación: *Ordenando Elementos Químicos (A dialogue between Chemistry and Physics about Mendeleev’s Table of Elements)*, en el programa “*Física para todos*” organizado por la “*XXXVII reunión Bial de la Real Sociedad Española de Física (RSEF)*” en el centro cultural El Patio de la Infanta de Zaragoza en el mes de julio.

La académica Sra. Doña María Victoria Arruga Laviña, en la tarea de divulgación de la Ciencia, ha publicado el artículo: *¿Hay uracilo en el ADN? Y si lo hay ¿para qué sirve?* publicado en El País, el 23 de Mayo y ha participado en el programa de divulgación científica de Aragón TV “*Aragón en abierto*”–*La vida que somos* el 8 de noviembre.

El académico Sr. D. Alberto Elduque Palomo ha organizado la XVI temporada del *Taller de Talento Matemático*, actividad dirigida a estudiantes de secundaria, desde 3º de ESO hasta 2º de Bachillerato, así como la *Fase Aragonesa de la Olimpiada Matemática Española*.

El académico Sr. D. Juan Marín Velázquez ha publicado en el repositorio Digital CSIC el trabajo de divulgación científica: *Organogénesis*, URL: <http://hdl.handle.net/10261/192626> accesible en el canal EEAD-CSIC en Youtube.

El académico Sr. D. Manuel Silva Suárez en el marco de la colección: *Técnica e Ingeniería en España*, ha editado los volúmenes: *Del noventayochismo al desarrollismo* (vol. **VIII**, 552 pp.), y *Trazas y reflejos culturales externos, 1898-1973* (vol. **IX**, 540 pp.) que han sido publicados por la Real Academia de Ingeniería / Institución Fernando el Católico / Prensas Universitarias de Zaragoza.

El académico Sr. D. Manuel Silva Suárez presentó los nuevos volúmenes **VIII** y **IX** de la colección en actos celebrados en Zaragoza y en Madrid y la colección completa (hasta ahora de diez tomos, unas 6.800 pp.) en actos, con diversos matices, celebrados en Logroño, Guadalajara (México), Valladolid, Gijón, Évora (Portugal), Lisboa (Portugal), y Barcelona.

Composición de la Academia a 1 de Enero de 2018

Junta de Gobierno

<i>Presidente:</i>	D. Antonio Elipe Sánchez
<i>Vicepresidente:</i>	D. Fernando José Lahoz Díaz
<i>Académico Editor:</i>	D. Enrique Artal Bartolo
<i>Académico Web:</i>	D. Pablo Alonso Gascón
<i>Académico Tesorero:</i>	D. Miguel Ángel Rebolledo Sanz
<i>Académico Secretario:</i>	D. Rafael Navarro Linares

Académicos Numerarios y Honorarios

A fecha 1 de Enero de 2020 hay 34 académicos de número, 2 académicos honorarios y 3 académicos nombrados que no han leído su discurso. Se han listado por secciones citando número de medalla y fecha de ingreso o de nombramiento.

Sección de Exactas

<i>Presidente:</i>	D. Mariano Gasca González	(medalla 1)	1 diciembre 1988
<i>Académicos:</i>	Doña María Teresa Lozano Imízcoz	(medalla 22)	22 enero 1998
	D. Manuel Calvo Pinilla	(medalla 25)	10 marzo 1998
	D. Eladio Domínguez Murillo	(medalla 27)	25 marzo 1999
	D. Antonio Elipe Sánchez	(medalla 16)	30 marzo 2000
	D. Jesús Bastero Eleizalde	(medalla 17)	9 noviembre 2000
	D. Alberto Elduque Palomo	(medalla 29)	23 febrero 2006
	D. Enrique Artal Bartolo	(medalla 4)	24 noviembre 2009
	D. Manuel Silva Suárez	(medalla 19)	20 octubre 2014
	D. José Esteban Galé Gimeno	(medalla 10)	31 enero 2018

Sección de Físicas*

<i>Presidente:</i>	D. Pablo Javier Alonso Gascón	(medalla 35)	16 mayo 2002
<i>Académicos:</i>	D. Miguel Ángel Rebolledo Sanz	(medalla 14)	11 mayo 2000
	D. José Fernando Cariñena Marzo	(medalla 33)	6 noviembre 2001
	D. Víctor Orera Clemente	(medalla 39)	14 junio 2007
	D. Fernando Solsona Motrel	(medalla 23)	14 febrero 2008
	D. Rafael Navarro Linares	(medalla 40)	4 junio 2009
	D. Juan Bartolomé Sanjoaquín	(medalla 3)	27 octubre 2016
	D. Ricardo Ibarra García	(medalla 20)	19 diciembre 2016
	D. Manuel Asorey Carballeira		Electo el 9 de octubre de 2019

***En esta sección hay una vacante**

Académicos Honorarios

D. Luis Joaquín Boya Balet	16 mayo 2019
D. Rafael Núñez Lagos Roglá	9 octubre 2019

Sección de Químicas

<i>Presidente:</i> D. Luis Antonio Oro Giral	(medalla 11)	4 junio 1981
<i>Académicos:</i> D. José Santiago Urieta Navarro	(medalla 5)	2 diciembre 1997
D. Carlos Gómez-Moreno Calera	(medalla 6)	21 octubre 1999
D. Juan Forniés Gracia	(medalla 24)	26 junio 2000
D. Ángel García de Jalón Comet	(medalla 30)	29 noviembre 2001
D. Juan Francisco Cacho Palomar	(medalla 13)	2 diciembre 2003
D. Miguel Pocoví Mieras	(medalla 32)	20 mayo 2004
D. José Luis Marqués Insa	(medalla 37)	24 noviembre 2005
D. José Luis Serrano Ostáriz	(medalla 26)	12 diciembre 2006
D. Fernando Lahoz Díaz	(medalla 2)	3 mayo 2017

Sección de Naturales*

<i>Presidente:</i> Doña María Victoria Arruga Laviña	(medalla 34)	10 diciembre 2015
<i>Académicos:</i> D. Juan Marín Velázquez	(medalla 15)	10 abril 1997
Doña María Caridad Sánchez Acedo	(medalla 9)	12 diciembre 2000
D. Juan Pablo Martínez Rica	(medalla 36)	24 octubre 2002
Doña María Luisa Peleato Sánchez	(medalla 21)	4 junio 2011
D. Andrés Pocoví Juan	(medalla 28)	4 abril 2019
Doña Gloria Cuenca Bescós		<i>Electa el 9 de octubre de 2019</i>
D. José Luis Simón Gómez		<i>Electo el 9 de octubre de 2019</i>

***En esta sección hay dos vacantes.**

Académicos Correspondientes

A fecha 1 de Enero hay 48 académicos correspondientes que se han distribuidos por secciones y ordenados por fechas de nombramiento

Sección de Exactas

D. Henry Mascart	(19 junio 1967)
D. José M. Montesinos Amilibia	(7 abril 1992)
D. Claude Brezinski	(9 mayo 2002)
D. Charles A. Micchelli	(9 mayo 2002)
D. José Luis Fernández Pérez	(24 septiembre 2002)
D. Gilles Pisier	(24 septiembre 2002)

D. José Ángel Docobo Durántez	(21 abril 2005)
D. Sylvio Ferraz Mello	(21 abril 2005)
D. Francisco Marcellán Español	(4 noviembre 2004)
D. Santos González Jiménez	(27 abril 2006)
D. José Luis Viviente Mateu	(5 octubre 2006)
D. Efim Zelmanov	(5 octubre 2011)
D. Manuel Doblaré Castellano	(13 febrero 2013)
D. Jesús Carlos Fernández Asensio	(7 junio 2013)
D. José Garay Pablo	(3 junio 2015)
D. Juan Luis Vázquez Suárez	(3 junio 2015)
D. Jesús Sanz Serna	(24 octubre 2018)

Sección de Físicas

D. Alberto Galindo Tisaire	(1 octubre 1967)
D. Eusebio Bernabeu Martínez	(1982)
D. Giuseppe Marmo	(9 mayo 2002)
Doña María Josefa Yzuel Giménez	(9 mayo 2002)
D. José Adolfo de Azcárraga	(25 septiembre 2008)
D. Albert Figueras Dagá	(25 septiembre 2008)
D. Fernando María Legarda Ibáñez	(25 septiembre 2008)
D. Javier Llorca Martínez	(25 septiembre 2008)
D. Miguel V. Andrés Bou	(23 marzo 2009)
D. Javier Sesma Bienzobas	(7 mayo 2014)
D. Juan Ignacio Cirac Sasturaín	(3 junio 2015))
D. Antonio Hernando Grandes	(16 Febrero 2017))
D. Francisco Javier Solís Céspedes	(4 Octubre 2017)

Sección de Químicas

D. Pascual Royo Gracia	(7 abril 1992)
D. Ekkehardt Hahn	(13 junio 2002)
D. Pierre Braunstein	(13 junio 2002)
D. José María Ordovás Muñoz	(13 febrero 2008)
Doña M ^a Carmen Orosia Claver Cabrero	(13 febrero 2008)
D. Avelino Corma Canós	(15 octubre 2015)
D. Fernando Cossío Mora	(15 octubre 2015)

Sección de Naturales

D. Leandro Sequeiros Sanromán	(9 mayo 2002)
D. Emiliano Aguirre Enríquez	(9 mayo 2002)
D. Luis Villar Pérez	(9 mayo 2002)
D. Adrian Michael Harvey	(13 junio 2002)
D. Mario Panizza	(13 junio 2002)

D. Carlos López Otín	(19 diciembre 2006)
D. Peter Carls	(8 mayo 2007)
D. Miguel Delibes de Castro	(23 febrero 2011)
D. Eladio Liñán Guijarro	(3 junio 2015)
D. Francisco García Novo	(15 octubre 2015)
D. Joaquín Villena Morales	(25 febrero 2016)

Zaragoza, diciembre de 2018

INSTRUCCIONES PARA LOS AUTORES

Resumen

The *Revista de la Real Academia de Ciencias* publishes original research contributions in the fields of Mathematics, Physics, Chemistry and Natural Sciences. All the manuscripts are peer reviewed in order to assess the quality of the work. On the basis of the referee's report, the Editors will take the decision either to publish the work (directly or with modifications), or to reject the manuscript.

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Para su publicación en esta Revista, los trabajos deberán remitirse a

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o bien electrónicamente a la cuenta `artal@unizar.es`.

La Revista utiliza el sistema de *offset* de edición, empleando el texto electrónico facilitado por los autores, que deberán cuidar al máximo su confección, siguiendo las normas que aquí aparecen.

Los autores emplearán un procesador de texto. Se recomienda el uso de \LaTeX , para el que se han diseñado los estilos `academia.sty` y `academia.cls` que pueden obtenerse directamente por internet en <http://www.raczar.es> o por petición a la cuenta de correo electrónico: `artal@unizar.es`.

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El texto de los trabajos, redactados en español, inglés o francés, no deberá exceder de 25 páginas, aunque se recomienda una extensión de 6 a 20 páginas como promedio. El texto de cada página ocupará una caja de 16×25 cm., con espacio y medio entre líneas.

2. Presentación del trabajo.

Los trabajos se presentarán con arreglo al siguiente orden: En la primera página se incluirán los siguientes datos:

- a) *Título del trabajo*: Conciso, pero ilustrativo, con mayúsculas.
- b) *Autor*: Nombre y apellidos del autor o autores, con minúscula.
- c) *Centro*: Centro donde se ha realizado, con su dirección postal.
- d) *Abstract*: En inglés y con una extensión máxima de 200 palabras.
- e) *Texto*

- A) Los encabezamientos de cada sección, numerados correlativamente, serán escritos con letras **minúsculas** en negrita. Los encabezamientos de subsecciones, numerados en la forma 1.1, 1.2, . . . , 2.1, 2.2, . . . , se escribirán en *cursiva*.
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3. Notas finales

La Revista permite la inclusión de fotografías o figuras en color, con un coste adicional que correrá a cargo de los autores.

Enrique Artal
Académico Editor

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6. *Anales de la Academia Nacional de Ciencias Exactas, Físicas y Naturales de Buenos Aires*
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26. *Functiones et Approximatio Commentarii Mathematici* - Poznań
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28. *Hiroshima Mathematical Journal*

29. *Hokkaido Mathematical Journal*
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