COMPUTATIONAL PHYSICS

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Numerical methods for matrices

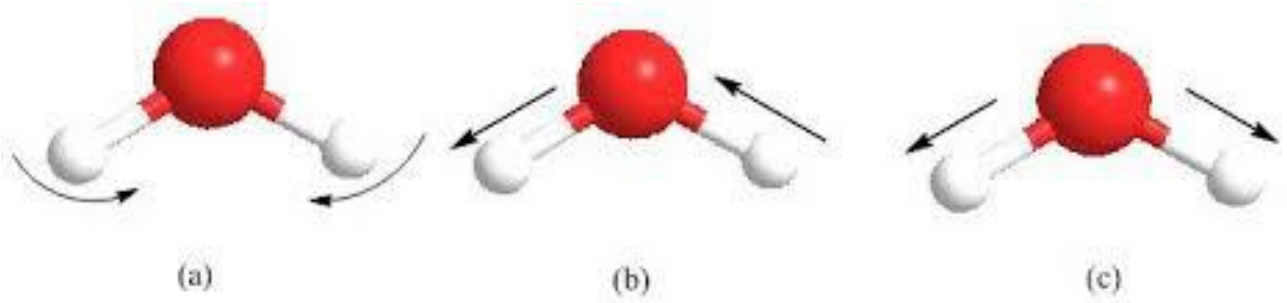
- Matrices in physics
- Basic matrix operations
- Linear equation systems
- Eigenvalue problems

Many problems in physics can be formulated in a matrix form

- Q: Where is matrix?
- A: Matrices are everywhere in physics!

- An eigenvalue problem given in the form of a partial differential equation can be rewritten as a matrix problem.
- A boundary-value problem after discretization is essentially a linear algebra problem.
- The vibrational spectrum of a molecule with n vibrational degrees of freedom can be also sloved using matrix methods.

Vibration of a Molecule



$$U(q_1, q_2, \cdots, q_n) \approx \frac{1}{2} \sum_{i,j=1}^{n} A_{ij} q_i q_j$$ Elastic energy

$$T(\dot{q}_1, \dot{q}_2, \cdots, \dot{q}_n) \approx \frac{1}{2} \sum_{i,j=1}^{n} M_{ij} \dot{q}_i \dot{q}_j$$ Kinetic energy

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0$$ Lagrange equation

$L=T-U$

$$\sum_{j=1}^{n} \left(A_{ij} q_j + M_{ij} \ddot{q}_j \right) = 0$$

Let: $q_j = x_j e^{-i\omega t} \Longrightarrow \sum_{j=1}^{n} (A_{ij} - \omega^2 M_{ij}) x_j = 0$

$$\begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \vdots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \lambda \begin{pmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & \vdots & \vdots \\ M_{n1} & \cdots & M_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

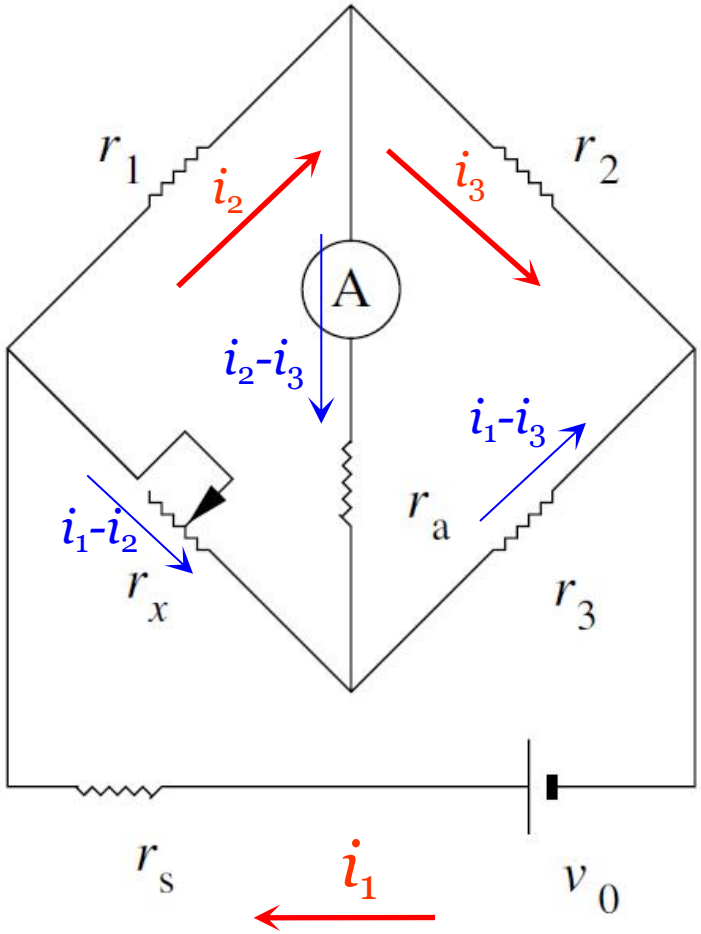
$$Ax = \lambda Mx \qquad \lambda = \omega^2$$

The determinant $\left| A - \lambda M \right| = 0$

The roots of this secular equation, λ_k with k = 1, 2, . . . , n, give all the possible vibrational angular frequencies $\omega_k^2 = \lambda_k$ of the molecule.

Kirchhoff Equations for Circuits

- The unbalanced Wheatstone bridge



$$r_s i_1 + r_1 i_2 + r_2 i_3 = \mathrm{v}_0,$$
$$-r_x i_1 + (r_1 + r_x + r_a) i_2 - r_a i_3 = 0,$$
$$-r_3 i_1 - r_a i_2 + (r_2 + r_3 + r_a) i_3 = 0,$$

Ohm's law $\mathrm{R}i = \mathrm{v}$

$$\mathrm{R} = \begin{pmatrix} r_s & r_1 & r_2 \\ -r_x & r_1 + r_x + r_a & -r_a \\ -r_3 & -r_a & r_2 + r_3 + r_a \end{pmatrix}$$

$$i = \mathrm{R}^{-1}\mathrm{v}$$

Matrix Quantum Mechanics

Choosing a set of bases: orthogonal, complete, unitary.
Then the Hamiltonian can be written as a matrix with the elements as: $H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle$

The Schrodinger equation $\hat{H} | \Psi_k \rangle = \varepsilon_k | \Psi_k \rangle$

- In fact, any operators can be written as matrices.
- For example: The spin -1/2 electron. Bases: spin up: |↑>; spin down: |↓>

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Basic matrix operations

- An *n* x *m* matrix A is defined through its elements A_{ij} with the row index i =1, 2, . . . , n and the column index j = 1, 2, . . . , m. It is called a square matrix if n=m.
- A variable array x with elements $x_1, x_2, \ldots, x_n$ arranged into a column is viewed as an n × 1 matrix, or an n-element column matrix.
- A typical set of linear algebraic equations is given by

$$\sum_{j=1}^{n} A_{ij} x_j = b_i \quad \Rightarrow \quad \mathbf{Ax} = \mathbf{b}$$

for i = 1, 2, . . . , n, where x_j are the unknowns to be solved, A_{ij} are the given coefficients, and b_i are the given constants.

The standard matrix multiplication:

$$C_{ij} = \sum_k A_{ik} B_{kj} \qquad \mathrm{C} = \mathrm{AB}$$

The summation over k requires the number of columns of the first matrix to be the same as the number of rows of the second matrix. Otherwise, the product does not exist.

The inverse of a square matrix A (written as A^{-1}) is defined by

$$\mathrm{A}^{-1}\mathrm{A} = \mathrm{A}\mathrm{A}^{-1} = \mathrm{I}$$

where I is a unit matrix with the elements $I_{ij}=\delta_{ij}$.

Determinant

The determinant of an n x n matrix A is defined as:

$$|\mathrm{A}| = \sum_{i=1}^{n} (-1)^{i+j} A_{ij} |R_{ij}|$$

- for any j = 1, 2, . . . , n, where $|R_{ij}|$ is the determinant of the residual matrix R_{ij} of A with its ith row and jth column removed.
- $C_{ij}=(-1)^{i+j}|R_{ij}|$ is called a cofactor of A_{ij}.

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

$$= aei + bfg + cdh - ceg - bdi - afh.$$

Inverse of A

- In principle, the inverse of A can be obtained through

$$A^{-1}{}_{ij} = \frac{C_{ji}}{|A|}$$

If a matrix has an inverse or nonzero determinant, it is called a nonsingular matrix. Otherwise, it is a singular matrix.

The trace of a matrix A is the sum of all its diagonal elements, written as

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

The transpose of a matrix A (written as A^T) has elements with the row and column indices of A interchanged, that is, $A_{ij}^T = A_{ji}$

We call A an orthogonal matrix if $A^T = A^{-1}$. The complex conjugate of A^T is called the Hermitian operation of A (written as $A^\dagger$) with $A^\dagger_{ij} = A^*_{ji}$.
We call A a Hermitian matrix if $A^\dagger = A$ and a unitary matrix if $A^\dagger = A^{-1}$.

code example

- To calculate the determinant, trace, transpose, and inverse of a square matrix.

- 5.1.Matrix.cpp

Triangular matrix

A matrix is called an upper-triangular (lower-triangular) matrix if the elements below (above) the diagonal are all zero.

$$U = \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} & \dots & u_{1,n} \\ & u_{2,2} & u_{2,3} & \dots & u_{2,n} \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & u_{n-1,n} \\ 0 & & & & u_{n,n} \end{bmatrix} L = \begin{bmatrix} l_{1,1} & & & & 0 \\ l_{2,1} & l_{2,2} & & & \\ l_{3,1} & l_{3,2} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ l_{n,1} & l_{n,2} & \dots & l_{n,n-1} & l_{n,n} \end{bmatrix}$$

Linear equation

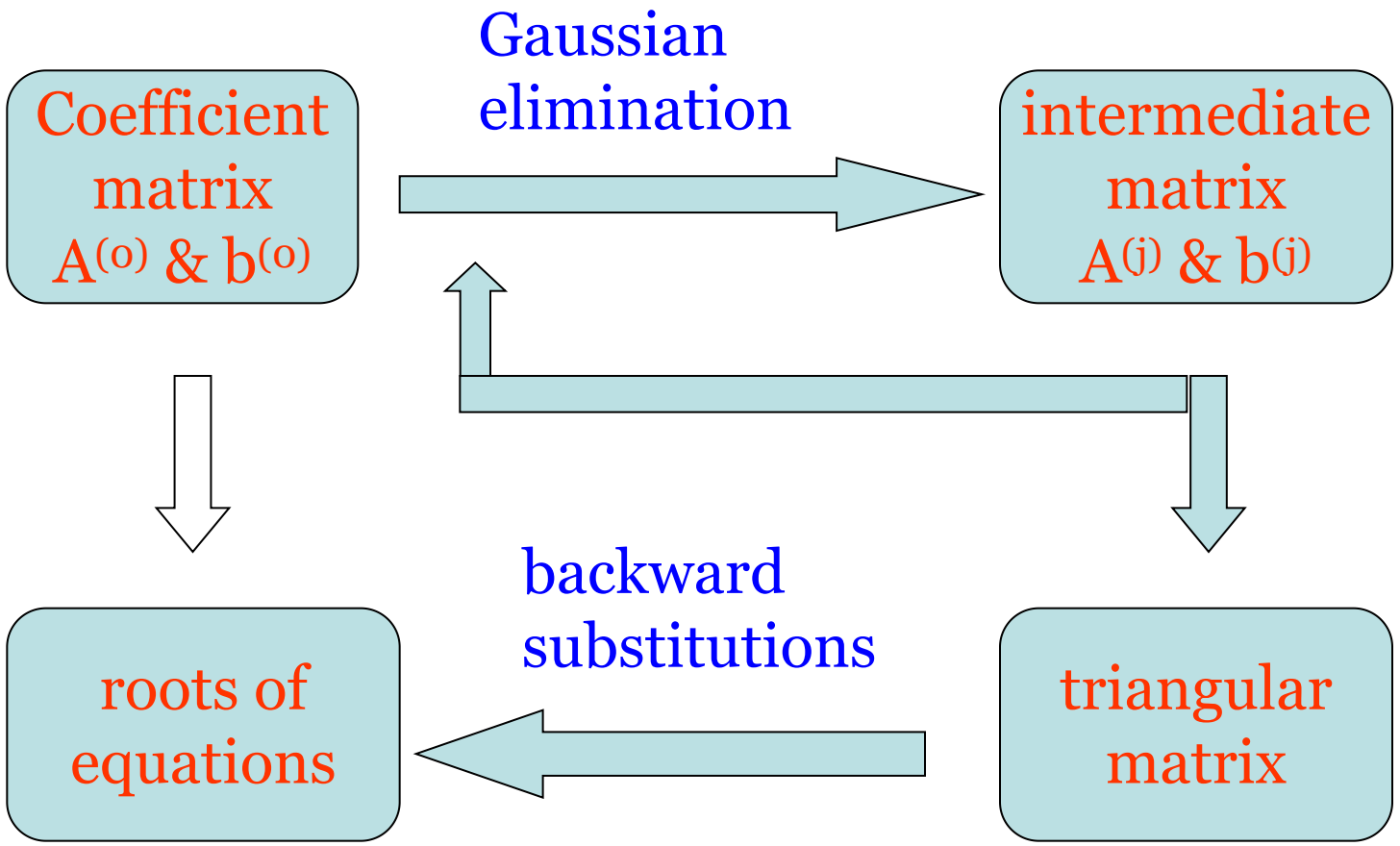
- $Ax = b$.
- $|A| \neq 0$ and $b \neq 0$ ----> a unique solution.

- Method: Gaussian elimination --- to transform the original matrix A to a triangular matrix

- The original matrix $A = A^{(0)}$
- $A^{(j)}$: the resultant matrix after j matrix operations.

- Similar notation is used for the transformed b: $b^{(j)}$

Gaussian elimination for linear equation systems



The inverse and the determinant of a matrix can also be obtained in such a manner.

$$\begin{pmatrix} A_{11}^{(0)} & A_{12}^{(0)} & \cdots & A_{1n}^{(0)} \\ A_{21}^{(0)} & A_{22}^{(0)} & \cdots & A_{2n}^{(0)} \\ \vdots & \vdots & \vdots & \vdots \\ A_{n1}^{(0)} & \cdots & \cdots & A_{nn}^{(0)} \end{pmatrix}$$

multiply the first equation by $-A_{i1}^{(0)} / A_{11}^{(0)}$

$$\begin{pmatrix} -A_{i1}^{(0)} & -\frac{A_{12}^{(0)} \times A_{i1}^{(0)}}{A_{11}^{(0)}} & \cdots & -\frac{A_{1n}^{(0)} \times A_{i1}^{(0)}}{A_{11}^{(0)}} \\ A_{21}^{(0)} & A_{22}^{(0)} & \cdots & A_{2n}^{(0)} \\ \vdots & \vdots & \vdots & \vdots \\ A_{n1}^{(0)} & \cdots & \cdots & A_{nn}^{(0)} \end{pmatrix}$$

add it to the ith equation for i > 1

$$\begin{pmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ 0 & A_{22}^{(1)} & \cdots & A_{2n}^{(1)} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & A_{nn}^{(1)} \end{pmatrix}$$

multiply the second equation by $-A_{i2}^{(1)} / A_{22}^{(1)}$

$$\begin{pmatrix} A_{11}^{(1)} & A_{12}^{(1)} & \cdots & A_{1n}^{(1)} \\ 0 & -A_{i2}^{(1)} & \cdots & -\frac{A_{2n}^{(1)} \times A_{i2}^{(1)}}{A_{22}^{(1)}} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & A_{nn}^{(1)} \end{pmatrix}$$

add it to the ith equation for i > 2

$$\begin{pmatrix} A_{11}^{(2)} & A_{12}^{(2)} & \cdots & A_{1n}^{(2)} \\ 0 & A_{22}^{(2)} & \cdots & A_{2n}^{(2)} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & A_{nn}^{(2)} \end{pmatrix}$$

continued with the third,fourth, . . . , and (n-1)th equations

$$\longrightarrow \quad \begin{pmatrix} A_{11}^{(n-1)} & A_{12}^{(n-1)} & \cdots & A_{1n}^{(n-1)} \\ 0 & A_{22}^{(n-1)} & \cdots & A_{2n}^{(n-1)} \\ 0 & 0 & 0 & \vdots \\ 0 & 0 & 0 & A_{nn}^{(n-1)} \end{pmatrix}$$

Then the coefficient matrix becomes an upper-triangular matrix $A^{(n-1)}$.

A linear equation set with an upper-triangular coefficient matrix can easily be solved with backward substitutions.

- Because all the diagonal elements are used in the denominators, the scheme would fail if any of them happened to be zero or a very small quantity.

- This problem can be circumvented in most cases by interchanging the rows to have the elements used for divisions being the ones with largest magnitudes possible.

- This is the so-called pivoting procedure.

- This procedure will not change the solutions of the linear equation set.

- The partial-pivoting scheme, which searches for the pivoting element only from the remaining elements of the given column.

- We first search for the element with the largest magnitude from $|A_{i1}^{(0)}|$ for i = 1, 2, . . . , n.

- Assuming that the element obtained is $A_{k_1 1}^{(0)}$, we then interchange the first row and the k_1th row and eliminate the first element of each row except the first row.

- Similarly, we can search for the second pivoting element with the largest magnitude from $|A_{i2}^{(1)}|$ for i = 2, 3, . . . , n.

Solution of a linear equation set

- After the Gaussian elimination, the solution of a linear equation set is then obtained through backward substitutions with

$$x_i = \frac{1}{A_{k_i i}^{(n-1)}} \left(b_{k_i}^{(n-1)} - \sum_{j=i+1}^{n} A_{k_i j}^{(n-1)} x_j \right)$$

$$\begin{pmatrix} A_{11}^{(n-1)} & A_{12}^{(n-1)} & \cdots & A_{1n}^{(n-1)} \\ 0 & A_{22}^{(n-1)} & \cdots & A_{2n}^{(n-1)} \\ 0 & 0 & 0 & \vdots \\ 0 & 0 & 0 & A_{nn}^{(n-1)} \end{pmatrix}$$

for i = n-1, n-2, . . . , 1, starting with $x_n = b_{k_n}^{(n-1)} / A_{k_n n}^{(n-1)}$

Determinant of a matrix

- The determinant of the original matrix can easily be obtained after we have transformed it into a triangular matrix through Gaussian elimination.

- The partial-pivoting Gaussian elimination does not change the value of the determinant only its sign, which can be fixed with the knowledge of the order of pivoting elements.

- For a triangular matrix, the determinant is given by the product of all its diagonal elements.

Inverse of a matrix

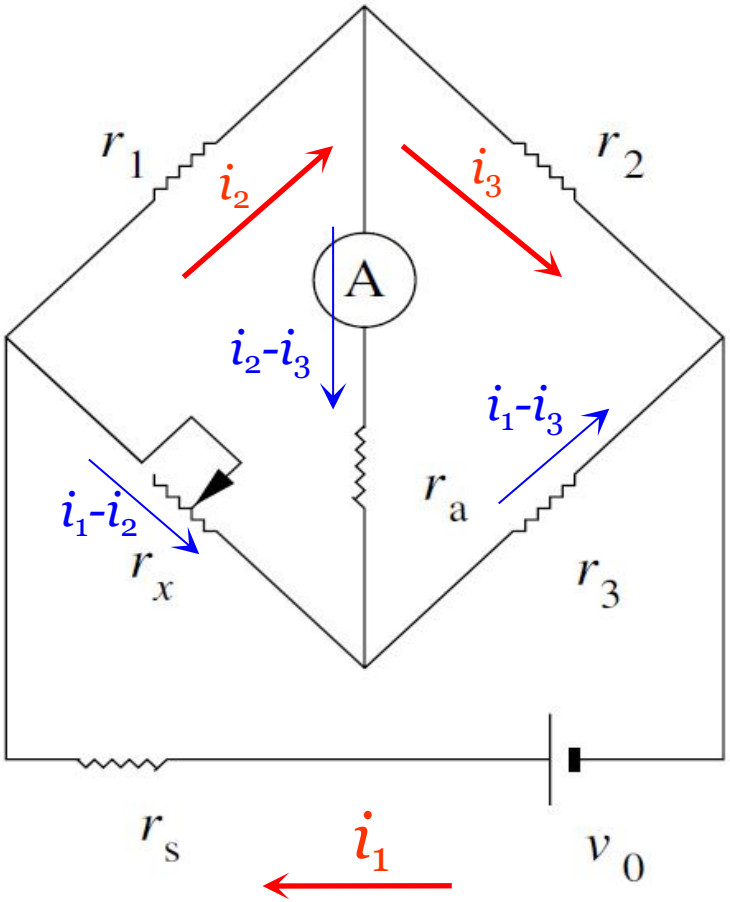
- The inverse of a matrix A can be obtained by solving the linear equation set.
- $AA^{-1}=I$. I: a unit matrix
- Let $A^{-1}_{ij} = x_{ij}$, for i, j = 1, 2, . . . , n, then x_{ij} is the solution of the equation $Ax_j = b_j$, with $b_{ij}=\delta_{ij}$.
- The solution of above equation corresponds to each column of the unit matrix forms the corresponding column of A^{-1}.

Code example

5.2.GaussianElimination.cpp

Homework

- Solve the unbalanced Wheatstone bridge.



Requirements:

Input the values of resistors.

Output the effective resistane of the circuit.

Matrix Eigenvalue

$$A\mathrm{x} = \lambda \mathrm{x}$$

where x and λ are an eigenvector and its corresponding eigenvalue of the matrix, respectively.

Determined from the secular equation:

$|A-\lambda I|=0$

An nxn matrix has a total of n eigenvalues.

- The eigenvalue problem is quite general in physics, which can come from many different problems.

- For example, the Lagrange equation for the vibrational modes of a large molecule, or the quantum mechanics Hamiltonian.

- In many problems in physics and related fields, the matrix in question is Hermitian with $A^{\dagger}=A$.

Eigenvalues of a Hermitian matrix

The simplicity of the Hermitian eigenvalue problem is due to three important properties:

1.the eigenvalues are all real;
2.the eigenvectors can be orthonormal;
3.can be transformed into a diagonal matrix with the same set of eigenvalues under a similarity transformation of a unitary matrix.

Similarity transformation: $B=P^{-1}AP$.
Unitary matrix: $P^{\dagger}P=I$, $P^{\dagger}=P^{-1}$; † means the conjugate transpose

- The eigenvalue problem of an n x n complex Hermitian matrix is equivalent to that of a 2n x 2n real symmetric matrix.

- Separate its real part from its imaginary part with $A = B + iC$.
- B is a real symmetric matrix: $B_{ij}=B_{ji}$
- C is a real skew symmetric matrix: $C_{ij}=-C_{ji}$.

- Decompose the eigenvector z in a similar fashion: $z=x+iy$.

The original eigenvalue problem becomes $(B+iC)(x+iy)=\lambda(x+iy)$, which is equivalent to

$$\begin{pmatrix} \mathbf{B} & -\mathbf{C} \\ \mathbf{C} & \mathbf{B} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

it becomes a real symmetric eigenvalue problem with the same set of eigenvalues that have an overall double degeneracy. Therefore we need to solve only the real symmetric eigenvalue problem if the matrix is Hermitian.

Diagonalization

- For a diagonal matrix, the eigenvalues are the diagonal elements.

$$\mathbf{D} = \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots \\ 0 & \lambda_2 & 0 & \cdots \\ 0 & 0 & \lambda_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

To obtain the eigenvalues of a Hermitian matrix

=

to transform it to a diagonal matrix by similarity transformations

Diagonalize a matrix -----> Diagonalization

Linear Algebra PACKage

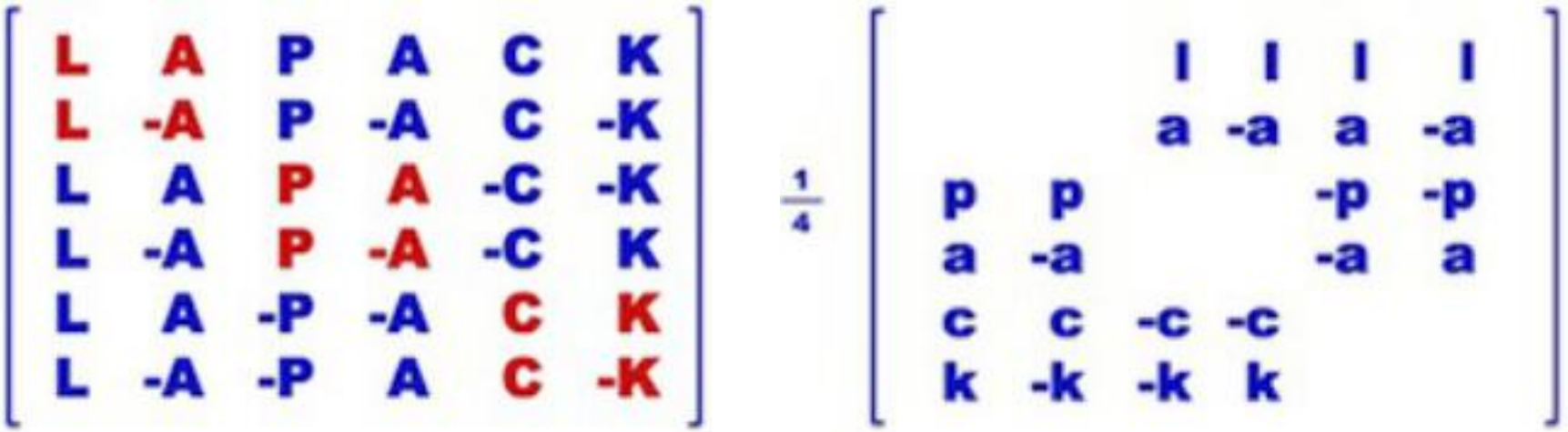
- LAPACK (Linear Algebra Package) is a software library for numerical linear algebra, provided by Univ. of Tennessee; Univ. of California, Berkeley; Univ. of Colorado, Denver; and NAG Ltd..

- It provides routines for solving systems of linear equations and linear least squares, eigenvalue problems, and singular value decomposition.

- The routines handle both real and complex matrices in both single and double precision.

- LAPACK was originally written in FORTRAN 77, but moved to Fortran 90 in version 3.2 (2008). The latest version is 3.8.0 (Nov. 2017).

- LAPACK is licensed under a three-clause BSD style license, a permissive free software license with few restrictions.
- Website *www.netlib.org/lapack*



More implements

- Lapack is also included (and may be optimized for specialized platforms) in MKL@Intel, ACML@AMD, Matlab, Mathematica, ……

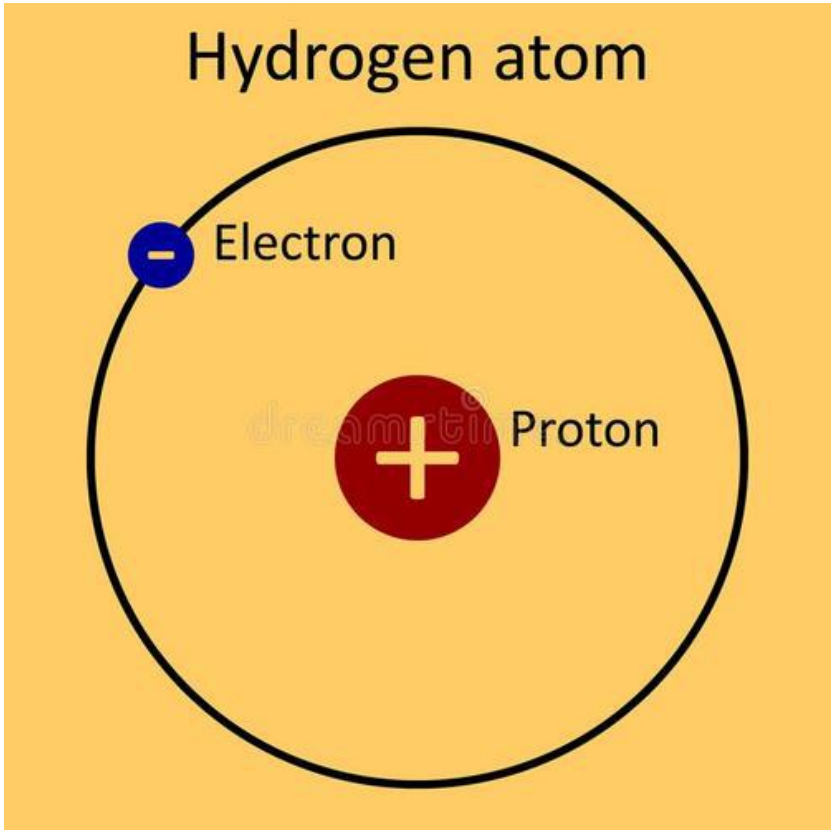
- It can be included in commercial software packages (and has been). Netlib only ask that proper credit be given to the authors.

Code example

- 5.3.Diagonalization.cpp
- 9.6.Diagonalization.cpp

http://www.netlib.org/lapack/lapacke.html

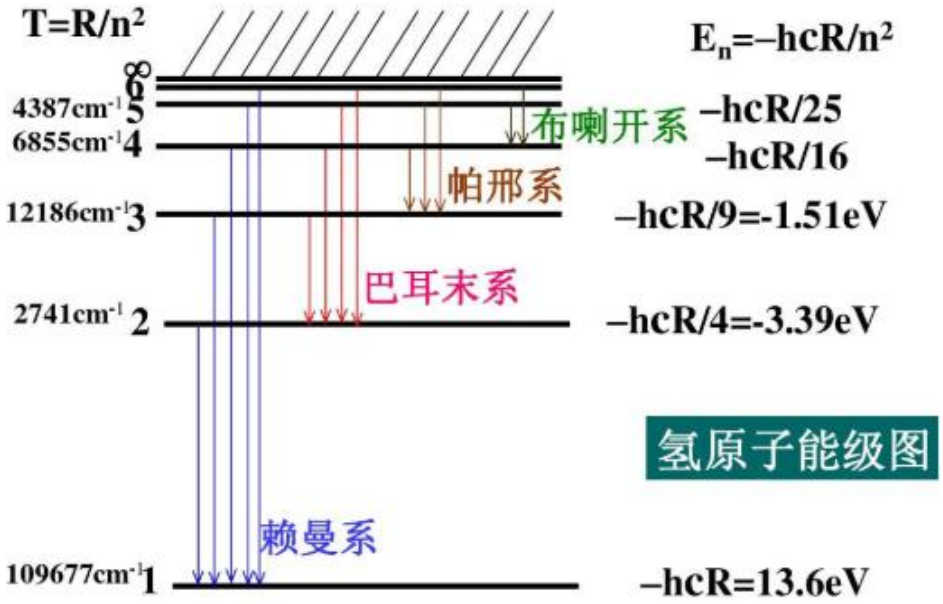
Hydrogen molecule



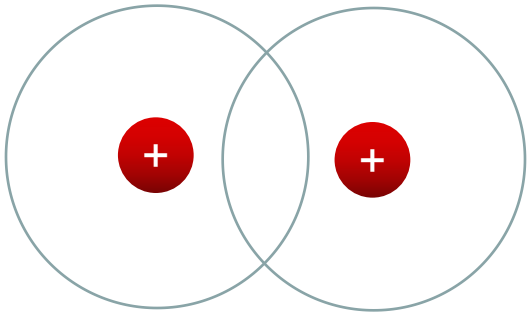
R=0.53 A

- H=K+U

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi + U\Psi = E\Psi$$



Hydrogen molecule



- H=K+U
- $=K_1+U_1+K_2+U_2+K_{12}$
- $=H_0+K_{12}$

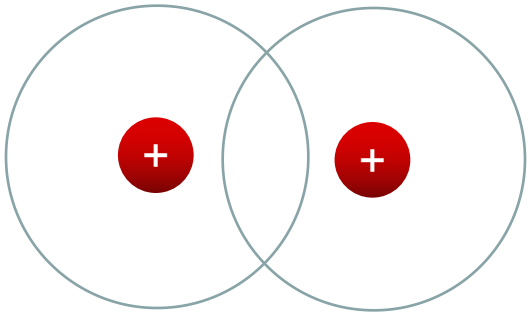
r=0.74 A

$$H_0 = V(n_1 + n_2) = V(c_1^\dagger c_1 + c_2^\dagger c_2)$$

$$K_{12} = -t(c_1^\dagger c_2 + c_2^\dagger c_1)$$

$$H = (c_1^\dagger, c_2^\dagger) \begin{pmatrix} V & -t \\ -t & V \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Hydrogen molecule



r=0.74 A

$$H = (c_1^\dagger, c_2^\dagger) \begin{pmatrix} V & -t \\ -t & V \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

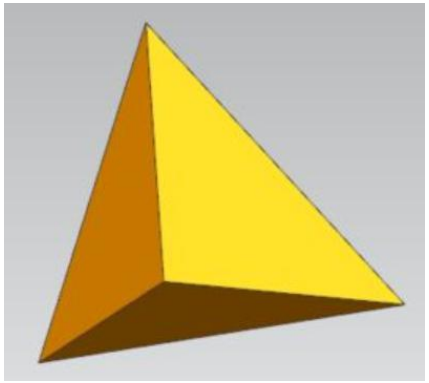
E=V+t
E=V-t

Reaction energy: 4.73 eV
t=2.365 eV

antibonding state: (|1>-|2>)/sqrt(2)

bonding state: (|1>+|2>)/sqrt(2)

Hydrogen pyramid



$$H_0 = V \sum_i c_i^\dagger c_i$$

$$K = -t \sum_{<ij>} (c_i^\dagger c_j + c_j^\dagger c_i)$$

$$H = (c_1^\dagger, c_2^\dagger, c_3^\dagger, c_4^\dagger) \begin{pmatrix} V & -t & -t & -t \\ -t & V & -t & -t \\ -t & -t & V & -t \\ -t & -t & -t & V \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

$$V - t \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

5.3.H4.cpp

Home work

- One dimensional hydrogen chain
- Eigen-energies?
- Surface (terminal) energy?