1. Mathematics for Quantum Mechanics

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Vector

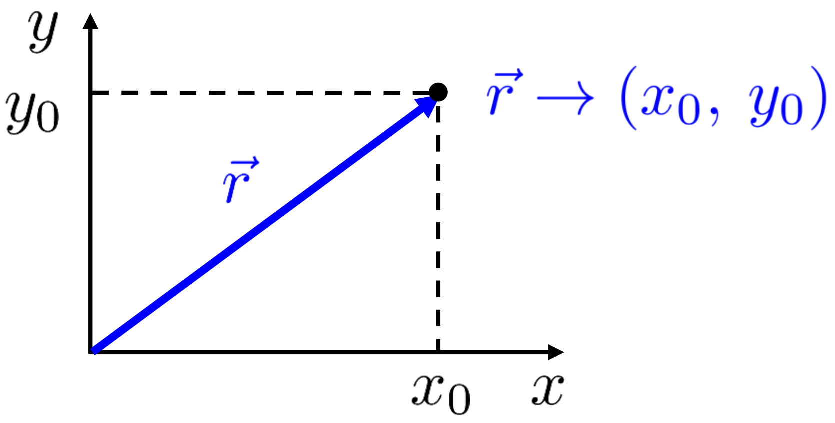
A vector is a mathematical object which has both magnitude and direction.

To represent a vector, we put a right arrow ($\rightarrow$) on top of an alphabet to express its directionality.

In 1-dimension, the vector is indistinguishable from a scalar, as the direction can be specified by the sign of a number.

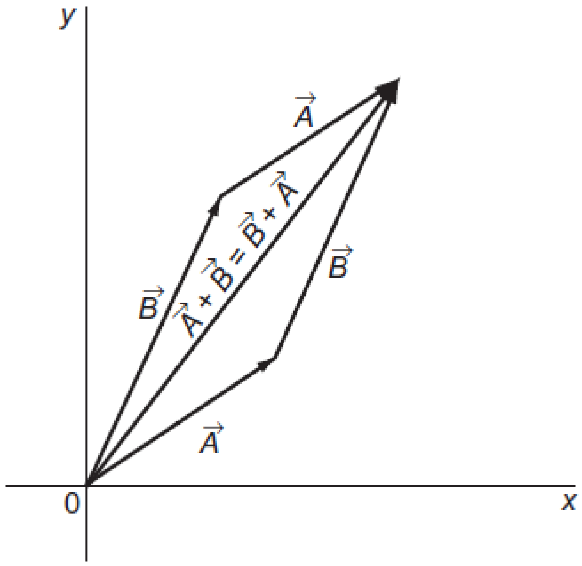
A vector does not change when shifted in space, as long as its direction and length remain constant.

Position Vector



An n-dimensional vector is assigned to a unique point in the n-dimensional space by putting its tail at the origin.

This assignment defines position vector.



The sum of the two vectors $\vec{A}$ and $\vec{B}$ can be calculated as the figure on the left.

The difference $\vec{A}-\vec{B}$ can be also calculated according to $\vec{A}+(-\vec{B})$.

Unit Vectors

The unit vectors $\mathbf{i}$ $(\hat{i})$ and $\mathbf{j}$ $(\hat{j})$ are defined as vectors of unit length along the directions of x- and y- axes, respectively.

We can represent any vectors in the xy-plane as

$$\mathbf{A} = A_x\mathbf{i} + A_y\mathbf{j} \quad \rightarrow \quad (A_x,\ A_y)$$

The coefficients A_x and A_y are called as x- and y- components, respectively.

$$a\mathbf{A} = (aA_x)\mathbf{i} + (aA_y)\mathbf{j} \quad \rightarrow \quad (aA_x,\ aA_y)$$
$$\mathbf{A} + \mathbf{B} = (A_x + B_x)\mathbf{i} + (A_y + B_y)\mathbf{j} \quad \rightarrow \quad (A_x + B_x,\ A_y + B_y)$$
$$\mathbf{A} - \mathbf{B} = (A_x - B_x)\mathbf{i} + (A_y - B_y)\mathbf{j} \quad \rightarrow \quad (A_x - B_x,\ A_y - B_y)$$

Scalar Product of Two Vectors

The scalar product (inner product, dot product) of the two vectors $\mathbf{A}$ and $\mathbf{B}$ is represented as $\mathbf{A} \cdot \mathbf{B}$ and calculated as

$$\mathbf{A} \cdot \mathbf{B} = |\mathbf{A}||\mathbf{B}| \cos \alpha$$

where $|\mathbf{A}|$ is the size of the vector $\mathbf{A}$ and α is the angle between $\mathbf{A}$ and $\mathbf{B}$.

$$|\mathbf{A}| = \sqrt{A_x^2 + A_y^2}$$

When the two vectors are parallel: $\mathbf{A} \cdot \mathbf{B} = |\mathbf{A}||\mathbf{B}|$

antiparallel: $\mathbf{A} \cdot \mathbf{B} = -|\mathbf{A}||\mathbf{B}|$

perpendicular (orthogonal): $\mathbf{A} \cdot \mathbf{B} = 0$

Scalar Product of Two Vectors

The scalar product can be also expressed by the components of the position vectors,

$$\begin{aligned}\mathbf{A}\cdot\mathbf{B} &= (A_x\mathbf{i}+A_y\mathbf{j})\cdot(B_x\mathbf{i}+B_y\mathbf{j})\\ &= A_xB_x(\mathbf{i}\cdot\mathbf{i})+A_xB_y(\mathbf{i}\cdot\mathbf{j})+A_yB_x(\mathbf{j}\cdot\mathbf{i})+A_yB_y(\mathbf{j}\cdot\mathbf{j})\\ &= A_xB_x+A_yB_y,\end{aligned}$$

which can be straightforwardly extended to arbitrary numbers of dimensions,

$$\mathbf{A}\cdot\mathbf{B} = \left(\sum_{j=1}^{N} A_j\mathbf{e}_j\right)\cdot\left(\sum_{k=1}^{N} B_k\mathbf{e}_k\right) = \sum_{j=1}^{N}\sum_{k=1}^{N} A_jB_k\delta_{jk} = \sum_{j=1}^{N} A_jB_j,$$

where $\{\mathbf{e}_j\}$ is a set of orthonormal unit vectors.

Scalar Product of Complex Vectors

Vectors can generally have complex components.

In such cases, the inner product between vectors $\mathbf{A}$ and $\mathbf{B}$ is defined as

$$\mathbf{A}^* \cdot \mathbf{B} = \left(\sum_{j=1}^{N} A_j^* \mathbf{e}_j \right) \cdot \left(\sum_{k=1}^{N} B_k \mathbf{e}_k \right) = \sum_{j=1}^{N} A_j^* B_j .$$

According to this definition, the inner product of a vector to itself is still equal to its length (norm),

$$\mathbf{A}^* \cdot \mathbf{A} = \sum_{j=1}^{N} A_j^* A_j = \sum_{j=1}^{N} |A_j|^2 = |\mathbf{A}|^2.$$

Matrix

A matrix is a list of quantities arranged in rows and columns.

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1n} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & A_{m3} & \cdots & A_{mn} \end{pmatrix}$$

The numbers $\{A_{mn}\}$are called matrix elements.

A matrix with m rows and n columns is called m-by-n matrix.

If $m = n$, the matrix is called a square matrix.

A single row and column are often called row vector and column vector, respectively, as they can be thought as one-dimensional arrays.

Matrix Algebra

A matrix is equal to another matrix if

- the number of rows and columns for the two matrices are identical,
- and all corresponding elements of the two matrices are also equal.

For two matrices and

$$\mathbf{A} = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{m1} & \cdots & B_{mn} \end{pmatrix},$$

the addition and scalar multiplication is defined as

$$\mathbf{A} + \mathbf{B} = \begin{pmatrix} A_{11} + B_{11} & \cdots & A_{1n} + B_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} + B_{m1} & \cdots & A_{mn} + B_{mn} \end{pmatrix} \text{ and } c\mathbf{A} = \begin{pmatrix} cA_{11} & \cdots & cA_{1n} \\ \vdots & \ddots & \vdots \\ cA_{m1} & \cdots & cA_{mn} \end{pmatrix}.$$

Matrix Algebra

The elements of the product matrix $\mathbf{C} = \mathbf{AB}$ is defined as

$$C_{mn} = \sum_k A_{mk} B_{kn}.$$

ex)

$$\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 2 & 1 \end{pmatrix} = ?$$

answer: $$\begin{pmatrix} 1 \times 0 + 2 \times 2 & 1 \times 1 + 2 \times 1 \\ 0 \times 0 + 1 \times 2 & 0 \times 1 + 1 \times 1 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 2 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 3 \\ 1 \end{pmatrix} = ?$$

answer: $$\begin{pmatrix} 1 \times 0 + 0 \times 3 + 2 \times 1 \\ 0 \times 0 + (-1) \times 3 + 1 \times 1 \\ 0 \times 0 + 0 \times 3 + 1 \times 1 \end{pmatrix} = \begin{pmatrix} 2 \\ -2 \\ 1 \end{pmatrix}$$

By definition, the multiplication can be only defined if the number of columns of $\mathbf{A}$ is equal to the number of rows of $\mathbf{B}$.

Matrix Algebra

Square matrices can be multiplied in any order, but they do not necessarily commute:

$$\mathbf{AB} \neq \mathbf{BA}.$$

Other than that, the matrix multiplication satisfies associativity and distributivity like scalars.

$$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC}),$$

$$\mathbf{A}(\mathbf{B}+\mathbf{C}) = \mathbf{AB} + \mathbf{AC}.$$

Example:

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Determinant

A square matrix $\mathbf{A}$ has a determinant $\det(\mathbf{A})$ which is a scalar.

For a 2-by-2 matrix, the determinant is

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \rightarrow \quad \det(\mathbf{A}) = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = A_{11}A_{22} - A_{12}A_{21}.$$

For higher-dimensional matrices, the determinants can be calculated by expansion by minors:

$$\begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = A_{11} \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix} - A_{12} \begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} + A_{13} \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix}$$

$$= A_{11}A_{22}A_{33} - A_{11}A_{32}A_{23} - A_{12}A_{21}A_{33} + A_{12}A_{31}A_{23} + A_{13}A_{21}A_{32} - A_{13}A_{31}A_{22}.$$

Determinant

ex) Calculate the determinant

$$\begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix}.$$

Linear Homogeneous Equations

Consider a set of linear simultaneous equation,

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = 0,$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = 0,$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = 0.$$

$$\underbrace{\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_{\mathbf{x}} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

It is apparent that we have

$$x_1 = x_2 = x_3 = 0$$

as a solution of the problem, which is called the trivial solution. However, such a simple solution is usually not very interesting.

The condition for solutions other than trivial solution (nontrivial solution) is $\det(\mathbf{A}) = 0$.

Linear Homogeneous Equations

ex)

a.

$$4x + 5y = 0,$$
$$6x + 8y = 0.$$

$$\underset{\mathbf{A}}{\begin{pmatrix} 4 & 5 \\ 6 & 8 \end{pmatrix}} \underset{\mathbf{x}}{\begin{pmatrix} x \\ y \end{pmatrix}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\det(\mathbf{A}) = 4 \times 8 - 5 \times 6 = 2$$

b.

$$3x + 4y = 0,$$
$$6x + 8y = 0.$$

$$\underset{\mathbf{A}}{\begin{pmatrix} 3 & 4 \\ 6 & 8 \end{pmatrix}} \underset{\mathbf{x}}{\begin{pmatrix} x \\ y \end{pmatrix}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\det(\mathbf{A}) = 3 \times 8 - 4 \times 6 = 0$$

Identity Matrix

An identity matrix $\mathbf{I}$ is a square matrix which satisfies

$$\mathbf{IA} = \mathbf{AI} = \mathbf{A},$$

and takes the form of

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}.$$

The elements can be summarized by using Kronecker delta δ_{ij},

$$I_{ij} = \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

Inverse Matrix

For a square matrix $\mathbf{A}$, its inverse matrix $\mathbf{A}^{-1}$ satisfies

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}.$$

The condition for the existence of an inverse matrix is $\det(\mathbf{A}) \neq 0$.

If the inverse exist, its elements $\{A^{-1}\}_{ij}$ satisfy a set of simultaneous equations

$$\sum_{k=1}^{n} A_{ik}(A^{-1})_{kj} = \delta_{ij}$$

which can be solved since the number of equations are equal to the number of unknowns.

Gauss-Jordan elimination: a systematic way to calculate the inverse

Matrix Terminologies

The trace of a matrix is the sum of its diagonal elements,

$$\mathrm{Tr}(A) = \sum_{i=1}^{n} A_{ii}.$$

An upper (lower) triangular matrix is a matrix with all the elements below (above) the diagonal are zero.

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & -1 \\ 0 & 0 & 2 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 2 & 0 & 0 \\ 1 & -1 & 0 \\ 2 & 2 & -2 \end{pmatrix}$$

If all elements of a matrix is zero, such a matrix is called null matrix or zero matrix.

Matrix Terminologies

The transpose $\mathbf{A}^{\mathrm{T}}$ of a matrix $\mathbf{A}$ is obtained by swapping the index of the column and row of all matrix elements.

$$A_{ij}^{\mathrm{T}} = A_{ji},$$

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 1+2i \\ -2 & i & -1 \\ 1 & 4 & 2 \end{pmatrix} \quad \rightarrow \quad \mathbf{A}^{\mathrm{T}} = \begin{pmatrix} 1 & -2 & 1 \\ 2 & i & 4 \\ 1+2i & -1 & 2 \end{pmatrix}.$$

The Hermitian transpose $\mathbf{A}^{\dagger}$ of a matrix $\mathbf{A}$ is obtained by taking the complex conjugate of the matrix and transposing it.

$$\mathbf{A}^{\dagger} = \left(\mathbf{A}^{\mathrm{T}}\right)^{*} = \begin{pmatrix} 1 & -2 & 1 \\ 2 & -i & 4 \\ 1-2i & -1 & 2 \end{pmatrix}.$$

Matrix Terminologies

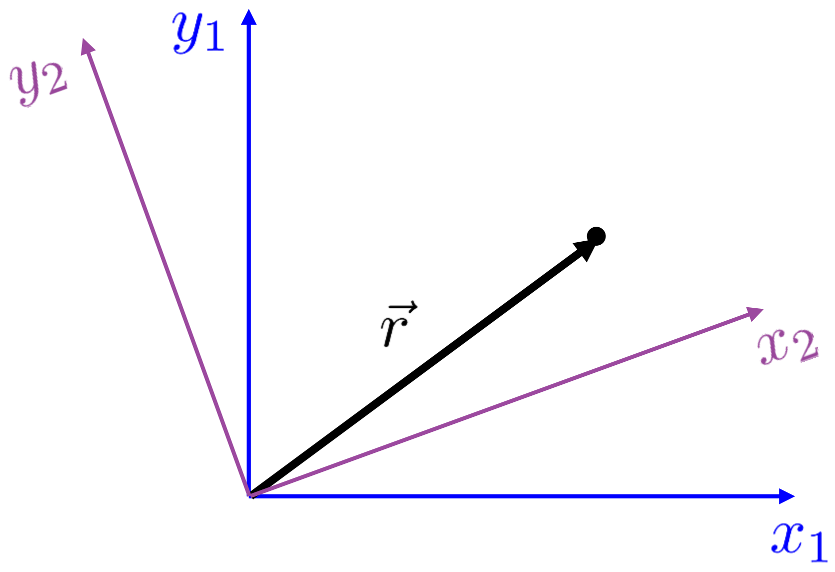
If a matrix is equal to its transpose ($\mathbf{A}^{\mathrm{T}} = \mathbf{A}$), it is called a symmetric matrix.

If a matrix is equal to its Hermitian transpose ($\mathbf{A}^{\dagger} = \mathbf{A}$), it is called a Hermitian matrix.

If the inverse of a matrix is equal to its transpose ($\mathbf{A}^{-1} = \mathbf{A}^{\mathrm{T}}$), such a matrix is called an orthogonal matrix.

If the inverse of a matrix is equal to its Hermitian transpose ($\mathbf{A}^{-1} = \mathbf{A}^{\dagger}$), such a matrix is called a unitary matrix.

Unitary Transformation



$$\vec{r} \rightarrow \begin{pmatrix} r\cos\theta_1 \\ r\sin\theta_1 \end{pmatrix}$$

$$= \begin{pmatrix} r\cos\theta_2 \\ r\sin\theta_2 \end{pmatrix} = \begin{pmatrix} r\cos(\theta_1 - \alpha) \\ r\sin(\theta_1 - \alpha) \end{pmatrix}$$

$$= \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} r\cos\theta_1 \\ r\sin\theta_1 \end{pmatrix}$$

When the coordinate axes undergo a rotation, the components of a position vector is transformed according to

$$\vec{r}_2 = \mathbf{U}^\dagger \vec{r}_1,$$

where $\vec{r}_1$ and $\vec{r}_2$ are the position vectors in each coordinate system and $\mathbf{U}^\dagger$ is (the Hermitian transpose of) a unitary matrix.

Unitary Transformation

As the position vectors undergo unitary transformation under the rotation of the coordinates, so do the matrices.

To observe this, we consider a scalar quantity

$$C = \vec{a}^\dagger \mathbf{M} \vec{b}$$

where $\vec{a}$ and $\vec{b}$ are column vector of length N and $\mathbf{M}$ is an $N \times N$ square matrix.

Now we insert two identities $\mathbf{I} = \mathbf{U}\mathbf{U}^\dagger$ and regroup the terms:

$$\begin{aligned} C = \vec{a}^\dagger \mathbf{U}\mathbf{U}^\dagger \mathbf{M} \mathbf{U}\mathbf{U}^\dagger \vec{b} &= (\vec{a}^\dagger \mathbf{U})(\mathbf{U}^\dagger \mathbf{M} \mathbf{U})(\mathbf{U}^\dagger \vec{b}) \\ &= (\vec{a}')^\dagger \mathbf{M}' \vec{b}', \end{aligned}$$

so that $\vec{a}'$, $\vec{b}'$, and $\mathbf{M}' = \mathbf{U}^\dagger \mathbf{M} \mathbf{U}$ are transformed vectors and matrix.

Matrix Eigenvalues and Eigenvectors

For a square matrix $\mathbf{A}$, if there are vectors which satisfy

$$\mathbf{A}\mathbf{x}_k = \lambda_k \mathbf{x}_k,$$

such vectors $\{\mathbf{x}_k\}$ and coefficients $\{\lambda_k\}$ are called eigenvectors and eigenvalues, which can be found by solving

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = 0.$$

The condition for nontrivial solutions is

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0.$$

Solving this equation gives the eigenvalues, which can be inserted in $\mathbf{A}\mathbf{x}_k = \lambda_k \mathbf{x}_k$ one-by-one to find the corresponding eigenvectors.

Matrix Eigenvalues and Eigenvectors

ex) Find the eigenvalues and eigenvectors of $\begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix}$.

Matrix Diagonalization

Suppose we have found eigenvalues $\{\lambda_k\}$ and eigenvectors $\{\mathbf{x}_k\}$ of a Hermitian 3-by-3 matrix $\mathbf{A}$:

$$\mathbf{A}\mathbf{x}_k = \lambda_k \mathbf{x}_k, \quad k = 1,\ 2,\ 3.$$

If we construct a square matrix $\mathbf{X}$ by using normalized $\{\mathbf{x}_k\}$ as its columns,

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix},$$

$\mathbf{X}$ is a unitary matrix:

$$\mathbf{X}^\dagger \mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\dagger \\ \mathbf{x}_2^\dagger \\ \mathbf{x}_3^\dagger \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^* \cdot \mathbf{x}_1 & \mathbf{x}_1^* \cdot \mathbf{x}_2 & \mathbf{x}_1^* \cdot \mathbf{x}_3 \\ \mathbf{x}_2^* \cdot \mathbf{x}_1 & \mathbf{x}_2^* \cdot \mathbf{x}_2 & \mathbf{x}_2^* \cdot \mathbf{x}_3 \\ \mathbf{x}_3^* \cdot \mathbf{x}_1 & \mathbf{x}_3^* \cdot \mathbf{x}_2 & \mathbf{x}_3^* \cdot \mathbf{x}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Matrix Diagonalization

We also have

$$\mathbf{AX} = \begin{pmatrix}\mathbf{Ax}_1 & \mathbf{Ax}_2 & \mathbf{Ax}_3\end{pmatrix} = \begin{pmatrix}\lambda_1\mathbf{x}_1 & \lambda_2\mathbf{x}_2 & \lambda_3\mathbf{x}_3\end{pmatrix} = \begin{pmatrix}\lambda_1 x_{11} & \lambda_2 x_{12} & \lambda_3 x_{13} \\ \lambda_1 x_{21} & \lambda_2 x_{22} & \lambda_3 x_{23} \\ \lambda_1 x_{31} & \lambda_2 x_{32} & \lambda_3 x_{33}\end{pmatrix}.$$

Which leads to

$$\mathbf{X}^\dagger\mathbf{AX} = \begin{pmatrix}\lambda_1\mathbf{x}_1^*\cdot\mathbf{x}_1 & \lambda_2\mathbf{x}_1^*\cdot\mathbf{x}_2 & \lambda_3\mathbf{x}_1^*\cdot\mathbf{x}_3 \\ \lambda_1\mathbf{x}_2^*\cdot\mathbf{x}_1 & \lambda_2\mathbf{x}_2^*\cdot\mathbf{x}_2 & \lambda_3\mathbf{x}_2^*\cdot\mathbf{x}_3 \\ \lambda_1\mathbf{x}_3^*\cdot\mathbf{x}_1 & \lambda_2\mathbf{x}_3^*\cdot\mathbf{x}_2 & \lambda_3\mathbf{x}_3^*\cdot\mathbf{x}_3\end{pmatrix} = \begin{pmatrix}\lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3\end{pmatrix} = \mathbf{D}.$$

A matrix which has nonzero elements only on its diagonal (such as $\mathbf{D}$) is called diagonal matrix.

Finding a unitary transform for making diagonal matrix is called diagonalization, which is only possible for symmetric matrix.

Matrix Diagonalization

A diagonal matrix satisfies

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & \cdots \\ 0 & \lambda_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \quad \rightarrow \quad \mathbf{D}^n = \begin{pmatrix} \lambda_1^n & 0 & \cdots \\ 0 & \lambda_2^n & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

This relation can be used to evaluate the powers of a diagonalizable symmetric matrix:

$$\mathbf{D} = \mathbf{X}^\dagger \mathbf{A} \mathbf{X} \quad \rightarrow \quad \mathbf{A} = \mathbf{X} \mathbf{D} \mathbf{X}^\dagger,$$

$$\mathbf{A}^n = \mathbf{X} \mathbf{D}^n \mathbf{X}^\dagger = \mathbf{X} \begin{pmatrix} \lambda_1^n & 0 & \cdots \\ 0 & \lambda_2^n & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \mathbf{X}^\dagger.$$

Matrix Diagonalization

The formula in the previous slide can be used to define the exponential of a diagonalizable symmetric matrix.

Based on the Taylor expansion of e^x, we can derive

$$e^{\mathbf{A}} = \sum_{j=0}^{\infty} \frac{\mathbf{A}^j}{j!} = \mathbf{X}\left(\sum_{j=0}^{\infty} \mathbf{D}^j\right)\mathbf{X}^\dagger$$

$$= \mathbf{X} \begin{pmatrix} e^{\lambda_1} & 0 & \cdots \\ 0 & e^{\lambda_2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \mathbf{X}^\dagger,$$

which is used as the most basic method for solving the Schrödinger equation.