In the name of $\mathcal{GOD}$

Computational Physics

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Outline

- Fortran-90 Programming
- Numerical calculus
- Approximation of a function
- Numerical methods for matrices
- Ordinary differential equations
- Partial differential equations
- Monte Carlo simulations
- Molecular dynamics simulations

$$U(q_1, q_2, \ldots, q_{n-1}, q_n) \approx \frac{1}{2}\sum_{i,j=1}^{n} A_{i,j} q_i q_j$$

q_i the generalized coordinates

$A_{i,j}$ the elements of the generalized elastic constant matrix

$$T(\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_{n-1}, \dot{q}_n) = \frac{1}{2}\sum_{i,j=1}^{n} M_{i,j} \dot{q}_i \dot{q}_j$$

$\dot{q}_i = \dfrac{dq_i}{dt}$ the generalized velocities,

$M_{i,j}$ the elements of the generalized mass matrix

$$\frac{d}{dt}\frac{\partial \ell}{\partial \dot{q}_i} - \frac{\partial \ell}{\partial q_i} = 0 \qquad , \qquad \ell = T - U$$

$$\sum_{j=1}^{n} (M_{i,j}\ddot{q}_j + A_{i,j}q_j) = 0 \qquad , \qquad i = 1,2,\dots,n$$

$$q_j = x_j e^{i\omega t}$$

$$e^{i\omega t}\left(\sum_{j=1}^{n} (-\omega^2 M_{i,j} + A_{i,j})x_j \right) = 0 \qquad , \qquad i = 1,2,\dots,n$$

$$\sum_{j=1}^{n}(-\omega^2 M_{i,j} + A_{i,j})x_j = 0 \qquad , \qquad i = 1,2,\ldots,n$$

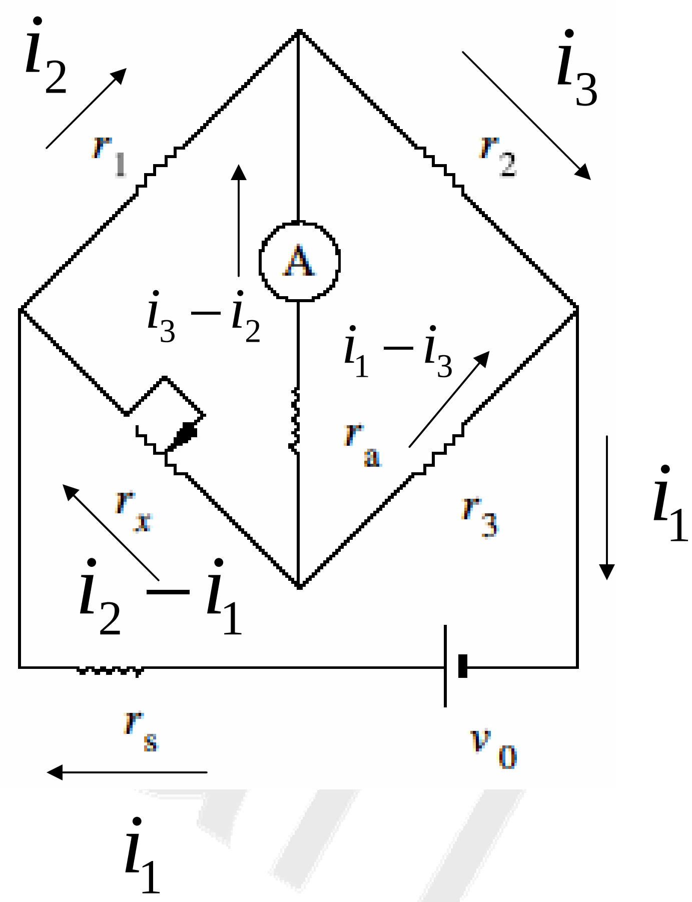
$$\begin{bmatrix} A_{11} & \ldots & A_{1n} \\ \vdots & \ldots & \vdots \\ A_{n1} & \ldots & A_{nn} \end{bmatrix}\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} - \lambda \begin{bmatrix} M_{11} & \ldots & M_{1n} \\ \vdots & \ldots & \vdots \\ M_{n1} & \ldots & M_{nn} \end{bmatrix}\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = 0$$

$$\lambda = \omega^2 \qquad Ax = \lambda M x$$

$$\begin{bmatrix} A_{11} - \lambda M_{11} & \ldots & A_{1n} - \lambda M_{1n} \\ \vdots & \ldots & \vdots \\ A_{n1} - \lambda M_{n1} & \ldots & A_{nn} - \lambda M_{nn} \end{bmatrix}\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = 0 \Rightarrow \left| A - \lambda M \right| = 0$$

Kirchhoff rules

$$r_s i_1 + r_1 i_2 + r_2 i_3 = v_0,$$
$$-r_x i_1 + (r_1 + r_x + r_a) i_2 - r_a i_3 = 0,$$
$$-r_3 i_1 - r_a i_2 + (r_2 + r_3 + r_a) i_3 = 0,$$



$$\begin{bmatrix} r_a & r_1 & r_2 \\ -r_x & r_1 + r_x + r_a & -r_a \\ -r_3 & -r_a & r_2 + r_3 + r_a \end{bmatrix} \begin{bmatrix} i_1 \\ i_2 \\ i_3 \end{bmatrix} = \begin{bmatrix} v_0 \\ 0 \\ 0 \end{bmatrix}$$

$$RI = V$$

$$I = \begin{bmatrix} i_1 \\ i_2 \\ i_3 \end{bmatrix} \quad , \quad V = \begin{bmatrix} v_0 \\ 0 \\ 0 \end{bmatrix}$$

$$I = R^{-1} V$$

Basic matrix operations

A typical set of linear algebraic equations is given by

$$\sum_{j=1}^{n} a_{i,j} x_j = b_i \qquad A = \begin{bmatrix} a_{1,1} & \dots & a_{1,n} \\ \vdots & \dots & \vdots \\ a_{n,1} & \dots & a_{n,n} \end{bmatrix} \quad , \qquad B = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$Ax = B$$

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

the standard matrix multiplication

$$A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,n} \\ \vdots & \cdots & \vdots \\ a_{n,1} & \cdots & a_{n,n} \end{bmatrix}_{n\times n} \quad , \quad B = \begin{bmatrix} b_{1,1} & \cdots & b_{1,n} \\ \vdots & \cdots & \vdots \\ b_{n,1} & \cdots & b_{n,n} \end{bmatrix}_{n\times n}$$

$$c_{ij} = \sum_{k}^{n} a_{ik} b_{kj}$$

$$AA^{-1} = A^{-1}A = I$$

$$|A| = \sum_{i,j=1}^{n} (-1)^{i+j} a_{i,j} |R_{i,j}|$$

$$TrA = \sum_{i=1}^{n} a_{i,i}$$

The transpose of a matrix

$$A^T_{i,j} = A_{j,i}$$

The orthogonal matrix

$$A^T = A^{-1}$$

The Hermitian operation of **A**

$$A^+ = \left(A^T\right)^*$$

The Hermitian matrix

$$A^+ = A$$

Eigenvalue problem

$$AX = \lambda X$$

x and *λ* are an eigenvector and its corresponding eigenvalue of the matrix

$$AX = \lambda MX$$

$$\xrightarrow{M^{-1}} M^{-1}AX = \lambda M^{-1}MX \xrightarrow{MM^{-1}=I} M^{-1}AX = \lambda X$$

$$M^{-1}AX = \lambda X \xrightarrow{A'=M^{-1}A} A'X = \lambda X$$

Linear equation systems

$$\sum_{j=1}^{n} a_{i,j} x_j = b_i$$

If we assume that $|A| \neq 0$ and $b \neq 0$, then the system has a unique solution.

Gaussian elimination

The basic idea of Gaussian elimination is to transform the original linear equation set to one that has an upper-triangular or lower-triangular coefficient matrix, but has the same solution. Here we want to transform the coefficient matrix into an **upper triangular matrix**.

Gaussian elimination

$$\begin{cases} -3x_1 - x_2 + 4x_3 = 8 \\ x_1 - x_2 + 3x_3 = 13 \\ 4x_1 - 2x_2 + x_3 = 15 \end{cases}$$

$$\begin{bmatrix} -3 & -1 & 4 \\ 1 & -1 & 3 \\ 4 & -2 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8 \\ 13 \\ 15 \end{bmatrix}$$

$$\left[\begin{array}{ccc:c} -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \\ 4 & -2 & 1 & 15 \end{array}\right]$$

$$\left[\begin{array}{ccc:c} -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \\ 4 & -2 & 1 & 15 \end{array}\right]$$

$$A = \{|-3|, |1|, |4|\} \rightarrow A = \{3,1,4\}$$

$$\boxed{Max(A) = 4}$$

Gaussian elimination

$$\left[\begin{array}{ccc|c} -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \\ 4 & -2 & 1 & 15 \end{array}\right] \qquad \left[\begin{array}{ccc|c} -3 & -1 & 4 & 8 \\ 1 & -1 & 3 & 13 \\ 4 & -2 & 1 & 15 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 1 & -1 & 3 & 13 \\ -3 & -1 & 4 & 8 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 1 & -1 & 3 & 13 \\ -3 & -1 & 4 & 8 \end{array}\right]$$

$$\xrightarrow{4R_2 - R_1} \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 1 & -1 & 3 & 13 \\ -3 & -1 & 4 & 8 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ -3 & -1 & 4 & 8 \end{array}\right]$$

Gaussian elimination

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ -3 & -1 & 4 & 8 \end{array}\right] \xrightarrow{4R_3+3R_1} \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ -3 & -1 & 4 & 8 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right]$$

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right]$$

Gaussian elimination

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right]$$

$$A=\{|-2|,|-10|\}\rightarrow A=\{2,10\} \qquad Max(A)=10$$

$$\left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -2 & 11 & 37 \\ 0 & -10 & 19 & 77 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -10 & 19 & 77 \\ 0 & -2 & 11 & 37 \end{array}\right]$$

Gaussian elimination

$$\xrightarrow{10R_3 - 2R_2} \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -10 & 19 & 77 \\ 0 & -2 & 11 & 37 \end{array}\right] \qquad \left[\begin{array}{ccc|c} 4 & -2 & 1 & 15 \\ 0 & -10 & 19 & 77 \\ 0 & 0 & -72 & -216 \end{array}\right]$$

$$\begin{cases} 4x_1 - 2x_2 + x_3 = 15 \\ -10x_2 + 19x_3 = 77 \\ -72x_3 = -216 \end{cases}$$

$$x_3 = 3, \;\; x_2 = -2, \;\; x_2 = 2$$

Gauss-Jordan Method

$$\begin{cases} 2x_2 + x_4 = 0 \\ 2x_1 + 2x_2 + 3x_3 + 2x_4 = -2 \\ 4x_1 - 3x_2 + x_4 = -7 \\ 6x_1 + x_2 - 6x_3 - 5x_4 = 6 \end{cases}$$

$$\begin{bmatrix} 0 & 2 & 0 & 1 & 0 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 6 & 1 & -6 & -5 & 6 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 2 & 0 & 1 & 0 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 6 & 1 & -6 & -5 & 6 \end{bmatrix} \qquad \begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Gauss-Jordan Method

$$\xrightarrow{\frac{1}{6}R_1}\begin{bmatrix} 6 & 1 & -6 & -5 & 6 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0.16667 & -1 & -0.83335 & 1 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Gauss-Jordan Method

$$\begin{array}{c} \\ \xrightarrow{R_2 - 2R_1} \\ \xrightarrow{R_3 - 4R_1} \\ \\ \end{array} \begin{bmatrix} 1 & 0.16667 & -1 & -0.83335 & 1 \\ 2 & 2 & 3 & 2 & -2 \\ 4 & -3 & 0 & 1 & -7 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{array}{c} \\ \xrightarrow{\frac{R_2}{1.6667}} \\ \\ \\ \end{array} \begin{bmatrix} 1 & 0.16667 & -1 & -0.83335 & 1 \\ 0 & 1.6667 & 5 & 3.6667 & -4 \\ 0 & -3.6667 & 4 & 4.3334 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Gauss-Jordan Method

$$\begin{bmatrix} 1 & 0.16667 & -1 & -0.83335 & 1 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & -3.6667 & 4 & 4.3334 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{array}{c} \xrightarrow{R_1 - 0.16667 R_2} \\ \\ \xrightarrow{R_3 + 3.6667 R_2} \\ \xrightarrow{R_4 - 2 R_2} \end{array} \begin{bmatrix} 1 & 0.16667 & -1 & -0.83335 & 1 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & -3.6667 & 4 & 4.3334 & -11 \\ 0 & 2 & 0 & 1 & 0 \end{bmatrix}$$

Gauss-Jordan Method

$$\begin{bmatrix} 1 & 0 & -1.5000 & -1.2000 & 1.4000 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & 0 & 15.000 & 12.400 & -19.800 \\ 0 & 0 & -5.9998 & -3.4000 & 4.8000 \end{bmatrix}$$

$$\xrightarrow{\frac{R_3}{15.000}} \begin{bmatrix} 1 & 0 & -1.5000 & -1.2000 & 1.4000 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & 0 & 15.000 & 12.400 & -19.800 \\ 0 & 0 & -5.9998 & -3.4000 & 4.8000 \end{bmatrix}$$

Gauss-Jordan Method

$$\begin{bmatrix} 1 & 0 & -1.5000 & -1.2000 & 1.4000 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & 0 & 1 & 0.8266 & -1.32 \\ 0 & 0 & -5.9998 & -3.4000 & 4.8000 \end{bmatrix}$$

$$\begin{array}{r} \xrightarrow{R_1+1.5000R_3} \\ \xrightarrow{R_2-2.9999R_3} \\ \\ \xrightarrow{R_3+5.999R_3} \end{array} \begin{bmatrix} 1 & 0 & -1.5000 & -1.2000 & 1.4000 \\ 0 & 1 & 2.9999 & 2.2000 & -2.4000 \\ 0 & 0 & 1 & 0.8266 & -1.32 \\ 0 & 0 & -5.9998 & -3.4000 & 4.8000 \end{bmatrix}$$

Gauss-Jordan Method

$$
\begin{array}{r}
\xrightarrow{R_1+1.5000R_3} \\
\xrightarrow{R_2-2.9999R_3} \\
\\
\xrightarrow{R_3+5.999R_3}
\end{array}
\begin{bmatrix}
1 & 0 & -1.5000 & -1.2000 & 1.4000 \\
0 & 1 & 2.9999 & 2.2000 & -2.4000 \\
0 & 0 & 1 & 0.8266 & -1.32 \\
0 & 0 & -5.9998 & -3.4000 & 4.8000
\end{bmatrix}
$$

$$
\begin{bmatrix}
1 & 0 & 0 & 0.0399 & -1.9 \\
0 & 1 & 0 & -0.2798 & 1.56 \\
0 & 0 & 1 & 0.8266 & -1.32 \\
0 & 0 & 0 & 1.5596 & -3.12
\end{bmatrix}
$$

Gauss-Jordan Method

$$\xrightarrow{\frac{R_4}{1.5596}}\begin{bmatrix} 1 & 0 & 0 & 0.0399 & -1.9 \\ 0 & 1 & 0 & -0.2798 & 1.56 \\ 0 & 0 & 1 & 0.8266 & -1.32 \\ 0 & 0 & 0 & 1.5596 & -3.12 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0.0399 & -1.9 \\ 0 & 1 & 0 & -0.2798 & 1.56 \\ 0 & 0 & 1 & 0.8266 & -1.32 \\ 0 & 0 & 0 & 1 & -2.00 \end{bmatrix}$$

Gauss-Jordan Method

$$
\begin{array}{c}
\xrightarrow{R_1 - 0.0399 R_4} \\
\xrightarrow{R_2 - 0.2798 R_4} \\
\xrightarrow{R_3 - 0.8266 R_4} \\

\end{array}
\begin{bmatrix}
1 & 0 & 0 & 0.0399 & -1.9 \\
0 & 1 & 0 & -0.2798 & 1.56 \\
0 & 0 & 1 & 0.8266 & -1.32 \\
0 & 0 & 0 & 1 & -2.00
\end{bmatrix}
$$

$$
\begin{bmatrix}
1 & 0 & 0 & 0 & -0.5 \\
0 & 1 & 0 & 0 & 1.0004 \\
0 & 0 & 1 & 0 & 0.33326 \\
0 & 0 & 0 & 1 & -2.00
\end{bmatrix}
$$

LU- decomposition

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} \boxed{a_{11} \quad a_{12} \quad a_{13} \quad a_{14}} \\ a_{21} \quad a_{22} \quad a_{23} \quad a_{24} \\ a_{31} \quad a_{32} \quad a_{33} \quad a_{34} \\ a_{41} \quad a_{42} \quad a_{43} \quad a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{11} = l_{11} \quad , \quad a_{12} = l_{11}u_{12} \quad , \quad a_{13} = l_{11}u_{13} \quad , \quad a_{14} = l_{11}u_{14}$$

$$l_{11} = a_{11} \quad , \quad u_{12} = \frac{a_{12}}{l_{11}} \quad , \quad u_{13} = \frac{a_{13}}{l_{11}} \quad , \quad u_{14} = \frac{a_{14}}{l_{11}}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{22} = l_{21}u_{12} + l_{22} \quad , \quad a_{32} = l_{31}u_{12} + l_{32} \quad , \quad a_{42} = l_{41}u_{12} + l_{42}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{21} = l_{21} \quad , \quad a_{22} = l_{21}u_{12} + l_{22}$$

$$a_{23} = l_{21}u_{13} + l_{22}u_{23} \quad , \quad a_{24} = l_{21}u_{14} + l_{22}u_{24}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ \boxed{a_{21} \quad a_{22} \quad a_{23} \quad a_{24}} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{21} = l_{21} \quad , \quad a_{22} = l_{21}u_{12} + l_{22}$$

$$a_{23} = l_{21}u_{13} + l_{22}u_{23} \quad , \quad a_{24} = l_{21}u_{14} + l_{22}u_{24}$$

$$\boxed{\begin{array}{l} l_{21} = a_{21} \quad , \quad l_{22} = a_{22} - l_{21}u_{12} \\ u_{23} = \dfrac{a_{23} - l_{21}u_{13}}{l_{22}} = \quad , \quad u_{24} = \dfrac{a_{24} - l_{21}u_{14}}{l_{22}} \end{array}}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{31} = l_{31} \quad , \quad a_{32} = l_{31}u_{12} + l_{32}$$

$$a_{33} = l_{31}u_{13} + l_{32}u_{23} + l_{33} \quad , \quad a_{34} = l_{31}u_{14} + l_{32}u_{24} + l_{33}u_{34}$$

$$\boxed{\begin{aligned} &l_{31} = a_{31} \quad , \quad l_{32} = a_{32} - l_{31}u_{12} \\ &l_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23} \quad , \quad u_{34} = \frac{a_{34} - l_{31}u_{14} - l_{32}u_{24}}{l_{33}} \end{aligned}}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

LU- decomposition

$$a_{41} = l_{41} \quad , \quad a_{42} = l_{41}u_{12} + l_{42}$$
$$a_{43} = l_{41}u_{13} + l_{42}u_{23} + l_{43} \quad , \quad a_{44} = l_{41}u_{14} + l_{42}u_{24} + l_{43}u_{34} + l_{44}$$

$$\boxed{\begin{aligned} &l_{41} = a_{41} \quad , \quad l_{42} = a_{42} - l_{41}u_{12} \\ &l_{43} = a_{43} - l_{41}u_{13} - l_{42}u_{23} \quad , \quad l_{44} = a_{44} - l_{41}u_{14} - l_{42}u_{24} - l_{43}u_{34} \end{aligned}}$$

LU- decomposition

$$\boxed{\begin{array}{l} l_{ij} = a_{ij} - \displaystyle\sum_{k=1}^{j-1} l_{ik} u_{kj}, \quad j \le i, \qquad i = 1,2,\ldots,n \\[2em] u_{ij} = \dfrac{a_{ij} - \displaystyle\sum_{k=1}^{i-1} l_{ik} u_{kj}}{l_{ii}}, \quad i \le j, \qquad j = 2,3,\ldots,n \end{array}}$$

$$Ax = B$$

$$LUx = B \xrightarrow{L^{-1}} L^{-1}LUx = L^{-1}B \rightarrow Ux = B'$$

$$B' = L^{-1}B$$

LU- decomposition

$$b_1' = \frac{b_1}{l_{11}},$$

$$b_i' = \frac{b_i - \sum_{k=1}^{i-1} l_{ik} b_k'}{l_{ii}}, \quad i = 2,3,\ldots,n$$

$$x_n = b_n',$$

$$x_j = b_j' - \sum_{k=j+1}^{n} u_{jk} x_k, \quad i = n-1, n-2, \ldots, 2, 1$$

LU- decomposition

Determinants and matrix Inversion

$$\det(A) = \det(LU) = \det(L) * \det(U) = \det(l) = \prod_{i=1}^{n} l_{ii}$$

Iterative Methods

$$\begin{cases} 6x_1 - 2x_2 + x_3 = 11 \\ x_1 + 2x_2 - 5x_3 = -1 \\ -2x_1 + 7x_2 + 2x_3 = 5 \end{cases}$$

$$\begin{cases} x_1 = (11 + 2x_2 - x_3)/6 \\ x_3 = -(-1 - x_1 - 2x_2)/5 \\ x_2 = (5 + 2x_1 - 2x_3)/7 \end{cases}$$

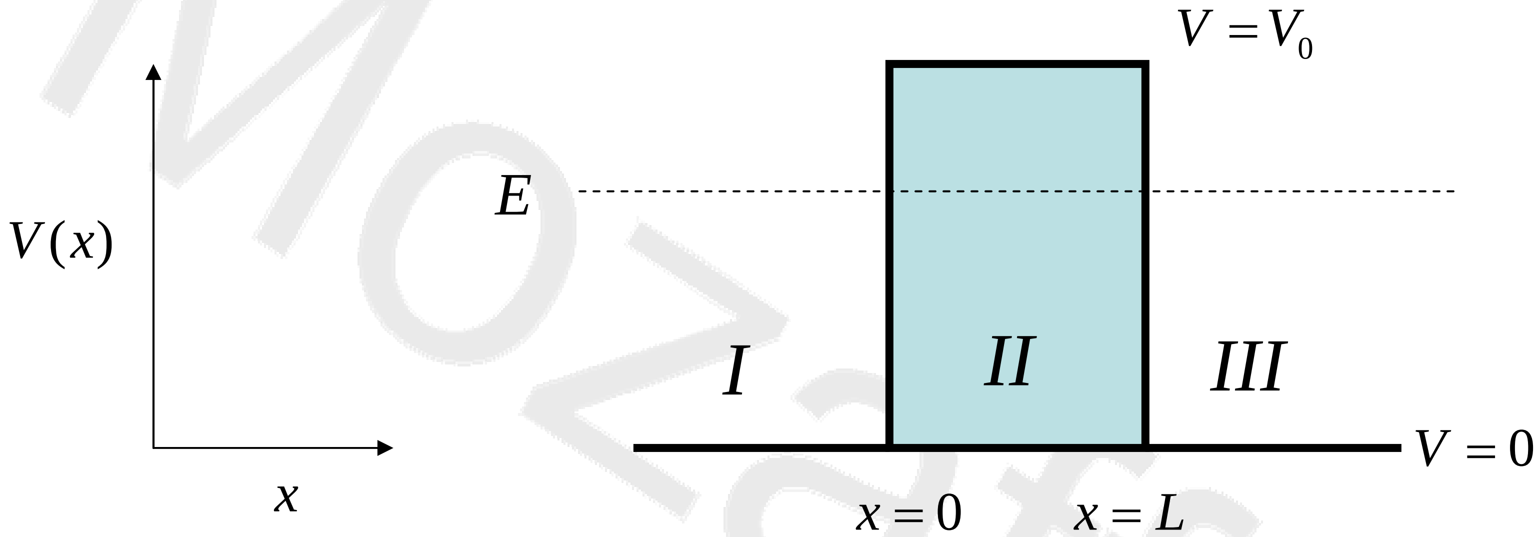
$$\begin{cases} x_1^{(n+1)} = (11 + 2x_2^{(n)} - x_3^{(n)})/6 \\ x_3^{(n+1)} = -(-1 - x_1^{(n)} - 2x_2^{(n)})/5 \\ x_2^{(n+1)} = (5 + 2x_1^{(n)} - 2x_3^{(n)})/7 \end{cases}$$

$$R^{(n)} = \sqrt{\left(x_1^n\right)^2 + \left(x_2^n\right)^2 + \left(x_3^n\right)^2}$$

$$R^{(n)} \rightarrow 0$$

	First	Second	Third	Fourth	Fifth	Sixth	…	Ninth
x_1	0	1.833	2.038	2.085	2.004	1.994	…	2
x_2	0	0.714	1.181	1.053	1.001	0.990	…	1
x_3	0	0.200	0.852	1.080	1.038	1.001	…	1

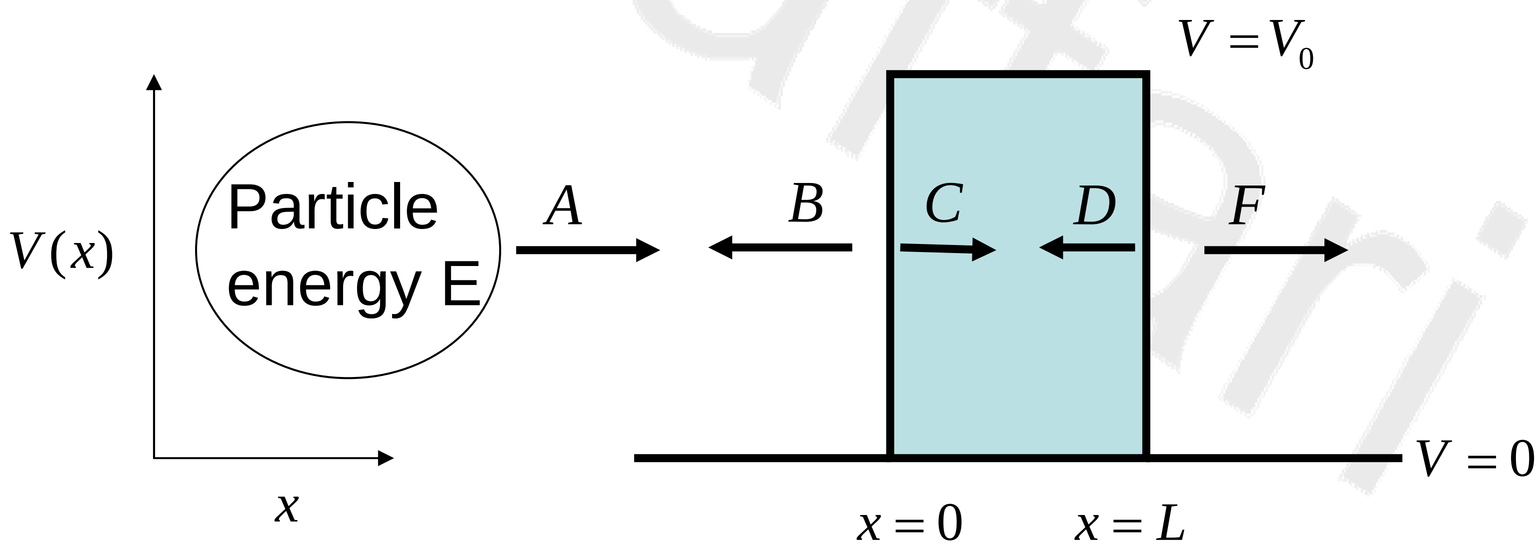
$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$



$$\begin{cases}\dfrac{d^2\psi(x)}{dx^2}=-\dfrac{2mE}{\hbar^2}\psi(x) \quad , \quad x<0\\[2ex] \dfrac{d^2\psi(x)}{dx^2}=-\dfrac{2m}{\hbar^2}(E-V_0)\psi(x) \quad , \quad 0<x<L\\[2ex] \dfrac{d^2\psi(x)}{dx^2}=-\dfrac{2mE}{\hbar^2}\psi(x) \quad , \quad x>L\end{cases}$$

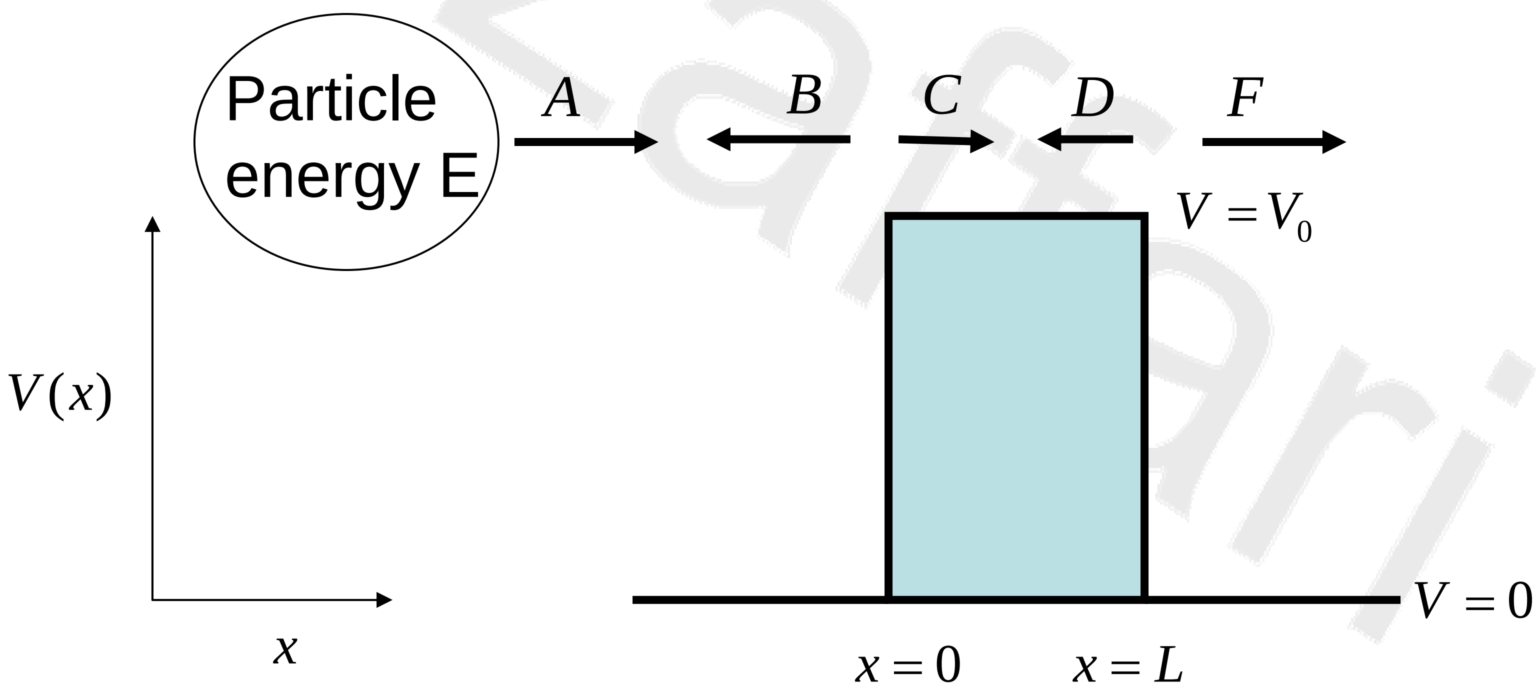
$$k^2 = \frac{2mE}{\hbar^2} \quad , \quad k'^2 = \frac{2m(E - V_0)}{\hbar^2} \quad , \quad E < V_0$$

$$\begin{cases} \dfrac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \Rightarrow \psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad , \quad x < 0 \\ \dfrac{d^2\psi(x)}{dx^2} + k'^2\psi(x) = 0 \Rightarrow \psi_{II}(x) = Ce^{k'x} + De^{-k'x} \quad , \quad 0 < x < L \\ \dfrac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \Rightarrow \psi_{III}(x) = Fe^{ikx} \quad , \quad x > L \end{cases}$$



$$k^2 = \frac{2mE}{\hbar^2} \quad , \quad k'^2 = \frac{2m(E - V_0)}{\hbar^2} \quad , \quad E > V_0$$

$$\begin{cases} \psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad , \quad x < 0 \\ \psi_{II}(x) = Ce^{ik'x} + De^{-ik'x} \quad , \quad 0 < x < L \\ \psi_{III}(x) = Fe^{ikx} \quad , \quad x > L \end{cases}$$

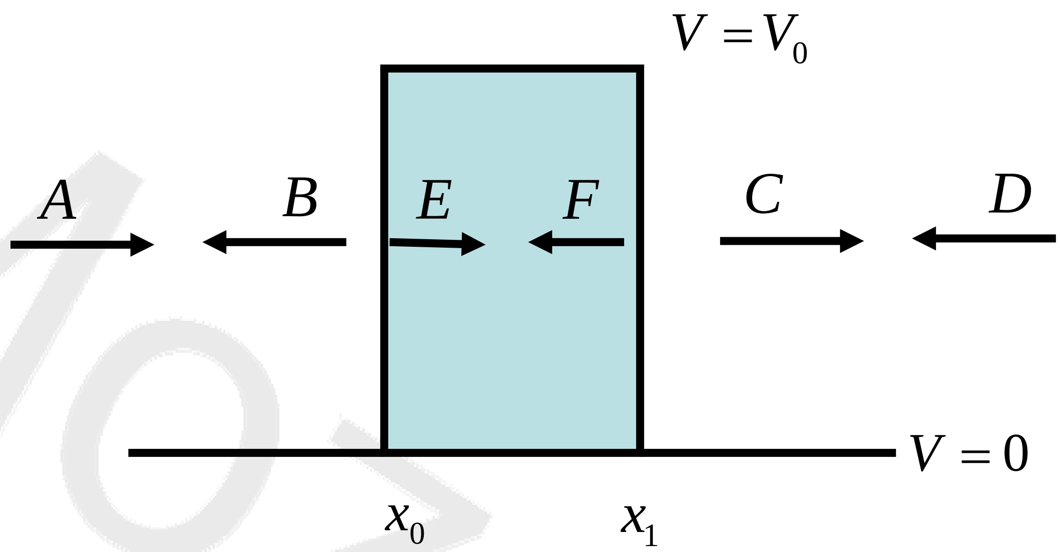


$$\begin{cases} \psi_I(x=0)=\psi_{II}(x=0) \Rightarrow A+B=C+D \\ \left.\dfrac{d\psi_I}{dx}\right|_{x=0} = \left.\dfrac{d\psi_{II}}{dx}\right|_{x=0} \Rightarrow ik(A-B)=k'(C-D) \end{cases}$$

$$\begin{cases} \psi_{II}(x=L)=\psi_{III}(x=L) \Rightarrow Ce^{k'L}+De^{-k'L}=Fe^{ikL} \\ \left.\dfrac{d\psi_{II}}{dx}\right|_{x=L} = \left.\dfrac{d\psi_{III}}{dx}\right|_{x=L} \Rightarrow k'(Ce^{k'L}-De^{-k'L})=ikFe^{ikL} \end{cases}$$

$$\begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix}=\begin{bmatrix} 1 & 1 \\ k' & -k' \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} e^{k'L} & e^{-k'L} \\ k'e^{k'L} & -k'e^{-k'L} \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix}=\begin{bmatrix} e^{ikL} & 0 \\ ike^{ikL} & 0 \end{bmatrix}\begin{bmatrix} F \\ 0 \end{bmatrix}$$



$$\begin{cases} Ae^{ikx_0} + Be^{-ikx_0} = Ee^{k'x_0} + Fe^{-k'x_0} \\ ik(Ae^{ikx_0} - Be^{-ikx_0}) = k'(Ee^{k'x_0} - Fe^{-k'x_0}) \end{cases}$$

$$\begin{cases} Ee^{k'x_1} + Fe^{-k'x_1} = Ce^{ikx_1} + De^{-ikx_1} \\ k'(Ee^{k'x_1} - Fe^{-k'x_1}) = ik(Ce^{ikx_1} - De^{-ikx_1}) \end{cases}$$

Boundary condition:

$$\begin{cases} Ae^{ikx_0} + Be^{-ikx_0} = Ee^{k'x_0} + Fe^{-k'x_0} \\ ik(Ae^{ikx_0} - Be^{-ikx_0}) = k'(Ee^{k'x_0} - Fe^{-k'x_0}) \end{cases}$$

$$\begin{cases} Ee^{k'x_1} + Fe^{-k'x_1} = Ce^{ikx_1} + De^{-ikx_1} \\ k'(Ee^{k'x_1} - Fe^{-k'x_1}) = ik(Ce^{ikx_1} - De^{-ikx_1}) \end{cases}$$

$$\begin{bmatrix} e^{ikx_0} & e^{-ikx_0} \\ ike^{ikx_0} & -ike^{-ikx_0} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{k'x_0} & e^{-k'x_0} \\ k'e^{k'x_0} & -k'e^{-k'x_0} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}$$

$$\begin{bmatrix} e^{k'x_1} & e^{-k'x_1} \\ k'e^{k'x_1} & -k'e^{-k'x_1} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

$$M_1\begin{bmatrix}A\\B\end{bmatrix}=M_2\begin{bmatrix}E\\F\end{bmatrix}$$

$$M_3\begin{bmatrix}E\\F\end{bmatrix}=M_4\begin{bmatrix}C\\D\end{bmatrix}$$

$$M_1=\begin{bmatrix}e^{ikx_0} & e^{-ikx_0}\\ ike^{ikx_0} & -ike^{-ikx_0}\end{bmatrix},\quad M_2=\begin{bmatrix}e^{k'x_0} & e^{-k'x_0}\\ k'e^{k'x_0} & -k'e^{-k'x_0}\end{bmatrix}$$

$$M_3=\begin{bmatrix}e^{k'x_1} & e^{-k'x_1}\\ k'e^{k'x_1} & -k'e^{-k'x_1}\end{bmatrix},\quad M_4=\begin{bmatrix}e^{ikx_1} & e^{-ikx_1}\\ ike^{ikx_1} & -ike^{-ikx_1}\end{bmatrix}$$

$$M_1\begin{bmatrix} A \\ B \end{bmatrix} = M_2\begin{bmatrix} E \\ F \end{bmatrix}$$

$$M_3\begin{bmatrix} E \\ F \end{bmatrix} = M_4\begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{cases} M_2^{-1}M_1\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} E \\ F \end{bmatrix} \\ M_4^{-1}M_3\begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix} \end{cases} \Rightarrow \begin{bmatrix} C \\ D \end{bmatrix} = M_4^{-1}M_3M_2^{-1}M_1\begin{bmatrix} A \\ B \end{bmatrix}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = M \begin{bmatrix} A \\ B \end{bmatrix} \qquad M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

$$M = M_4^{-1} M_3 M_2^{-1} M_1 \qquad k^2 = \frac{2mE}{\hbar^2} \quad , \quad k'^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$M_1 = \begin{bmatrix} e^{ikx_0} & e^{-ikx_0} \\ ike^{ikx_0} & -ike^{-ikx_0} \end{bmatrix} \quad , \quad M_2 = \begin{bmatrix} e^{k'x_0} & e^{-k'x_0} \\ k'e^{k'x_0} & -k'e^{-k'x_0} \end{bmatrix}$$

$$M_3 = \begin{bmatrix} e^{k'x_1} & e^{-k'x_1} \\ k'e^{k'x_1} & -k'e^{-k'x_1} \end{bmatrix} \quad , \quad M_4 = \begin{bmatrix} e^{ikx_1} & e^{-ikx_1} \\ ike^{ikx_1} & -ike^{-ikx_1} \end{bmatrix}$$

We know : $\boxed{A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \quad , \quad A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}}$

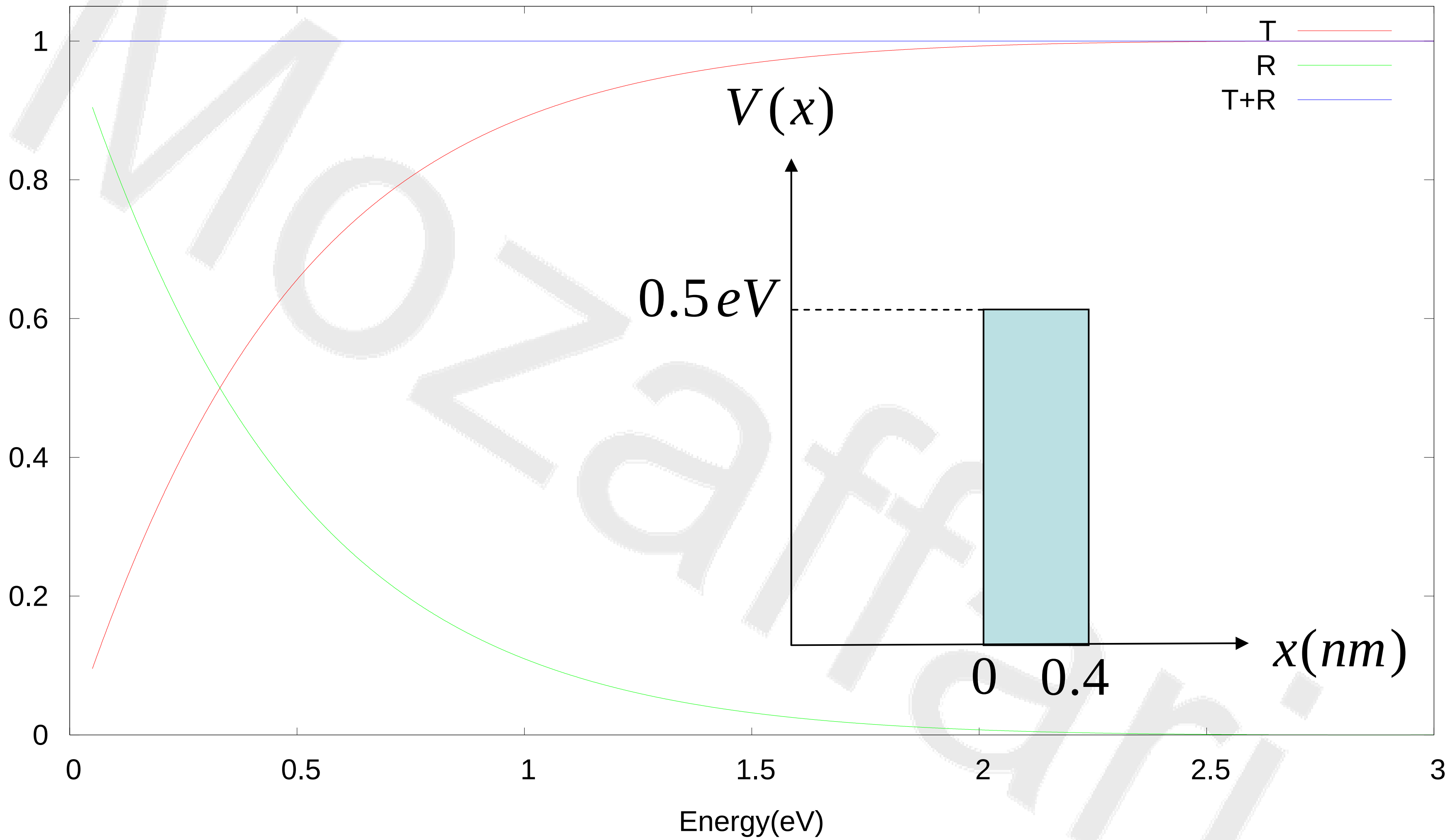
$$\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

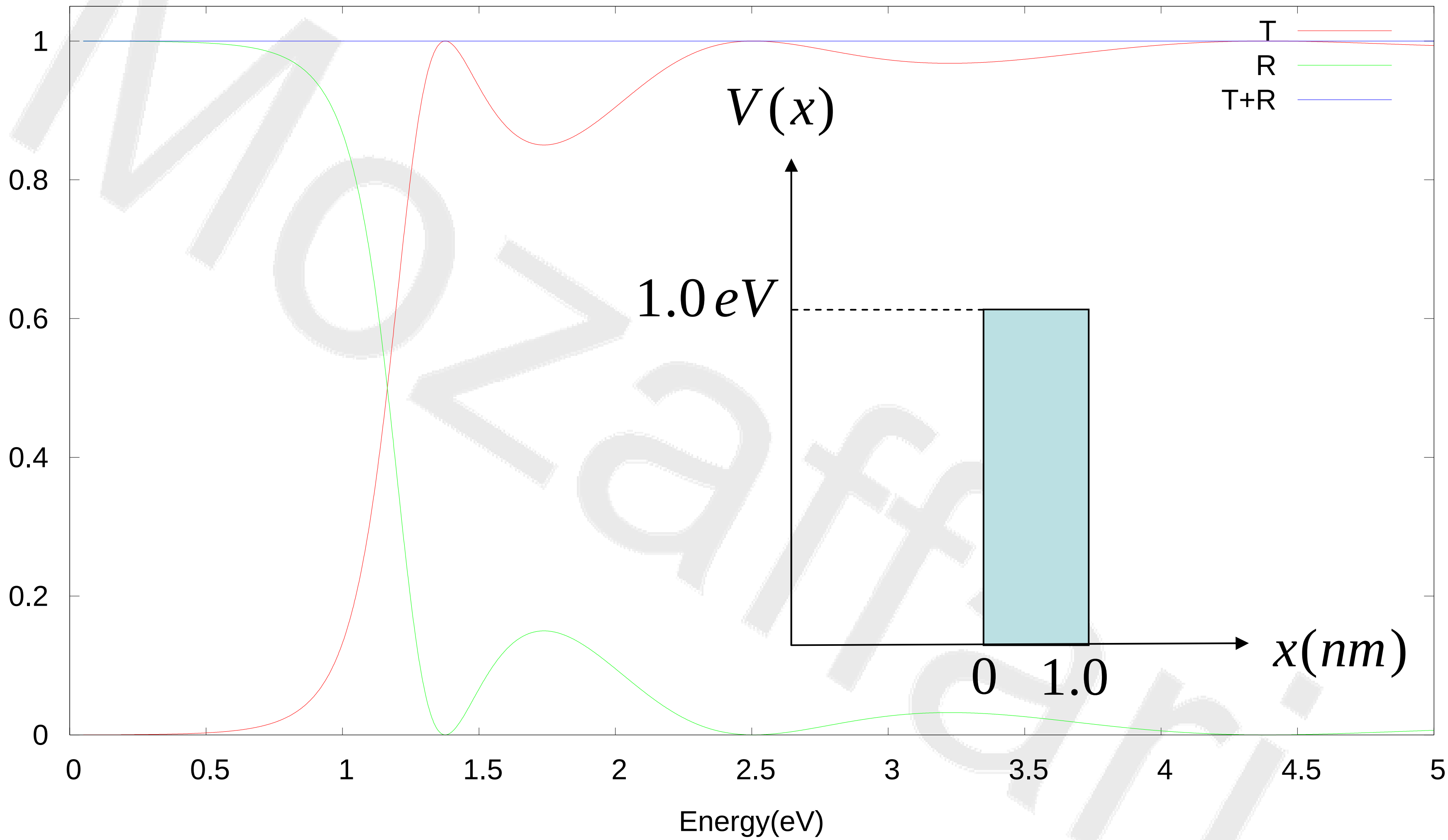
$$M_{11}A + M_{12}B = C \longrightarrow \frac{C}{A} = M_{11} + M_{12}\frac{B}{A} \Rightarrow \frac{C}{A} = M_{11} - \frac{M_{12}M_{21}}{M_{22}}$$

$$M_{21}A + M_{22}B = D \xrightarrow{D=0} \frac{B}{A} = -\frac{M_{21}}{M_{22}}$$

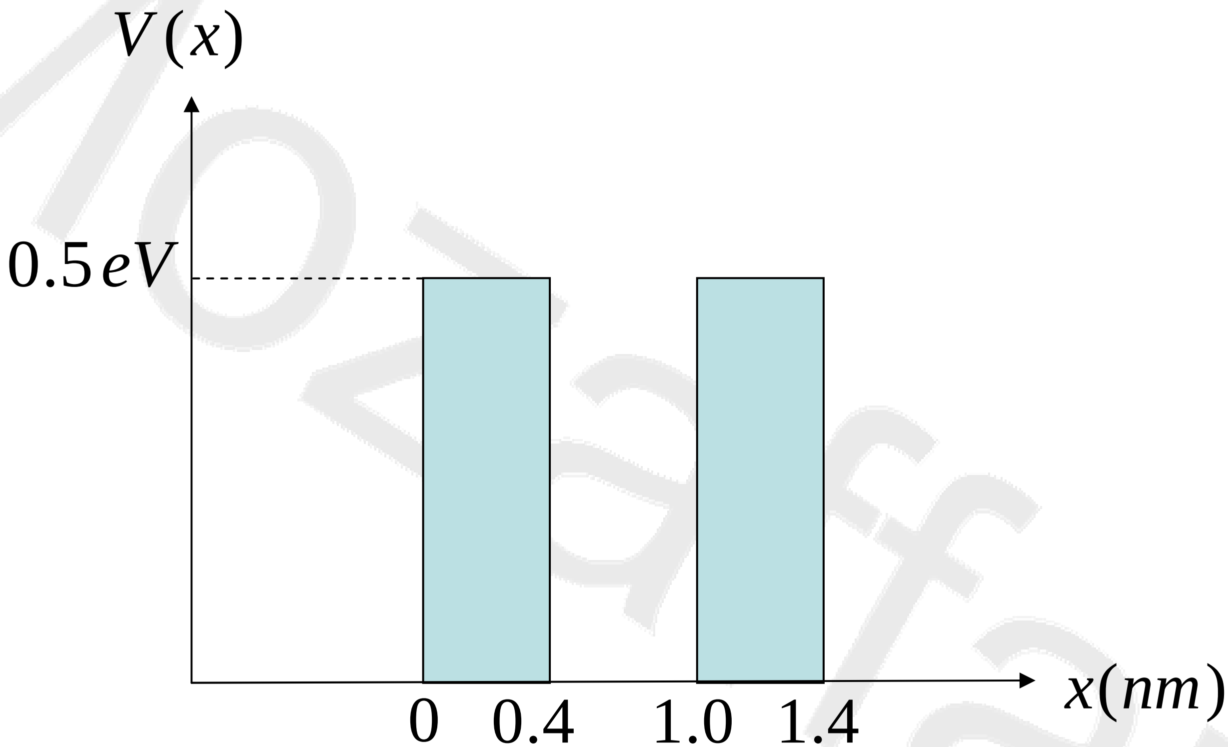
$$\begin{cases} \dfrac{C}{A} = M_{11} - \dfrac{M_{12}M_{21}}{M_{22}} \\ \dfrac{B}{A} = -\dfrac{M_{21}}{M_{22}} \end{cases} \Rightarrow \begin{cases} T(E) = \left|\dfrac{C}{A}\right|^2 \\ R(E) = \left|\dfrac{B}{A}\right|^2 \end{cases}$$

$$T(E) + R(E) = 1$$

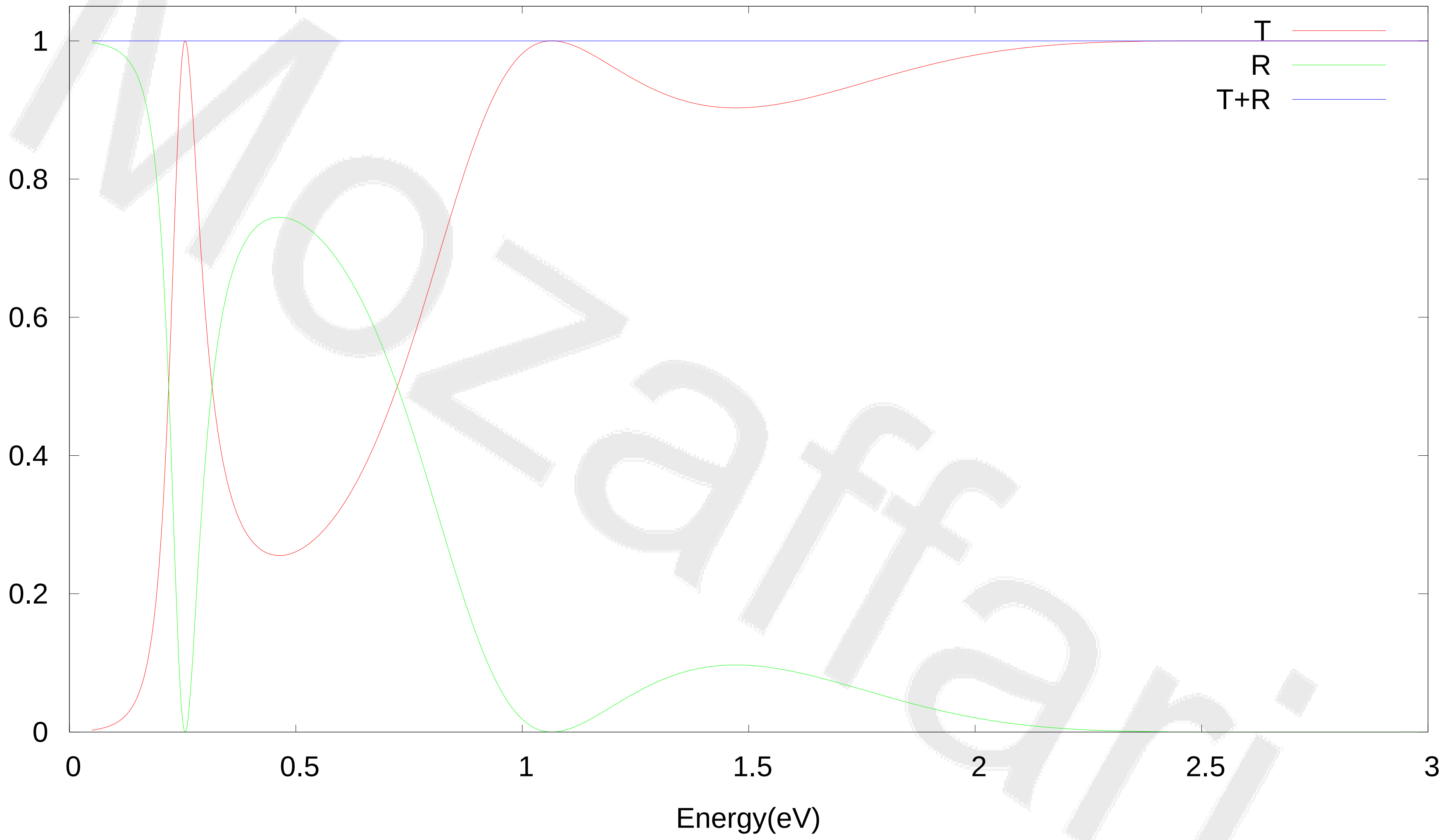

T
R
T+R
$V(x)$
$0.5eV$
$x(nm)$
0
0.4
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5
3
Energy(eV)

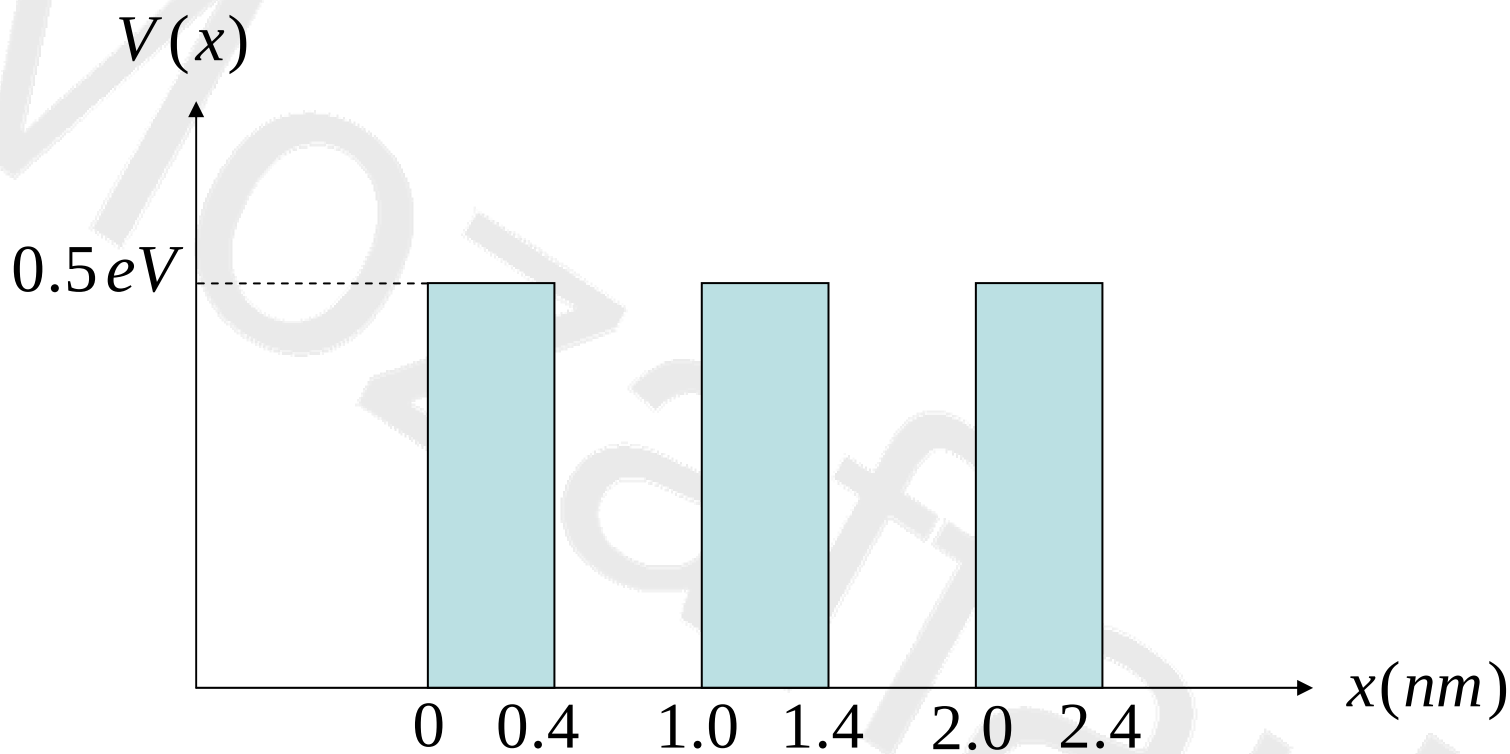


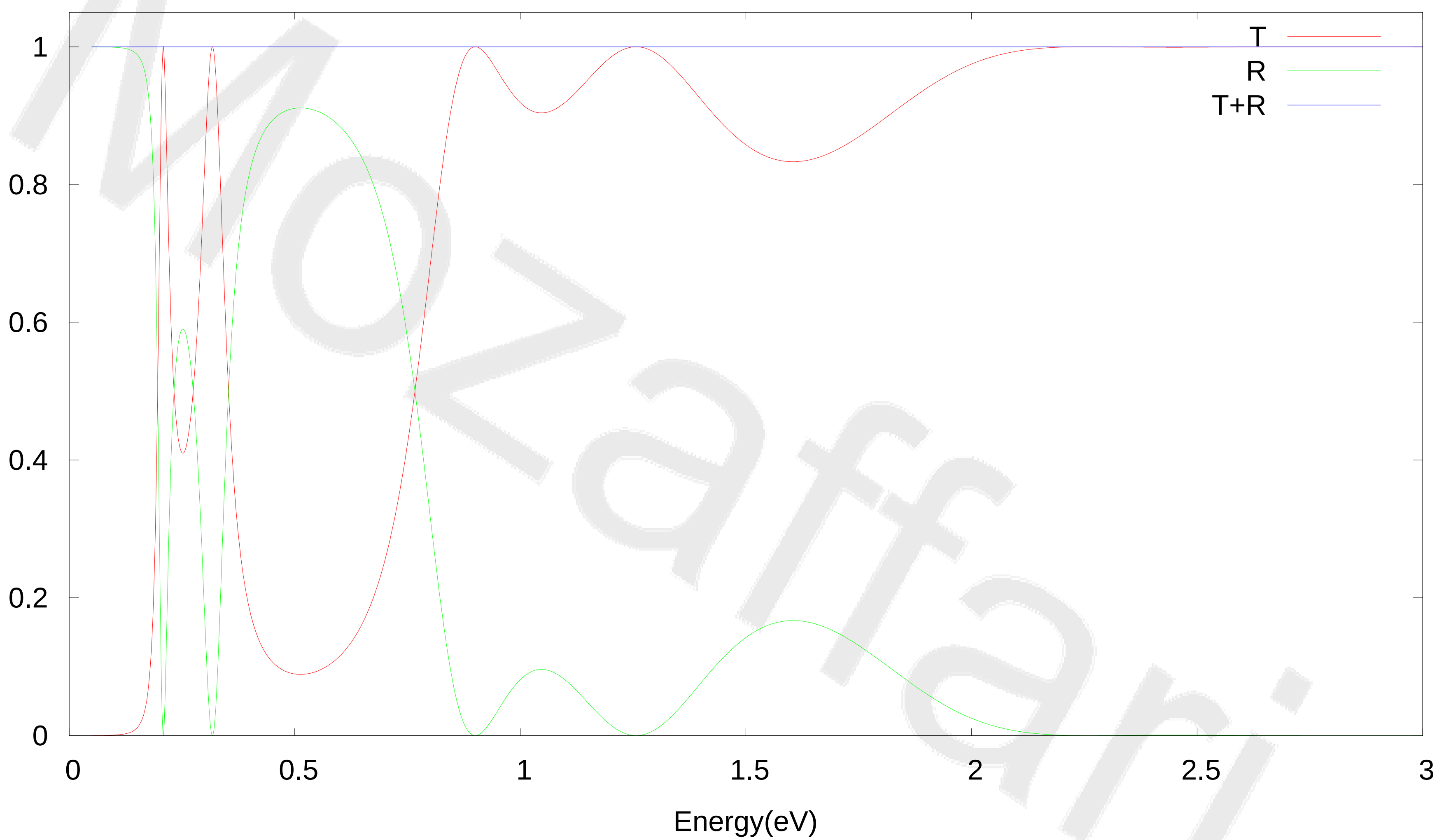
T
R
T+R
V(x)
1.0 eV
x(nm)
0
1.0
0
0.2
0.4
0.6
0.8
1
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Energy(eV)

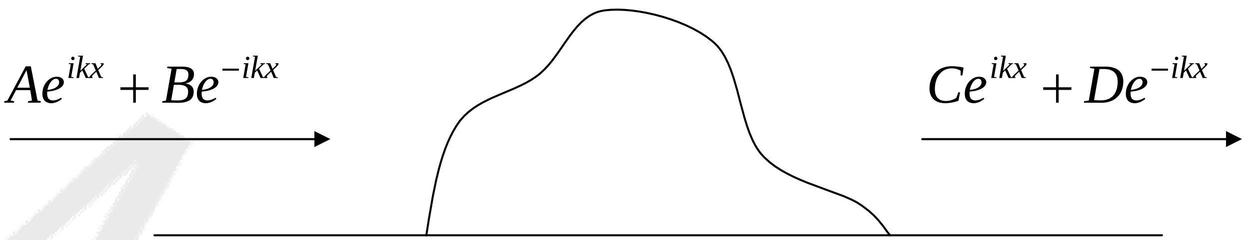


$V(x)$
$0.5eV$
0
0.4
1.0
1.4
$x(nm)$


T
R
T+R
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5
3
Energy(eV)


$V(x)$
$0.5\,eV$
$x(nm)$
0
0.4
1.0
1.4
2.0
2.4


T
R
T+R
1
0.8
0.6
0.4
0.2
0
0
0.5
1
1.5
2
2.5
3
Energy(eV)



Scattering matrix : $$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$$

$$\begin{cases} C = S_{11}A + S_{12}D \\ B = S_{21}A + S_{22}D \end{cases} \Rightarrow \begin{bmatrix} C \\ B \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix}$$

$$\xrightarrow{D=0} \begin{cases} \dfrac{C}{A} = S_{11} \Rightarrow T = \left|S_{11}\right|^2 \\ \dfrac{B}{A} = S_{21} \Rightarrow R = \left|S_{21}\right|^2 \end{cases}$$

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$$

Properties:

$$\begin{cases} |S_{11}|^2 + |S_{21}|^2 = 1 \\ |S_{12}|^2 + |S_{22}|^2 = 1 \\ S_{11}S^*{}_{12} + S_{21}S^*{}_{22} = 0 \end{cases}$$

$$T + R = 1$$