Operators and Matrices

Let ν be an inner-product vector space with an ONB $\{|e_j\rangle\}$, so that $\forall|x\rangle \in \nu$ there exists a unique representation

$$|x\rangle \,=\, \sum_j x_j|e_j\rangle\,, \qquad\qquad x_j \,=\, \langle e_j|x\rangle\,. \tag{1}$$

[We remember that if the dimensionality of the vector space is finite, then the sum is finite. In an infinite-dimensional vector space, like, e.g., $\mathcal{L}_2$, the sum is infinite and is called Fourier series.] The isomorphism of the vector spaces allows one to map our space ν onto the vector space $\tilde{\nu}$ formed by the coordinates of the vector with respect to our fixed ONB (see section Vector Spaces):

$$|x\rangle \;\longleftrightarrow\; (x_1, x_2, x_3, \ldots) \,\in\, \tilde{\nu}\,. \tag{2}$$

In the context of this isomorphism—which is very important for practical applications, since it allows one to work with just the numbers instead of abstract vectors—the following question naturally arises. Suppose A is some linear operator that acts on some $|x\rangle \in \nu$ producing corresponding vector $|y\rangle \in \nu$:

$$|y\rangle \,=\, A|x\rangle\,. \tag{3}$$

By the isomorphism,

$$|y\rangle \;\longleftrightarrow\; (y_1, y_2, y_3, \ldots) \,\in\, \tilde{\nu}\,, \tag{4}$$

and we realize that it is crucially important to understand how $(y_1, y_2, y_3, \ldots)$ is obtained from $(x_1, x_2, x_3, \ldots)$ *directly* in the space $\tilde{\nu}$. To this end, we note that

$$y_j \,=\, \langle e_j|y\rangle \,=\, \langle e_j|A|x\rangle \,=\, \langle e_j|A\sum_s x_s|e_s\rangle\,, \tag{5}$$

and, taking into account linearity of the operator A, find that

$$y_j \,=\, \sum_s A_{js}\, x_s\,, \tag{6}$$

where

$$A_{js} \,=\, \langle e_j|A|e_s\rangle\,. \tag{7}$$

We see that the set of numbers $\{A_{js}\}$ defined in accordance with Eq. (7) completely defines the action of the operator A on any vector $|x\rangle$ (in terms

of the coordinates with respect to a given ONB). This set of numbers is called *matrix* of the operator A with respect to the given ONB. If the ONB is fixed or at least is not being explicitly changed, then it is convenient to use the same letter A for both operator A and its matrix (with respect to our ONB). Each particular element A_{js} (say, A_{23}) is called matrix element of the operator A (with respect to the given ONB). In Mathematics, by matrix one means a two-subscript set of numbers (normally represented by a table, which, however is not necessary, and not always convenient) with a ceratin rules of *matrix addition, multiplication of a matrix by a number*, and *matrix multiplication*. These rules, forming *matrix algebra*, are naturally derivable from the properties of linear operators in the vector spaces which, as we have seen above, can be represented by matrices. Let us derive these rules.

Addition. The sum, $C = A + B$, of two operators, A and B, is naturally defined as an operator that acts on vectors as follows.

$$C|x\rangle \;=\; A|x\rangle \;+\; B|x\rangle \;. \tag{8}$$

Correspondingly, the matrix elements of the operator $C = A + B$ are given by

$$C_{ij} \;= A_{ij} \;+\; B_{ij} \;, \tag{9}$$

and this is exactly how a sum of two matrices is defined in matrix theory.

Multiplication by a number. The product $B = \lambda A$ of a number λ and an operator A is an operator that acts as follows.

$$B|x\rangle \;=\; \lambda(A|x\rangle) \;. \tag{10}$$

The product $C = A\lambda$ of an operator A and a number λ is an operator that acts as follows.

$$C|x\rangle \;=\; A(\lambda|x\rangle) \;. \tag{11}$$

If A is a linear operator (which we will be assuming below), then $B = C$, and we do not need to pay attention to the order in which the number and the operator enter the product. Clearly, corresponding matrix is

$$C_{ij} \;=\; B_{ij} \;=\; \lambda A_{ij} \;, \tag{12}$$

and this is how a product of a number and a matrix is defined in the theory of matrices.

Multiplication. The product, $C = AB$, of two operators, A and B, is defined as an operator that acts on vectors as follows

$$C|x\rangle \;=\; A(B|x\rangle) \;. \tag{13}$$

That is the rightmost operator, B, acts first, and then the operator A acts on the vector resulting from the action of the operator B.

The operator multiplication is associative: for any three operators A, B, and C, we have $A(BC) = (AB)C$. But the operator multiplication is not commutative: generally speaking, $AB \neq BA$.

It is easy to check that the matrix elements of the operator $C = AB$ are given by

$$C_{ij} = \sum_s A_{is} B_{sj} \ . \tag{14}$$

And this is exactly how a product of two matrices is defined in matrix theory.

Each linear operator is represented by corresponding matrix, and the opposite is also true: each matrix generates corresponding linear operator.

Previously we introduced the notion of an adjoint (Hermitian conjugate) operator (see Vector Spaces chapter). The operator $A^\dagger$ is adjoint to A if $\forall\, |x\rangle, |y\rangle \in \nu$

$$\langle y|Ax\rangle \ = \ \langle A^\dagger y|x\rangle \ = \ \overline{\langle x|A^\dagger y\rangle} \ . \tag{15}$$

Expanding $|x\rangle$ and $|y\rangle$ in terms of our ONB, one readily finds that

$$\langle y|Ax\rangle \ = \ \sum_{ij} A_{ij}\, y_i^* x_j \ , \tag{16}$$

$$\overline{\langle x|A^\dagger y\rangle} \ = \ \sum_{ij} (A^\dagger_{ji})^*\, x_j y_i^* \ , \tag{17}$$

and, taking into account that Eq. (15) is supposed to take place for *any* $|x\rangle$ and $|y\rangle$, concludes that

$$A^\dagger_{ji} \ = \ A^*_{ij} \ . \tag{18}$$

We see that the matrix of an operator adjoint to a given operator A is obtained from the matrix A by interchanging the subscripts and complex conjugating. In the matrix language, the matrix which is obtained from a given matrix A by interchanging the subscripts is called *transpose* of A and is denoted as A^{T}. By a complex conjugate of the matrix A (denoted as A^*) one understands the matrix each element of which is obtained from corresponding element of A by complex conjugation. Speaking this language, the matrix of the adjoint operator is a complex conjugate transpose of the matrix of the original operator. They also say that the matrix $A^\dagger$ is the Hermitian conjugate of the matrix A. In fact, all the terminology applicable to linear operators is automatically applicable to matrices, because of the above-established isomorphism between these two classes of objects.

For a self-adjoint (Hermitian) operator we have

$$A = A^\dagger \qquad \Leftrightarrow \qquad A_{ji} = A^*_{ij} \, . \tag{19}$$

Corresponding matrices are called Hermitian. There are also anti-Hermitian operators and matrices:

$$A = -A^\dagger \qquad \Leftrightarrow \qquad -A_{ji} = A^*_{ij} \, . \tag{20}$$

There is a close relationship between Hermitian and anti-Hermitian operators/matrices. If A is Hermitian, then iA is anti-Hermitian, and vice versa.

An identity operator, I, is defined as

$$I|x\rangle = |x\rangle \, . \tag{21}$$

Correspondingly,

$$I_{ij} = \delta_{ij} \, . \tag{22}$$

It is worth noting that an identity operator can be non-trivially written as the sum over projectors onto the basis vectors:

$$I = \sum_j |e_j\rangle\langle e_j| \, . \tag{23}$$

Equation (23) is also known as the *completeness* relation for the orthonormal system $\{|e_j\rangle\}$, ensuring that it forms a basis. For an incomplete orthonormal system, corresponding operator is not equal to the identity operator. [It projects a vector onto the sub-space of vectors spanned by this ONS.]

In a close analogy with the idea of Eq. (23), one can write a formula explicitly restoring an operator from its matrix in terms of the operations of inner product and multiplication of a vector by a number:

$$A = \sum_{ij} |e_i\rangle A_{ij} \langle e_j| \, . \tag{24}$$

Problem 26. The three 2×2 matrices, A, B, and C, are defined as follows.

$$A_{12} = A_{21} = 1 \, , \qquad A_{11} = A_{22} = 0 \, , \tag{25}$$

$$-B_{12} = B_{21} = i \, , \qquad B_{11} = B_{22} = 0 \, , \tag{26}$$

$$C_{12} = C_{21} = 0 \, , \qquad C_{11} = -C_{22} = 1 \, . \tag{27}$$

Represent these matrices as 2×2 tables. Make sure that (i) all the three matrices are Hermitian, and (ii) feature the following properties.

$$AA = BB = CC = I\,, \tag{28}$$

$$BC = iA\,, \qquad CA = iB\,, \qquad AB = iC\,, \tag{29}$$

$$CB = -iA\,, \qquad AC = -iB\,, \qquad BA = -iC\,. \tag{30}$$

For your information. Matrices A, B, and C are the famous Pauli matrices. In Quantum Mechanics, these matrices and the above relations between them play a crucial part in the theory of spin.

Problem 27. Show that:
(a) For any two linear operators A and B, it is always true that $(AB)^\dagger = B^\dagger A^\dagger$.
(b) If A and B are Hermitian, the operator AB is Hermitian *only* when $AB = BA$.
(c) If A and B are Hermitian, the operator $AB - BA$ is *anti*-Hermitian.

Problem 28. Show that under canonical boundary conditions the operator $A = \partial/\partial x$ is anti-Hermitian. Then make sure that for the operator B defined as $B|f\rangle = xf(x)$ (that is the operator B simply multiplies any function $f(x)$ by x) and for the above-defined operator A the following important commutation relation takes place

$$AB - BA = I\,. \tag{31}$$

Problem 29. In the Hilbert space $\mathcal{L}_2[-1,1]$, consider a subspace spanned by the following three vectors.

$$e_1(x) = \frac{1}{\sqrt{2}}\,, \tag{32}$$

$$e_2(x) = \frac{1}{\sqrt{2}}\left(\sin\frac{\pi}{2}x + \cos\pi x\right)\,, \tag{33}$$

$$e_3(x) = \frac{1}{\sqrt{2}}\left(\sin\frac{\pi}{2}x - \cos\pi x\right)\,. \tag{34}$$

(a) Make sure that the three vectors form an ONB in the space spanned by them (that is show that they are orthogonal and normalized).
(b) Find matrix elements of the Laplace operator $B = \partial^2/\partial x^2$ in this ONB. Make sure that the matrix B is Hermitian.

Problem 30. In the Hilbert space $\mathcal{L}_2[-1,1]$, consider a subspace spanned by the following three vectors.

$$e_1(x) \,=\, \frac{1}{\sqrt{2}}\,, \tag{35}$$

$$e_2(x) \,=\, \sin \pi x\,, \tag{36}$$

$$e_3(x) \,=\, \cos \pi x\,. \tag{37}$$

(a) Make sure that the three vectors form an ONB in the space spanned by them (that is show that they are orthogonal and normalized).
(b) Show that the subspace is closed with respect to the operator $A = \partial/\partial x$ and find matrix elements of the operator A in the given ONB.
(c) Find matrix elements of the Laplace operator $B = \partial^2/\partial x^2$ in the given ONB.
(d) By matrix multiplication, check that $B = AA$.

Unitary matrices and operators

Consider two different ONB's, $\{|e_j\rangle\}$ and $\{|\tilde{e}_j\rangle\}$. [For example, two different Cartesian systems in the space of geometric vectors.] A vector $|x\rangle$ can be expanded in terms of each of the two ONB's

$$|x\rangle \,=\, \sum_j x_j |e_j\rangle \,=\, \sum_j \tilde{x}_j |\tilde{e}_j\rangle\,. \tag{38}$$

and a natural question arises of what is the relation between the two sets of coordinates. A trick based on the completeness relation immediately yields an answer:

$$\tilde{x}_i \,=\, \langle \tilde{e}_i|x\rangle \,=\, \langle \tilde{e}_i|I|x\rangle \,=\, \sum_j \langle \tilde{e}_i|e_j\rangle\langle e_j|x\rangle \,=\, \sum_j U_{ij}\, x_j\,, \tag{39}$$

where

$$U_{ij} \,=\, \langle \tilde{e}_i|e_j\rangle\,. \tag{40}$$

Analogously,

$$x_i \,=\, \sum_j \tilde{U}_{ij}\, \tilde{x}_j\,, \tag{41}$$

where

$$\tilde{U}_{ij} \,=\, \langle e_i|\tilde{e}_j\rangle \,=\, \overline{\langle \tilde{e}_j|e_i\rangle} \,=\, U^*_{ji}\,. \tag{42}$$

We arrive at an important conclusion that the transformation of coordinates of a vector associated with changing the basis formally looks like the action of a linear operator on the coordinates treated as vectors from $\tilde{\nu}$. The matrix of the operator that performs the transformation $\{x_j\} \to \{\tilde{x}_j\}$ is U, the matrix elements being defined by (40). The matrix of the operator that performs the transformation $\{\tilde{x}_j\} \to \{x_j\}$ is $\tilde{U}$, the matrix elements being defined by (42). Eq. (42) demonstrates that the two matrices are related to each other through the procedure of Hermitian conjugation:

$$\tilde{U} \,=\, U^{\dagger}\,, \qquad U \,=\, \tilde{U}^{\dagger}\,. \tag{43}$$

Since the double transformations $\{x_j\} \to \{\tilde{x}_j\} \to \{x_j\}$ and $\{\tilde{x}_j\} \to \{x_j\} \to \{\tilde{x}_j\}$ are, by construction, just identity transformations, we have

$$\tilde{U}U \,=\, I\,, \qquad U\tilde{U} \,=\, I\,. \tag{44}$$

Then, with Eq. (43) taken into account, we get

$$U^{\dagger}U \,=\, I\,, \qquad UU^{\dagger} \,=\, I\,. \tag{45}$$

The same is automatically true for $\tilde{U} = U^{\dagger}$, which plays the same role as U. The matrices (operators) that feature the property (45) are termed *unitary* matrices (operators).

One of the most important properties of unitary operators, implied by Eq. (45), is that $\forall\, |x\rangle, |y\rangle \in \nu$ we have

$$\langle\, Ux \,|\, Uy \,\rangle \,=\, \langle\, x \,|\, y \,\rangle\,. \tag{46}$$

In words, a unitary transformation of any two vectors does not change their inner product. This fact has a very important immediate corollary. If we take in (46), $|x\rangle \,=\, |e_i\rangle$, $|y\rangle \,=\, |e_j\rangle$ and denote the transformed vectors according to $U|x\rangle = |l_i\rangle$, $U|y\rangle = |l_j\rangle$, we obtain

$$\langle\, l_i \,|\, l_j \,\rangle \,=\, \langle\, Ue_i \,|\, Ue_j \,\rangle \,=\, \langle\, e_i \,|\, e_j \,\rangle = \delta_{i\,j}\,, \tag{47}$$

meaning that an ONB $\{|e_i\rangle\}$ is transformed by U into another ONB, $\{|l_i\rangle\}$. Note, that in two- and three-dimensional real-vector spaces, (47) implies that U can only consist of rotations of the basis as a whole and flips of some of the resulting vectors into the opposite direction (mirror reflections). A bit jargonically, they say that the operator U *rotates* the vectors of the original space ν.

So far, we were dealing with the action of the matrix U in the vector space $\tilde{\nu}$ of the coordinates of our vectors. Let us now explore the action

of corresponding operator U in the original vector space ν. To this end we formally restore the operator from its matrix by Eq. (24):

$$U \;=\; \sum_{ij} |e_i\rangle U_{ij} \langle e_j| \;=\; \sum_{ij} |e_i\rangle \langle \tilde{e}_i | e_j \rangle \langle e_j| \;. \tag{48}$$

Now using the completeness relation (23), we arrive at the most elegant expression

$$U \;=\; \sum_{i} |e_i\rangle \langle \tilde{e}_i| \;, \tag{49}$$

from which it is directly seen that

$$U|\tilde{e}_i\rangle \;=\; |e_i\rangle \;. \tag{50}$$

That is the operator U takes the i-th vector of the *new* basis and transforms it into the i-th vector of the *old* basis.

Note an interesting subtlety: in terms of the *coordinates*—as opposed to the basis vectors, the matrix U is responsible for transforming *old* coordinates into the *new* ones.

Clearly, the relations for the matrix/operator $\tilde{U}$ are identical, up to interchanging tilded and non-tilde quantities.

Any unitary operator U acting in the vector space ν can be *constructed* by its action on some ONB $\{|e_i\rangle\}$. In view of the property (47), this transformation will always produce an ONB and will have a general form of (50). Hence, we can write down the transformation $\{|e_i\rangle\} \to \{|\tilde{e}_i\rangle\}$ explicitly as

$$U|e_i\rangle \;=\; |\tilde{e}_i\rangle \quad \Longleftrightarrow \quad U \;=\; \sum_{i} |\tilde{e}_i\rangle \langle e_i| \;. \tag{51}$$

Applying the identity operator $I = \sum_j |e_j\rangle\langle e_j|$ to the left hand side of the first equation, we arrive at the expansion of the new basis in terms of the old one

$$|\tilde{e}_i\rangle \;=\; \sum_j U_{ji}\, |e_j\rangle, \tag{52}$$

where the matrix U_{ij} is given by

$$U_{ij} \;=\; \langle e_i|U|e_j\rangle \;=\; \langle e_i|\tilde{e}_j\rangle \;. \tag{53}$$

(Compare to Eq. (40).) Thus, for any vector $|x\rangle$ transformed by U, its coordinates in the basis $\{|e_i\rangle\}$ are transformed according to

$$x'_i = \sum_j U_{ij}\, x_j. \tag{54}$$

Note that, in contrast to (39), $\{x_i\}$ and $\{x'_i\}$ are the coordinates of the original vector and the "rotated" one in the *same* basis $\{|e_i\rangle\}$. Interestingly, since the coordinates of the vector $|e_j\rangle$ itself are $x_k = 0$ for all k except $k = j$, $x_j = 1$, the matrix element U_{ij} is nothing but the i-th coordinate of the transform of $|e_j\rangle$. The latter property can be also used to explicitly construct U_{ij}.

Rotations in real-vector spaces

Rotations in two- and three- dimensional real-vector spaces are a common application of unitary operators. [In classical and quantum mechanics, operators of spacial rotations are crucially important being fundamentally related to the angular momentum.]

To be specific, let us consider the following problem. Suppose we are dealing with a rigid body—a body that cannot change its shape—which pivots on a single fixed point. How can we describe its orientation? Obviously, there are many ways to do that. The most natural one is to associate an ONB $\{|\tilde{e}_i\rangle\}$ with the body (stick it to the body); the coordinates of any point on the body with respect to this basis stay constant. We can describe the current position of the body in terms of the rotation U required to bring some reference ONB $\{|e_i\rangle\}$ to coincide with $\{|\tilde{e}_i\rangle\}$. Thus, we have reduced our problem to finding the corresponding unitary transformation U. In the following examples, we shall explicitly obtain the rotation matrices in 2D and 3D.

2D case. Let us fix the reference frame by choosing the basis $|e_1\rangle = \hat{x}$, $|e_2\rangle = \hat{y}$, where $\hat{x}$ and $\hat{y}$ are the unit vectors of the two-dimensional Cartesian coordinate system. Consider a counterclockwise rotation by some angle φ around the origin. The rotation brings the basis $\{|e_i\rangle\}$ to $\{|\tilde{e}_i\rangle\}$. Thus, the corresponding rotation matrix is straightforwardly obtained from (53) using the geometrical representation for the inner product in real-vector spaces,

$$\langle a|b\rangle = ab\cos\theta, \tag{55}$$

where $a = \sqrt{\langle a|a\rangle}$, $b = \sqrt{\langle b|b\rangle}$ and θ is the angle between $|a\rangle$ and $|b\rangle$. The answer is:

$$\begin{aligned} U_{11} &= \cos\varphi, \qquad U_{12} = -\sin\varphi \\ U_{21} &= \sin\varphi, \qquad U_{22} = \cos\varphi \end{aligned} \tag{56}$$

3D case. In three dimensions, the situation is more complicated. Apart from special cases, the direct approach using Eqs. (53),(55) is rather inconvenient. To start with, one can wonder how many variables are necessary to describe an arbitrary rotation. The answer is given by the Euler's rotation theorem, which claims that an arbitrary rotation in three dimensions can be represented by only three parameters. We shall prove the theorem by explicitly obtaining these parameters.

The idea is to represent an arbitrary rotation by three consecutive simple rotations (the representation is not unique and we shall use one of the most common). Here, by a simple rotation we mean a rotation around one of the axes of the Cartesian coordinate system. For example, the matrix of rotation around the z-axis by angle α, $A_{ij}(\alpha)$, is easily obtained by a generalization of (56). We just have to note that the basis vector $|e_3\rangle = \hat{z}$ is unchanged by such rotation—it is an eigenvector of the rotation operator with the eigenvalue 1. Thus, Eq. (52) implies that $A_{13} = A_{23} = A_{31} = A_{32} = 0$ and $A_{33} = 1$. Clearly, the remaining components coincide with those of U_{ij} in (56), so for $A_{ij}(\alpha)$ we get

$$\begin{aligned} A_{11} = \cos\alpha, \quad A_{12} = -\sin\alpha, \quad A_{13} = 0, \\ A_{21} = \sin\alpha, \quad A_{22} = \cos\alpha, \quad A_{23} = 0, \\ A_{31} = 0, \quad A_{32} = 0, \quad A_{33} = 1. \end{aligned} \tag{57}$$

The convention for the sign of α is such that α is positive if the rotation observed along the vector $-\hat{z}$ is counterclockwise. We shall also need a rotation around the x-axis, $B_{ij}(\beta)$, which by analogy with (57) is given by

$$\begin{aligned} B_{11} = 1, \quad B_{12} = 0, \quad B_{13} = 0, \\ B_{21} = 0, \quad B_{22} = \cos\beta, \quad B_{23} = -\sin\beta, \\ B_{31} = 0, \quad B_{32} = \sin\beta, \quad B_{33} = \cos\beta. \end{aligned} \tag{58}$$

Now we are ready to construct an arbitrary rotation of the Cartesian system xyz to XYZ. Fig. 1 explains the procedure explicitly. It consists of three steps:

1. Rotation around the z axis by angle α, the angle between the x-axis and the line of intersection of the planes xy and XY, so called line of nodes N. As a result the new axis x' coincides with N.

2. Rotation around N (the x' axis) by angle β, the angle between z and Z. As a result the axis z coincides with Z.

3. Rotation around $Z \equiv z$ by angle γ, the angle between N and X, which finally brings the coordinate systems together.

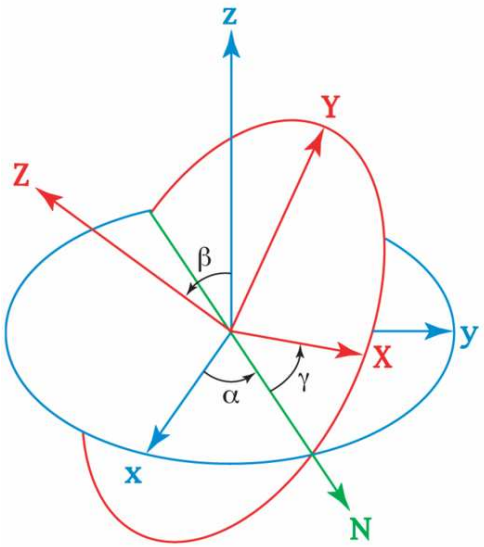

Figure 1: Rotation in 3D. Euler angles.

The angles α, β, γ are the famous Euler angles. To make them unique for the procedure described above, we set their range according to

$$0 \leq \alpha < 2\pi \ , \quad 0 \leq \beta < \pi \ , \quad 0 \leq \gamma < 2\pi \ . \tag{59}$$

Finally, the total rotation is described by

$$U_{ij} = \sum_{k,l} A_{ik}(\gamma)\ B_{kl}(\beta)\ A_{lj}(\alpha). \tag{60}$$

Note an interesting fact: after the first transformation, $A(\alpha)$, the position of the x-axis has changed, but the following rotation matrix $B(\beta)$ has exactly the same form as for the rotation around the original axis (analogously for the following $A(\gamma)$). This is correct because B_{ij} in (60) is actually the matrix element evaluated as $\langle e'_i|B|e'_j\rangle$, where $\{|e'_j\rangle\}$ is already the result of the first transformation, $A(\alpha)$, and thus B has the form (58). [One can see that by straightforwardly proving (60) using Eq. (52).]

Transformation of Matrices

Let us return to the problem of coordinate transformation when one switches from one ONB to another, Eq. (38). One may wonder what matrix corresponds to an operator A in the new basis. To answer that, consider the action of A in the vector space ν,

$$A|x\rangle = |y\rangle, \tag{61}$$

which is independent of a particular choice of ONB and, for the two expansions (38), we write

$$\begin{aligned} \sum_j A_{ij} x_j &= y_i, \\ \sum_j \tilde{A}_{ij} \tilde{x}_j &= \tilde{y}_i, \end{aligned} \tag{62}$$

where $A_{ij} = \langle e_i|A|e_j\rangle$ and $\tilde{A}_{ij} = \langle \tilde{e}_i|A|\tilde{e}_j\rangle$. Thus, the problem is to express $\tilde{A}_{ij}$ in terms of A_{ij}.

Replacing in the first line of (62) x_i, y_i in terms of $\tilde{x}_i, \tilde{y}_i$ according to (41) yields

$$\begin{aligned} A\tilde{U}\tilde{x} &= \tilde{U}\tilde{y}, \\ \tilde{A}\tilde{x} &= \tilde{y}, \end{aligned} \tag{63}$$

where we employed short hand notations for matrix and matrix-vector products denoting the vectors as $x = (x_1, x_2, \ldots)$. Now we can multiply the first line of (63) from the left by $\tilde{U}^\dagger$ and in view of (45) obtain

$$\begin{aligned} \tilde{U}^\dagger A\tilde{U}\,\tilde{x} &= \tilde{y}, \\ \tilde{A}\tilde{x} &= \tilde{y}, \end{aligned} \tag{64}$$

Therefore, since the vectors $|x\rangle$ and $|y\rangle$ were arbitrary, we arrive at

$$\tilde{A} = \tilde{U}^\dagger A\tilde{U}. \tag{65}$$

Note that instead of employing the academic approach of introducing $|x\rangle$ and $|y\rangle$ we can derive (65) straightforwardly by the definition, $\tilde{A}_{ij} = \langle \tilde{e}_i|A|\tilde{e}_j\rangle$, if we use the convenient expression for the operator A in terms of its matrix elements A_{ij}: $A = \sum_{ij} |e_i\rangle A_{ij} \langle e_j|$.

Trace of a Matrix

In many cases, abundant in physics, matrices affect specific quantities only through some function of their elements. Such a function associates a single number with the whole set of matrix elements A_{ij}. One example is matrix *determinant*, which we shall define and extensively use later in the course. Another frequently used function of a matrix A is called *trace* (also known as *spur*) and is denoted by $\mathrm{Tr}A$. Trace is defined only for square matrices ($n \times n$) by the expression

$$\mathrm{Tr}A \;=\; A_{11} + A_{22} + \ldots A_{nn} \;=\; \sum_{i=1}^{n} A_{ii}. \tag{66}$$

Thus, trace is simply an algebraic sum of all the diagonal elements. Here are the main properties of trace, which simply follow from the definition (66) (A and B are both $n \times n$ matrices):

$$\mathrm{Tr}(A^{\mathrm{T}}) = \mathrm{Tr}A \tag{67}$$

$$\mathrm{Tr}(A^{\dagger}) = (\mathrm{Tr}A)^{*} \tag{68}$$

$$\mathrm{Tr}(A + B) = \mathrm{Tr}A + \mathrm{Tr}B, \tag{69}$$

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) \tag{70}$$

Systems of linear equations

In the most general case, a system of linear equations (SLE) has the form

$$\begin{aligned} a_{11}\,x_1 \;+\; a_{12}\,x_2 \;+\; \ldots \;+\; a_{1n}\,x_n \;&=\; b_1 \\ a_{21}\,x_1 \;+\; a_{22}\,x_2 \;+\; \ldots \;+\; a_{2n}\,x_n \;&=\; b_2 \\ &\vdots \\ a_{m1}\,x_1 \;+\; a_{m2}\,x_2 \;+\; \ldots \;+\; a_{mn}\,x_n \;&=\; b_m\,. \end{aligned} \tag{71}$$

There is a convenient way of rewriting Eq. (71) in a matrix form,

$$\sum_{j=1}^{n} a_{ij}\,x_j \;=\; b_j \quad \Leftrightarrow \quad A\,x \;=\; b\,, \tag{72}$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \tag{73}$$

is an $n \times m$ matrix,

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}. \tag{74}$$

In terms of (73), (74) we can also represent Eq. (71) as

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}. \tag{75}$$

Yet another way of representing Eq. (71), which will prove most convenient for solving the system in practice, is by a single $(n+1) \times m$ matrix, constructed from A by extending it to include an extra column that consists of the vector b,

$$A' = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} & b_1 \\ a_{21} & a_{22} & \dots & a_{2n} & b_2 \\ \vdots & & \ddots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} & b_m \end{bmatrix}. \tag{76}$$

Matrix A' is called *enlarged* matrix of the SLE (71).

In the following, we shall be interested in finding solutions of a SLE in the most general case. A vector $x = (x_1, x_2, \dots, x_n)$ is called a solution of a SLE (71) if, upon its substitution to (71), it turns *every* equation in (71) into an identity. A system of equations is said to be solved if (and only if) *all* its possible solutions are found.

The problem of solving SLE is common in various fields of science and engineering. In physics, it can be a part of such fundamental problem as solving for eigenvectors of operators.

Two equations with two unknowns.

Before solving a complex problem in general, to get an insight, it is always a good idea to study a simple special case first. Consider the simplest non-trivial SLE given by two constraints on two unknowns

$$\begin{array}{l} a_{11}\,x_1 \,+\, a_{12}\,x_2 \,=\, b_1 \\ a_{21}\,x_1 \,+\, a_{22}\,x_2 \,=\, b_2 \end{array} \quad \Leftrightarrow \quad \left[\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right] = \left[\begin{array}{c} b_1 \\ b_2 \end{array}\right] . \tag{77}$$

As you probably know, the standard way of solving this problem is by transforming it to an *equivalent* system of equations—a system of equations that has the same solutions as the original one and no other solutions—of a simpler form. If x is a solution of (77), then each equation in the system is an identity and we can multiply both sides of any of the equations by some non-zero number transforming thereby the system into an equivalent one. Another frequently used trick is to formally "add" two identities, that is add their left-hand sides and their right-hand sides separately and equate the results. Then replacing one of the "added" equations by this "sum" of equations produces an equivalent system. The goal of these transformations is to reduce the original equations to ones with only one unknown by nullifying the coefficient in front of the other. The idea is obviously generalizable to the case of more than two unknowns. Actually, as wee shall see soon, that is exactly how we can solve (71).

In our special case (77), we can multiply the first equation by a_{22}, the second one by a_{12} and subtracting the results obtain an equation on x_1 only. Then, eliminating x_1 analogously, we obtain

$$\begin{array}{l} (a_{11}\,a_{22} \,-\, a_{12}\,a_{21})\,x_1 \,=\, b_1\,a_{22} \,-\, b_2\,a_{12} \\ (a_{11}\,a_{22} \,-\, a_{12}\,a_{21})\,x_2 \,=\, b_2\,a_{11} \,-\, b_1\,a_{21} \end{array} . \tag{78}$$

We can rewrite these equations conveniently if we introduce the notion of *determinant* of a 2×2 matrix A:

$$\det A \,=\, \det \left[\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right] = a_{11}\,a_{22} \,-\, a_{12}\,a_{21} . \tag{79}$$

Thus, obtain

$$x_i \,\det A = \det(B_i) , \quad i = 1, 2 , \tag{80}$$

where

$$B_1 \,=\, \left[\begin{array}{cc} b_1 & a_{12} \\ b_2 & a_{22} \end{array}\right] , \quad B_2 \,=\, \left[\begin{array}{cc} a_{11} & b_1 \\ a_{21} & b_2 \end{array}\right] . \tag{81}$$

If the matrix A is such that $\det A \neq 0$, in which case the matrix A is call *non-singular*, then the solution of (80) is given by the formula $x_i = \det B_i / \det A$, $i = 1, 2$.

If, however, $\det A = 0$ (correspondingly, A is called *singular*) then the problem requires further consideration. For example, the system of equations

$$\begin{array}{l} 2x_1 + 2x_1 = 0 \\ 3x_1 + 3x_2 = 0 \end{array} , \tag{82}$$

which has $\det A = 0$, is equivalent to just one equation, $x_1 + x_2 = 0$, and thus for any complex number c, $(x_1 = c,\ x_2 = -c)$ is a solution of (82). It is easy to show that the opposite is also true: there is an infinite number of solutions, each of which can be expressed (in the vector form) as

$$x \ = \ c \begin{bmatrix} 1 \\ -1 \end{bmatrix} , \tag{83}$$

where c is some complex number.

We could also have a system like this

$$\begin{array}{l} 2x_1 + 2x_1 = 1 \\ 3x_1 + 3x_2 = 0 \end{array} , \tag{84}$$

which has the same matrix A with $\det A = 0$, but no solutions at all.

For now, putting aside the case of $\det A = 0$, we can formulate the following rule for finding the solutions of any system of n equations with n unknowns when the corresponding matrix A is non-singular. It is called *Cramer's rule* and is essentially a straightforward generalization of the 2×2 case.

Cramer's rule

If a SLE (71) has $n = m$ and the corresponding square matrix A (73) is non-singular, that is $\det A \neq 0$, then the SLE has one and only one solution $x = (x_1, x_2, \ldots, x_n)$ given by

$$x_i \ = \ \det B_i \,/\, \det A \ , \quad i = 1, \ldots, n \ , \tag{85}$$

where the matrix B_i is an $n \times n$ matrix obtained from A by replacing its i-th column with the vector b (74). For example,

$$A \ = \ \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \quad \Rightarrow \quad B_2 \ = \ \begin{bmatrix} a_{11} & b_1 & a_{13} \\ a_{21} & b_2 & a_{23} \\ a_{31} & b_3 & a_{33} \end{bmatrix} . \tag{86}$$

The definition of determinant in the general case follows below.

Matrix determinant

For any square $n \times n$ matrix $A = \{a_{ij}\}$ its determinant is a single number given by the recursive formula

$$\begin{aligned} &\text{if } n = 1\,, \quad \det A \,=\, \det[a_{11}] \,=\, a_{11}\,, \\ &\text{if } n > 1\,, \quad \det A \,=\, \sum_j (-1)^{i+j}\, a_{ij}\, M_{ij} \,=\, \sum_j (-1)^{j+i}\, a_{ji}\, M_{ji}\,, \end{aligned} \tag{87}$$

where M_{ij} is a determinant of an $(n-1)\times(n-1)$ matrix obtained from A by removing its i-th row and j-th column, M_{ij} is called *minor*. In this formula, the index i is arbitrary: $1 \le i \le n$, and, apparently, it also does not matter whether the summation is over the row (first) index or a column (second) index, the choice being a matter of convenience for a particular form of A.

Note that M_{ij} being a determinant itself is calculated according to (87), but for a smaller matrix $(n-1) \times (n-1)$. Minors of the latter would be determinants of $(n-2) \times (n-2)$ matrices and so on until we get to 1×1 matrices, for which the answer is explicit. Thus, the formula for the 2×2 case (79) clearly follows from this general procedure. As an example, let us find the determinant of a 3×3 matrix, choosing the expansion with respect to the first row (that is, in (87) choose summation over the second index and take $i = 1$)

$$\begin{aligned} &\det \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \\ &a_{11}\, \det \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} - a_{12}\, \det \begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix} + a_{13}\, \det \begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}. \end{aligned} \tag{88}$$

Here the determinants in the right-hand side are known due to (79).

Properties of determinants

We can formulate some properties of matrix determinants, which one can prove straightforwardly from the definition (87). If A and B are $n \times n$

matrices and λ is a complex number, then

$$\det(A^{\mathrm{T}}) \,=\, \det A \,, \tag{89}$$

$$\det(A^{\dagger}) \,=\, \det\big((A^{*})^{\mathrm{T}}\big) \,=\, (\det A)^{*} \,, \tag{90}$$

$$\det(\lambda A) \,=\, \lambda^{n} \det A \,, \tag{91}$$

$$\det(A\,B) \,=\, \det A \, \det B \,. \tag{92}$$

A very important set of determinant properties involves the following class of operations with matrices.

Elementary row and column operations with matrices:

1. Multiplying a row (column) by a non-zero complex number. For example,

$$E_1 \left[\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \left[\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ \lambda a_{21} & \lambda a_{22} & \lambda a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right] , \tag{93}$$

where E_1 is the corresponding operator (that is a matrix) and λ is a complex number.

2. Multiplying a row (column) by a complex number and adding it to another row (column). For example,

$$E_2 \left[\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \left[\begin{array}{ccc} a_{11} + \lambda a_{21} & a_{12} + \lambda a_{22} & a_{13} + \lambda a_{23} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right] , \tag{94}$$

where E_2 is the corresponding operator and λ is a complex number.

3. Interchanging two rows (columns). For example,

$$E_3 \left[\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \left[\begin{array}{ccc} a_{21} & a_{22} & a_{23} \\ a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \end{array} \right] , \tag{95}$$

where E_3 is the corresponding operator.

Now, we can formulate the properties of determinants with respect to $E_{1,2,3}$ (also directly following from (87)):

$$\det(\, E_1 \, A \,) = \lambda \det A \,, \tag{96}$$

$$\det(\, E_2 \, A \,) = \det A \,, \tag{97}$$

$$\det(\, E_3 \, A \,) = -\det A \,. \tag{98}$$

Calculating determinants

In case of sufficiently large matrices (in practice, 4×4 and larger) using Eq. (87) to calculate determinants becomes highly inefficient. An alternative route is to first transform the matrix using the elementary row and column operations into some special form, the determinant of which is easily calculable, and then use the properties (96)-(98) to find the answer. In fact, it is sufficient to use only the elementary operation of type 2, with respect to which the corresponding determinant is invariant, Eq. (97). By consequently applying this operation to different rows (columns) with different factors, one can always reduce the original matrix to either one or the other of the following forms:

1. *Zero row or column.* If a square matrix has a zero row or column its determinant is zero. For a matrix $A = \{a_{ij}\}$, we can write

$$\begin{aligned} &\exists i: \ \forall j, \ a_{ij} = 0 \ \Rightarrow \ \det A = 0 \, , \\ &\exists j: \ \forall i, \ a_{ij} = 0 \ \Rightarrow \ \det A = 0 \, . \end{aligned} \tag{99}$$

2. *Upper or Lower triangular form.* If a square matrix $A = \{a_{ij}\}$ has $a_{ij} = 0$ for $j > i$ it is called *lower triangular*. For example,

$$\begin{bmatrix} a_{11} & 0 & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \, . \tag{100}$$

Analogously, if $a_{ij} = 0$ for $i > j$, the matrix is called *upper triangular*. For example,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix} \, . \tag{101}$$

If A is lower or upper triangular, its determinant is given by

$$\det A \ = \ a_{11} \, a_{22} \ldots a_{nn} \ = \ \prod_i a_{ii} \, . \tag{102}$$

SLE: General Solution

Solving SLE of a generic form (71), one would like to know whether or not its solution exists in the first place. Obviously, the analysis involving

determinant of A is irrelevant in the general case, since we don't restrict ourselves with $m = n$ anymore. However, one can introduce a general characteristic of matrices that allows to infer important information about their structure and thus about the corresponding SLE. First, let us define a *submatrix*.

A *submatrix* of a matrix A is a matrix that can be formed from the elements of A by removing one, or more than one, row or column. We already used submartices implicity in the definition of minors.

The key notion in the analysis of SLE is *rank* of a matrix, defined as follows: an integer number r is rank of a matrix A if A has an $r \times r$ (r rows and r columns) submatrix S_r such that $\det S_r \neq 0$, and any $r_1 \times r_1$ submatrix S_{r_1}, $r_1 > r$, either does not exist or $\det S_{r_1} = 0$. We shall write $\operatorname{rank} A = r$. Note that, if A is an $m \times n$ matrix, then $\operatorname{rank} A$ can not be greater than the smaller number among m and n. In some cases, it is more convenient to use an equivalent definition: $\operatorname{rank} A$ is the maximum number of linearly independent rows (columns) in A.

To prove equivalence of the two definitions, recall the method of calculating determinants using the elementary row and column operations. If $\det S_r \neq 0$, transforming S_r by multiplying any its row by a number and adding it to another row we can not nullify any row in S_r completely (otherwise, that would immediately give $\det S_r = 0$). In other words, *none* of the rows in S_r can be reduced to a linear combination of other rows, and thus there are r linearly independent rows in S_r. But S_r is a submatrix of A, therefore there are *at least* r linearly independent rows in A. On the other hand, there is no more than r linearly independent rows in A. Indeed, $\det S_{r_1} = 0$ implies that rows of S_{r_1} must be linearly dependent and thus any set of $r_1 > r$ rows in A is linear dependent, which means that r is the maximum number of linearly independent rows. Vice versa: if r is the maximum number of linearly independent rows in A, then composing a submatrix S_r of size $r \times r$ consisting of these rows gives $\det S_r \neq 0$. Since any $r_1 > r$ rows are linearly dependent, for any $r_1 \times r_1$ submatrix S_{r_1}, we get $\det S_{r_1} = 0$. Analogously, one proves that r is the number of linearly independent columns.

Thereby, we proved an interesting fact: in any matrix, the maximum number of linearly independent rows is equal to the maximum number of linearly independent columns. There is also an important property of $\operatorname{rank} A$, that follows directly from its definition in the second form. That is $\operatorname{rank} A$ is invariant with respect to elementary row and column operations applied to A.

Now, we can formulate the following criterion.

Theorem (*Kronecker-Capelli*). A SLE (71) has at least one solution if and only if rank of the matrix A (73) is equal to the rank of the enlarged matrix A' (76).

The proof is very simple. Prove the "if" part first: if $\operatorname{rank} A = \operatorname{rank} A'$, then enlarging A to include the column b (74) does not change the number of linearly independent columns, meaning that the column b is a linear combination of the columns of matrix A:

$$x_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} + x_2 \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{bmatrix} + \ldots + x_n \begin{bmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} . \quad (103)$$

Comparing with (71), we see that the coefficients in the linear combination are actually a solution, $x = (x_1, x_2, \ldots, x_n)$, of SLE (71).

Prove the "only if" part: If there is a solution $x = (x_1, x_2, \ldots, x_n)$ of SLE (71), then it satisfies (103). On the other hand, Eq. (103) is a way to write that b is a linear combination of the columns of A and therefore $\operatorname{rank} A' = \operatorname{rank} A$.

As we shall see below, the meaning of $\operatorname{rank} A'$ for the SLE (71) is that, actually, $\operatorname{rank} A'$ is the number of independent equations in (71), that is the rest are simply their consequence.

The general method of finding the solutions of SLE is based on the simple idea that we already used in the analyzing the special case of two equations with two unknowns. That is we can simplify the problem significantly by reducing a SLE to an equivalent one multiplying equations by a number and adding them in the aforementioned sense. Such a transformation of a SLE result in a transformation of the corresponding enlarged matrix A' by the elementary row operations. In other words, since we can obviously restore a SLE from its enlarged matrix A', elementary row operations applied to A' transform the corresponding SLE to an equivalent one. Correspondingly, the goal of these transformations should be to reduce A' to the most simple form possible. In the following set of instructions, we shall describe the general procedure of how it can be done and see what the simplest form is.

Simplifying a matrix

This instructions are rather general and can be applied to any matrix. Let's assume that we are dealing with an $m \times n$ matrix $A = \{a_{ij}\}$, $i = 1, \ldots, m$, $j = 1, \ldots, n$.

1. In general, it is possible that the first few columns of A are zeros. Let j_1 be the number of the leftmost column containing a non-zero element $a_{i_1 j_1}$.

(a) Divide the row i_1 by $a_{i_1\, j_1}$, so that its first non-zero element is 1,

(b) interchange rows in order to put the row i_1 in the first place,

(c) by multiplying the first row by specific numbers and adding it to the other rows, nullify all the remaining elements in the j_1-th column (obviously, except the first one, which is 1).

Denoting the resulting matrix by $A^{(1)}$, we can write

$$A^{(1)} \;=\; \begin{pmatrix} 0 & \dots & 0 & 1 & \dots \\ 0 & \dots & 0 & 0 & \dots \\ \vdots & & \vdots & \vdots & \ddots \\ 0 & \dots & 0 & 0 & \dots \end{pmatrix}, \tag{104}$$

where $a^{(1)}_{1\, j_1} = 1$. If all the elements in the last $m-1$ lines are equal to zero, we are done. In this case $\operatorname{rank} A = 1$. Otherwise, continue.

2. Let j_2 be the index of the leftmost column which has a non-zero element $a^{(1)}_{i_2\, j_2}$ in the last $m-1$ rows.

(a) Divide the row i_2 by $a^{(1)}_{i_2\, j_2}$, so that its first non-zero element is 1,

(b) interchange rows in order to make the row i_2 second

(c) as in 1(c), by multiplying the second row by specific numbers and adding it to the other rows, nullify all the elements in the column i_2, except for the second element, which is 1. Note that these transformations will not change the first $j_2 - 1$ columns, since the first $j_2 - 1$ elements of the second row are zeros.

Denoting the resulting matrix by $A^{(2)}$, obtain

$$A^{(1)} \;=\; \begin{bmatrix} 0 & \dots & 0 & 1 & * & \dots & * & 0 & \dots \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & 1 & \dots \\ \vdots & \dots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \ddots \\ 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 & \dots \end{bmatrix}, \tag{105}$$

where the stars denote unknown elements. If all the elements in the last $m-2$ lines are equal to zero, we are done. In this case $\operatorname{rank} A = 2$. Otherwise, continue the procedure analogously until all the elements in the last $m - r$ lines are zero or you run out of lines, $r = m$. Thus $r = \operatorname{rank} A$.

Finally, we have just proven that:

By means of elementary row operations, any $m \times n$ matrix of rank r can be transformed into the following simplified form. Some r columns coincide

with the first r columns of an $m \times m$ identity matrix. If $r < m$, then the last $m - r$ rows consist of zeros.

In particular, if $r = n = m$ ($\det A \neq 0$), than the simplified matrix is simply an $n \times n$ identity matrix.

Thus, if the matrices A' and A both have rank r (that is ther is a solution) simplifying the matrix A' (76) by the described procedure will lead us to the following equivalent to the original SLE (71) system of r equations

$$\begin{aligned} x_1 &= \tilde{b}_1 - (\tilde{a}_{1\,(r+1)}\, x_{r+1} + \ldots + \tilde{a}_{1n}\, x_n)\,, \\ &\vdots \\ x_r &= \tilde{b}_r - (\tilde{a}_{r\,(r+1)}\, x_{r+1} + \ldots + \tilde{a}_{rn}\, x_n)\,, \end{aligned} \tag{106}$$

where the matrix elements with tildes are those of the simplified matrix A', which we shall call $\tilde{A}'$. Here, without loss of generality, we assumed that the r columns of the identity matrix in $\tilde{A}'$ are the first r columns—interchanging any columns in $\tilde{A}'$ except the last one we only rename our unknowns x_i.

Note that if $\mathrm{rank}A'$ were larger than $r = \mathrm{rank}A$ (the only way $\mathrm{rank}A' \neq \mathrm{rank}A$ is possible) then the simplified form of A' would have an extra non-zero row. But since A' is different from A only by having an extra rightmost column, it means that the last non-zero line in $\tilde{A}'$ is $a_{(r+1)\,i} = 0$, $i = 1, \ldots, n$, $b_{r+1} = 1$. This line therefore corresponds to the equation $0 = 1$.

Interestingly, in the case of $n = m = r$, when the Cramer's rule is applicable, the simplified matrix $\tilde{A}'$ immediately gives the solution by (106) as $x_i = \tilde{b}_i$, $i = 1, \ldots, n$. Also, for the case $n = m$, (106) proves that if $\det A = 0$, we can only have either infinitely many solutions (if $\mathrm{rank}\, A' = \mathrm{rank}\, A$) or no solutions at all ($\mathrm{rank}\, A' > \mathrm{rank}\, A$).

Fundamental system of solutions

The general solution to (106) can be written in a transparent and very convenient form. In order to do that, let us first study the *homogenous* SLE, corresponding to SLE (71)

$$\begin{aligned} a_{11}\, x_1 + a_{12}\, x_2 + \ldots + a_{1n}\, x_n &= 0 \\ a_{21}\, x_1 + a_{22}\, x_2 + \ldots + a_{2n}\, x_n &= 0 \\ &\vdots \\ a_{m1}\, x_1 + a_{m2}\, x_2 + \ldots + a_{mn}\, x_n &= 0\,, \end{aligned} \tag{107}$$

or, equivalently,

$$A\,x = 0\,, \tag{108}$$

where A is given by (73). Simplifying the matrix A, Eqs. (107) are reduced to an equivalent system of $r = \mathrm{rank}A$ equations

$$\begin{aligned} x_1 &= -\,(\,\tilde{a}_{1\,(r+1)}\,x_{r+1} + \ldots + \tilde{a}_{1n}\,x_n\,)\,, \\ &\vdots \\ x_r &= -\,(\,\tilde{a}_{r\,(r+1)}\,x_{r+1} + \ldots + \tilde{a}_{rn}\,x_n\,)\,. \end{aligned} \tag{109}$$

The importance of the homogenous SLE is due to the following theorem.

Theorem. Let the vector y^0 be the solution of SLE (71), then vector y is also a solution of (71) if and only if there exists a solution of the corresponding homogeneous SLE (71) x, such that $y = y^0 + x$.

The proof is obvious: if $Ay^0 = b$ and $Ay = b$, then $A(y - y^0) = 0$, thus $y - y^0 = x$ is a solution of the homogeneous system; vice versa: if $Ay^0 = 0$ and $Ax = 0$, then, for $y = y^0 + x$, we get $Ay^0 = b$.

Most importantly, the theorem implies that a *general* solution of SLE (71) is a sum of some *particular* solution of (71) and a *general* solution of the homogeneous SLE (107). A particular solution of (71) $y^0 = (y^0_1, \ldots, y^0_n)$ can be obtained, for example, by setting all the variables in the right hand side of (106) to zero and calculating the rest from the same system of equations:

$$y^0 \;=\; \begin{bmatrix} \tilde{b}_1 \\ \vdots \\ \tilde{b}_r \\ 0 \\ \vdots \\ 0 \end{bmatrix}\,. \tag{110}$$

Now, to obtain the general solution of SLE (71), it is sufficient solve a simpler system of equations (107). First note that unlike the inhomogeneous SLE (71) this system always has a trivial solution $x = 0$.

A general solution of homogeneous SLE (107) can be expressed in terms of the so-called *fundamental system of solutions* (FSS), which is simply a set of $n - r$ linearly independent vectors satisfying (107) (or, equivalently, (109)):

Theorem. Suppose $x^1 = (x^1_1, \ldots, x^1_n)$, $\ldots$, $x^{n-r} = (x^{n-r}_1, \ldots, x^{n-r}_n)$ is some FSS of the homogeneous SLE (107). Then, any solution of the

homogeneous SLE (107) x is a linear combination of the FSS,

$$x \;=\; \sum_{i=1}^{n-r} c_i x^i \;, \tag{111}$$

where c_i are some complex numbers.

The proof. Compose a matrix X, the columns of which are the solutions $x, x^1, \ldots, x^{n-r}$. This matrix has at least $n-r$ linearly independent columns and thus its rank is not smaller than $n-r$. On the other hand, rank$X$ can not be larger than $n-r$. Indeed, each of the rows of X satisfies (109), that is the first r rows are linear combinations of the last $n-r$ rows. Thus, rank$X = n-r$ and therefore x must be a linear combination of $x^1, \ldots, x^{n-r}$.

To prove existence of a FSS, we can obtain it explicitly by the following procedure. To obtain the first vector, x^1, we can set in the right hand side of (109) $x^1_{r+1} = 1$, and $x^1_i = 0$, $i = r+2, \ldots, n$ and solve for the components in the left hand side, which gives $x^1 = (-\tilde{a}_{1\,(r+1)}, \ldots, -\tilde{a}_{r\,(r+1)},$ $1, 0 \ldots, 0)$. Then, chose $x^2_{r+2} = 1$, $x^2_i = 0$, $i = r+1, r+3, \ldots, n$ and solve for the remaining components of x^2. Repeating this procedure analogously for the remaining variables in the right hand side of (109) leads to a set of vectors in the form

$$x^1 = \begin{bmatrix} -\tilde{a}_{1\,(r+1)} \\ \vdots \\ -\tilde{a}_{r\,(r+1)} \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad x^2 = \begin{bmatrix} -\tilde{a}_{1\,(r+2)} \\ \vdots \\ -\tilde{a}_{r\,(r+2)} \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \quad \ldots \;, \quad x^{n-r} = \begin{bmatrix} -\tilde{a}_{1\,n} \\ \vdots \\ -\tilde{a}_{r\,n} \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \tag{112}$$

By construction the vectors in () are linearly independent and satisfy (107). Therefore the vectors () form a FSS. Obviously, the FSS is not unique. In the form of (), with zeros and ones in the last $n-r$ components of x^i, the FSS is called the *normal* FSS.

To summarize, the general solution of a SLE (71) is given by

$$y \;=\; y^0 \;+\; \sum_{i=1}^{n-r} c_i x^i \;, \tag{113}$$

where $r = \operatorname{rank} A = \operatorname{rank} A'$, y_0 is some particular solution of SLE (71), $\{x^i\}$, $i = i, \ldots, n-r$ is some FSS of the homogeneous SLE (107) and c_i are

complex numbers. In practice, we shall typically use the normal FSS, for which the latter formula becomes (taking into account (110) and ())

$$y = \begin{bmatrix} \tilde{b}_1 \\ \vdots \\ \tilde{b}_r \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_1 \begin{bmatrix} -\tilde{a}_{1\,(r+1)} \\ \vdots \\ -\tilde{a}_{r\,(r+1)} \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} -\tilde{a}_{1\,(r+2)} \\ \vdots \\ -\tilde{a}_{r\,(r+2)} \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix} + \ldots + c_{n-r} \begin{bmatrix} -\tilde{a}_{1\,n} \\ \vdots \\ -\tilde{a}_{r\,n} \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} . \tag{114}$$

Inverse Matrix

Given some operator A, we naturally define an inverse to it operator A^{-1} by the requirements

$$A^{-1}A \,=\, AA^{-1} \,=\, I \,. \tag{115}$$

This definition implies that if A^{-1} is inverse to A, then A is inverse to A^{-1}. [Note, in particular, that for any unitary operator U we have $U^{-1} \equiv U^{\dagger}$.] It is important to realize that the inverse operator not always exists. Indeed, the existence of A^{-1} implies that the mapping

$$|x\rangle \,\to\, |y\rangle \,, \tag{116}$$

where

$$|y\rangle \,=\, A|x\rangle \,, \tag{117}$$

is a one-to-one mapping, since only in this case we can unambiguously restore $|x\rangle$ from $|y\rangle$. For example, the projector $P_{|a\rangle} \,=\, |a\rangle\langle a|$ does not have an inverse operator in the spaces of dimensionality larger than one.

If the linear operator A is represented by the matrix A, the natural question is: What matrix corresponds to the inverse operator A^{-1}?—Such matrix is called inverse matrix. Also important is the question of the *criterion* of existence of the inverse matrix (in terms of the given matrix A).

The previously introduced notions of the determinant and minors turn out to be central to the theory of the inverse matrix. Given a matrix A,

define the matrix B:

$$b_{ij} \,=\, (-1)^{i+j} M_{ji}\,, \tag{118}$$

where M's are corresponding minors of the matrix A. Considering the product AB, we get

$$(AB)_{ij} \,=\, \sum_s a_{is} b_{sj} \,=\, \sum_s a_{is} (-1)^{s+j} M_{js} \,=\, \begin{cases} \det A\,, & \text{if} \quad i = j\,, \\ 0\,, & \text{if} \quad i \neq j\,. \end{cases} \tag{119}$$

Indeed, in the case $i = j$ we explicitly deal with Eq. (87). The case $i \neq j$ is also quite simple. We notice that here we are dealing with the determinant of a new matrix $\tilde{A}$ obtained from A by replacing the j-th row with the i-th row, in which case the matrix $\tilde{A}$ has two identical rows and its determinant is thus zero. Rewriting Eq. (119) in the matrix form we get

$$AB \,=\, [\det A]\, I\,. \tag{120}$$

Analogously, we can get

$$BA \,=\, [\det A]\, I\,, \tag{121}$$

and this leads us to the conclusion that

$$A^{-1} \,=\, [\det A]^{-1} B\,, \tag{122}$$

provided $\det A \neq 0$. The latter requirement thus forms the necessary and sufficient condition of the existence of the inverse matrix.

The explicit form for the inverse matrix, Eqs. (122), (118), readily leads to the Cramer's rule (85). Indeed, given the linear system of equations

$$A\vec{x} \,=\, \vec{b}\,, \tag{123}$$

with A being $n \times n$ matrix with non-zero determinant, we can act on both sides of the equation with the operator A^{-1} and get

$$\vec{x} \,=\, A^{-1}\vec{b} \,=\, [\det A]^{-1} B\vec{b}\,. \tag{124}$$

Then we note that the i-th component of the vector $B\vec{b}$ is nothing but the determinant of the matrix B_i obtained from A by replacing its i-th column with the vector $\vec{b}$.

Eigenvector/Eigenvalue Problem

Matrix form of Quantum Mechanics. To reveal the crucial importance of the eigenvector/eigenvalue problem for physics applications, we start with the matrix formulation of Quantum Mechanics. At the mathematical level, this amounts to considering the Schrödinger's equation

$$i\hbar \frac{d}{dt}|\psi\rangle \;=\; H|\psi\rangle \tag{125}$$

[where $|\psi\rangle$ is a vector of a certain Hilbert space, H is a Hermitian operator (called Hamiltonian), and $\hbar$ is the Plank's constant] in the representation where $|\psi\rangle$ is specified by its coordinates in a certain ONB (we loosely use here the sign of equality),

$$|\psi\rangle \;=\; (\psi_1, \psi_2, \psi_3, \ldots)\;, \tag{126}$$

and the operator H is represented by its matrix elements H_{js} with respect to this ONB. In the matrix form, Eq. (125) reads

$$i\hbar \dot{\psi}_j \;=\; \sum_s H_{js}\,\psi_s\;. \tag{127}$$

Suppose we know all the eigenvectors $\{|\phi^{(n)}\rangle\}$ of the operator H (with corresponding eigenvalues $\{E_n\}$):

$$H|\phi^{(n)}\rangle \;=\; E_n|\phi^{(n)}\rangle\;. \tag{128}$$

Since the operator H is Hermitian, without loss of generality we can assume that $\{|\phi^{(n)}\rangle\}$ is an ONB, so that we can look for the solution of Eq. (125) in the form

$$|\psi\rangle \;=\; \sum_n C_n(t)|\phi^{(n)}\rangle\;. \tag{129}$$

Plugging this into (125) yields

$$i\hbar \dot{C}_n \;=\; E_n C_n \qquad \Rightarrow \qquad C_n(t) \;=\; C_n(0)\mathrm{e}^{-iE_n t/\hbar}\;. \tag{130}$$

The initial values of the coefficients C are given by

$$C_n(0) \;=\; \langle\phi^{(n)}|\psi(t=0)\rangle \;=\; \sum_s (\phi_s^{(n)})^* \psi_s(t=0)\;, \tag{131}$$

where $\phi_s^{(n)}$ is the s-th component of the vector $|\phi^{(n)}\rangle$. In components, our solution reads

$$\psi_j(t) \,=\, \sum_n C_n(0)\, \phi_j^{(n)} \mathrm{e}^{-iE_n t/\hbar} \,. \tag{132}$$

We see that if we know E_n's and $\phi_j^{(n)}$'s, we can immediately solve the Schrödingers's equation. And to find E_n's and $\phi_s^{(n)}$'s we need to solve the problem

$$\sum_s H_{js}\phi_s \,=\, E\phi_j \,, \tag{133}$$

which is the eigenvalue/eigenvector problem for the matrix H.

In the standard mathematical notation, the eigenvalue/eigenvector problem for a matrix A reads

$$Ax \,=\, \lambda x \,, \tag{134}$$

where the eigenvector x is supposed to be found simultaneously with corresponding eigenvalue λ. Introducing the matrix

$$\tilde{A} \,=\, A - \lambda I \,, \tag{135}$$

we see that formally the problem looks like the system of linear homogeneous equations:

$$\tilde{A}x \,=\, 0 \,. \tag{136}$$

However, the matrix elements of the matrix $\tilde{A}$ depend on the yet unknown parameter λ. Now we recall that from the theory of the inverse matrix it follows that if $\det \tilde{A} \neq 0$, then $x = \tilde{A}^{-1}\, 0 \,=\, 0$, and there is no non-trivial solutions for the eigenvector. We thus arrive at

$$\det \tilde{A} \,=\, 0 \tag{137}$$

as the necessary condition for having non-trivial solution for the eigenvector of the matrix A. This condition is also a sufficient one. It guarantees the existence of at least one non-trivial solution for corresponding λ. The equation (137) is called *characteristic equation*. It defines the set of eigenvalues. With the eigenvalues found from (137), one then solves the system (136) for corresponding eigenvectors.

If A is a $n \times n$ matrix, then the determinant of the matrix $\tilde{A}$ is a polynomial function of the parameter λ, the degree of the polynomial being equal to n:

$$\det \tilde{A} \,=\, a_0 + a_1\lambda^1 + a_2\lambda^2 + \ldots + a_n\lambda^n \,=\, P_n(\lambda) \,, \tag{138}$$

where $a_0, a_1, \ldots, a_n$ are the coefficients depending on the matrix elements of the matrix A. The polynomial $P_n(\lambda)$ is called *characteristic polynomial*. The algebraic structure of the characteristic equation for an $n \times n$ matrix is thus

$$P_n(\lambda) \;=\; 0\;. \tag{139}$$

In this connection, it is important to know that for any polynomial of degree n the *Fundamental Theorem of Algebra* guarantees the existence of exactly n complex roots (if repeated roots are counted up to their multiplicity). For a Hermitian matrix, all the roots of the characteristic polynomial will be real, in agreement with the theorem which we proved earlier for the eigenvalues of Hermitian operators.

Problem 31. Find the eigenvalues and eigenvectors for all the three Pauli matrices (see Problem 26).

Problem 32. Solve the (non-dimensionalized) Schrödinger's equation for the wave function $|\psi\rangle = (\psi_1, \psi_2)$,

$$i\dot{\psi}_j \;=\; \sum_{s=1}^{2} H_{js}\psi_s \qquad (j = 1, 2)\;, \tag{140}$$

with the matrix H given by

$$H \;=\; \left[\begin{array}{cc} 0 & \xi \\ \xi & 0 \end{array}\right]\;, \tag{141}$$

and the initial condition being

$$\psi_1(t=0) \;=\; 1\,, \qquad \psi_2(t=0) \;=\; 0\;. \tag{142}$$

Functions of Operators

The operations of addition and multiplication (including multiplication by a number) allow one to introduce *functions* of operators/matrices by utilizing the idea of a series. [Recall that we have already used this idea to introduce

the functions of a complex variable.] For example, given an operator A we can introduce the operator e^A by

$$\mathrm{e}^A \,=\, \sum_{n=0}^{\infty} \frac{1}{n!} A^n \,. \tag{143}$$

The exponential function plays a crucial role in Quantum Mechanics. Namely, a formal solution to the Schrödinger's equation (125) can be written as

$$|\psi(t)\rangle \,=\, \mathrm{e}^{-iHt/\hbar}|\psi(0)\rangle \,. \tag{144}$$

The equivalence of (144) to the original equation (125) is checked by explicit differentiating (144) with respect to time:

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle \,=\, i\hbar\left[\frac{d}{dt}\mathrm{e}^{-iHt/\hbar}\right]|\psi(0)\rangle \,=\, i\hbar\left[\frac{-iH}{\hbar}\,\mathrm{e}^{-iHt/\hbar}\right]|\psi(0)\rangle \,= \\ =\, H\,\mathrm{e}^{-iHt/\hbar}|\psi(0)\rangle \,=\, H|\psi(t)\rangle \,. \end{aligned} \tag{145}$$

Note that in a general case differentiating a function of an operator with respect to a parameter the operator depends on is non-trivial because of non-commutativity of the product of operators. Here this problem does not arise since we differentiate with respect to a parameter which enters the expressions as a pre-factor, so that the operator H behaves like a number.

The exponential operator in (144) is called *evolution operator*. It "evolves" the initial state into the state at a given time moment.

In a general case, the explicit calculation of the evolution operator is not easier than solving the Schrödinger equation. That is why we refer to Eq. (144) as formal solution. Nevertheless, there are cases when the evaluation is quite straightforward. As a typical and quite important example, consider the case when H is proportional to one of the three Pauli matrices (see Problem 26). In this case,

$$\mathrm{e}^{-iHt/\hbar} \,=\, \mathrm{e}^{-i\mu\sigma t} \,, \tag{146}$$

where σ stands for one of the three Pauli matrices and μ is a constant. The crucial property of Pauli matrices that allows us to do the algebra is $\sigma^2 \,=\, I$. It immediately generalizes to $\sigma^{2m} \,=\, I$ and $\sigma^{2m+1} \,=\, \sigma$, where $m = 0, 1, 2, \ldots$. With these properties taken into account we obtain

(grouping even and odd terms of the series)

$$\mathrm{e}^{-i\mu\sigma t} \;=\; \sum_{m=0}^{\infty} \frac{(-i)^{2m}\,(\mu t)^{2m}}{(2m)!}\,\sigma^{2m} \;+\; \sum_{m=0}^{\infty} \frac{(-i)^{2m+1}\,(\mu t)^{2m+1}}{(2m+1)!}\,\sigma^{2m+1} \;=$$

$$=\; I \sum_{m=0}^{\infty} \frac{(-1)^{m}\,(\mu t)^{2m}}{(2m)!} \;-\; i\sigma \sum_{m=0}^{\infty} \frac{(-1)^{2m}\,(\mu t)^{2m+1}}{(2m+1)!} \;=$$

$$=\; I\cos\mu t \;-\; i\sigma \sin\mu t\;. \tag{147}$$

In the explicit matrix form, for each of the three matrices,

$$\sigma_1 \;=\; \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\;, \qquad \sigma_2 \;=\; \begin{bmatrix} 0 & -\,i \\ i & 0 \end{bmatrix}\;, \qquad \sigma_3 \;=\; \begin{bmatrix} 1 & 0 \\ 0 & -\,1 \end{bmatrix}\;, \tag{148}$$

we have

$$\mathrm{e}^{-i\mu\sigma_1 t} \;=\; \begin{bmatrix} \cos\mu t & -\,i\sin\mu t \\ -i\sin\mu t & \cos\mu t \end{bmatrix}\;, \tag{149}$$

$$\mathrm{e}^{-i\mu\sigma_2 t} \;=\; \begin{bmatrix} \cos\mu t & -\sin\mu t \\ \sin\mu t & \cos\mu t \end{bmatrix}\;, \tag{150}$$

$$\mathrm{e}^{-i\mu\sigma_3 t} \;=\; \begin{bmatrix} \mathrm{e}^{-i\mu t} & 0 \\ 0 & \mathrm{e}^{i\mu t} \end{bmatrix}\;. \tag{151}$$

Eq. (144) allows one to draw an interesting general conclusion about the character of quantum-mechanical evolution. To this end, we first note that for any Hermitian operator A, the operator

$$U \;=\; \mathrm{e}^{iA} \tag{152}$$

is unitary. Indeed, applying the operation of Hermitian conjugation to the exponential series, and taking into account that $A^{\dagger} = A$, we find

$$\left[\mathrm{e}^{iA}\right]^{\dagger} \;=\; \mathrm{e}^{-iA}\;. \tag{153}$$

Then we utilize the fact that for any two commuting operators—and thus behaving with respect to each other as numbers—one has

$$\mathrm{e}^{A}\,\mathrm{e}^{B} \;=\; \mathrm{e}^{A+B} \qquad\quad (\text{if and only if } AB = BA)\;. \tag{154}$$

This yields (below O is the matrix of zeroes)

$$\mathrm{e}^{iA}\,\mathrm{e}^{-iA} \;=\; \mathrm{e}^{O} \;=\; I\;, \tag{155}$$

and proves that $UU^{\dagger} = I$. We thus see that the evolution operator is unitary. This means that *the evolution in Quantum Mechanics is equivalent to a certain rotation in the Hilbert space of states.*

Systems of Linear Ordinary Differential Equations with Constant Coefficients

The theory of matrix allows us to develop a simple general scheme for solving systems of ordinary differential equations with constant coefficients.

We start with the observation that without loss of generality we can deal only with the first-order derivatives, since higher-order derivatives can be reduced to the first-order one at the expense of introducing new unknown functions equal to corresponding derivatives. Let us illustrate this idea with the differential equation of the harmonic oscillator:

$$\ddot{x} + \omega^2 x \;=\; 0\;. \tag{156}$$

The equation is the second-order differential equation, and there is only one unknown function, $x(t)$. Now if we introduce two functions, $x_1 \equiv x$, and $x_2 \equiv \dot{x}$, we can equivalently rewrite (156) as the system of two equations (for which we use the matrix form)

$$\left[\begin{array}{c} \dot{x}_1 \\ \dot{x}_2 \end{array}\right] \;=\; \left[\begin{array}{cc} 0 & 1 \\ -\omega_0^2 & 0 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \end{array}\right]\;. \tag{157}$$

Analogously, *any* system of ordinary differential equations with constant coefficients can be reduced to the canonical vector form

$$\dot{x} \;=\; Ax\;, \tag{158}$$

where $x = (x_1, x_2 \ldots x_m)$ is the vector the components of which correspond to the unknown functions (of the variable t), and A is an $m \times m$ matrix. In addition to the equation (158), the initial condition $x(t = 0)$ is supposed to be given.

In a general case, the matrix A has m different eigenvectors with corresponding eigenvalues :

$$Au^{(n)} \,=\, \lambda_n u^{(n)} \qquad\qquad (n = 1, 2, 3, \ldots, m)\ . \tag{159}$$

As can be checked by direct substitution, each eigenvector/eigenvalue yields an elementary solution of Eq. (158) of the form

$$s^{(n)}(t) \,=\, c_n\, \mathrm{e}^{\lambda_n t}\, u^{(n)}\ , \tag{160}$$

where c_n is an arbitrary constant. The linearity of the equations allows us to write the general solution as just the sum of elementary solutions.

$$x(t) \,=\, \sum_{n=1}^{m} c_n\, \mathrm{e}^{\lambda_n t}\, u^{(n)}\ . \tag{161}$$

In components, this reads

$$x_j(t) \,=\, \sum_{n=1}^{m} c_n\, \mathrm{e}^{\lambda_n t}\, u_j^{(n)} \qquad\qquad (j = 1, 2, 3, \ldots, m)\ . \tag{162}$$

To fix the constants c_n, we have to use the initial condition. In the special case of so-called normal matrix (see also below), featuring an ONB of eigenvectors, finding the constants c_n is especially simple. As we have seen it many times in this course, it reduces to just forming the inner products:

$$c_n \,=\, \sum_{j=1}^{m} [u_j^{(n)}]^* x_j(0) \qquad\qquad (\text{if } u'\text{s form an ONB})\ . \tag{163}$$

In a general case, we have to solve the system of linear equations

$$\sum_{n=1}^{m} u_j^{(n)}\, c_n \,=\, x_j(0) \qquad\qquad (j = 1, 2, 3, \ldots, m)\ , \tag{164}$$

in which $u_j^{(n)}$'s play the role of the matrix, c_n's play the role of the components of the vector of unknowns, and $x(0)$ plays the role of the r.h.s. vector.

Problem 33. Solve the system of two differential equations

$$\left\{ \begin{array}{l} 3\dot{x}_1 \,=\, -4x_1 + x_2 \\ 3\dot{x}_2 \,=\, 2x_1 - 5x_2 \end{array} \right. \tag{165}$$

for the two unknown functions, $x_1(t)$ and $x_2(t)$, with the initial conditions

$$x_1(0) = 2 , \qquad x_2(0) = -1 . \tag{166}$$

Normal Matrices/Operators

By definition, a normal matrix—for the sake of briefness, we are talking of matrices, keeping in mind that a linear operator can be represented by a matrix—is the matrix that features an ONB of its eigenvectors. [For example, Hermitian and unitary matrices are normal.] A necessary and sufficient criterion for a matrix to be normal is given by the following theorem. The matrix A is normal if and only if

$$AA^\dagger = A^\dagger A , \tag{167}$$

that is if A commutes with its Hermitian conjugate.

Proof. Let us show that Eq. (167) holds true for each normal matrix. In the ONB of its eigenvectors, the matrix A is diagonal (all the non-diagonal elements are zeros), and so has to be the matrix $A^\dagger$, which then immediately implies commutativity of the two matrices, since any two diagonal matrices commute.

To show that Eq. (167) implies the existence of an ONB of eigenvectors, we first prove an important lemma saying that any eigenvector of the matrix A with the eigenvalue λ is also an eigenvector of the matrix $A^\dagger$ with the eigenvalue λ^*. Let x be an eigenvector of A:

$$Ax = \lambda x . \tag{168}$$

The same is conveniently written as

$$\tilde{A}x = 0 , \qquad \tilde{A} = A - \lambda I . \tag{169}$$

Note that if $AA^\dagger = A^\dagger A$, then $\tilde{A}\tilde{A}^\dagger = \tilde{A}^\dagger \tilde{A}$, because

$$\tilde{A}\tilde{A}^\dagger = AA^\dagger - \lambda A^\dagger - \lambda^* A + |\lambda|^2 , \tag{170}$$

$$\tilde{A}^\dagger \tilde{A} = A^\dagger A - \lambda^* A - \lambda A^\dagger + |\lambda|^2 = \tilde{A}\tilde{A}^\dagger . \tag{171}$$

[Here we took into account that $\tilde{A}^\dagger = A^\dagger - \lambda^* I$.] Our next observation is

$$\langle \tilde{A}^\dagger x | \tilde{A}^\dagger x \rangle \;=\; \langle x | \tilde{A}\tilde{A}^\dagger | x \rangle \;=\; \langle x | \tilde{A}^\dagger \tilde{A} | x \rangle \;=\; \langle \tilde{A} x | \tilde{A} | x \rangle \;=\; 0 \,, \tag{172}$$

implying the statement of the lemma:

$$|\tilde{A}^\dagger x\rangle \;=\; 0 \qquad \Leftrightarrow \qquad A^\dagger\, x = \lambda^* x \,. \tag{173}$$

With the above lemma, the rest of the proof is most simple to the that for the Hermitian operator. Once again we care only about the orthogonality of the eigenvectors with different eigenvalues, since the eigenvectors of the same eigenvalue form a subspace, so that if the dimensionality of this subspace is greater than one, we just use the Gram-Schmidt orthogonalization within this subspace. Suppose we have

$$A x_1 \;=\; \lambda_1\, x_1 \,, \tag{174}$$

$$A x_2 \;=\; \lambda_2\, x_2 \,. \tag{175}$$

By our lemma, we have

$$A^\dagger x_2 \;=\; \lambda_2^*\, x_2 \,. \tag{176}$$

From (174) we find

$$\langle x_2 | A | x_1 \rangle \;=\; \lambda_1 \langle x_2 | x_1 \rangle \,, \tag{177}$$

while (176) yields

$$\langle x_1 | A^\dagger | x_2 \rangle \;=\; \lambda_2^* \langle x_1 | x_2 \rangle \,. \tag{178}$$

The latter equation can be re-written as

$$\langle A x_1 | x_2 \rangle \;=\; \lambda_2^* \langle x_1 | x_2 \rangle \,. \tag{179}$$

Complex-conjugating both sides we get

$$\langle x_2 | A | x_1 \rangle \;=\; \lambda_2 \langle x_2 | x_1 \rangle \,. \tag{180}$$

Comparing this with (177) we see that

$$\lambda_1 \langle x_2 | x_1 \rangle \;=\; \lambda_2 \langle x_2 | x_1 \rangle \,, \tag{181}$$

which at $\lambda_1 \neq \lambda_2$ is only possible if $\langle x_2 | x_1 \rangle \;=\; 0$.