Theoretical Mechanics

理论力学

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Syllabus

- Chapter 0 Preface
- Chapter 1 Survey of the Elementary Principles
- Chapter 2 Variational Principle and Lagrange's Equations
- Chapter 3 The Central Force Problem
- Chapter 4 The Kinematics of Rigid Body Motion

Mid-term exam

- Chapter 5 The Rigid Body Equations of Motion
- Chapter 6 Oscillations
- Chapter 7 The Classical Mechanics of the Special Theory of Relativity
- Chapter 8 The Hamilton Equations of Motion
- Chapter 9 Canonical Transformations

Final term exam

- Chapter 10 Introduction to the Lagrangian and Hamiltonian Formulations for Continuous Systems and Fields

6.2 The Eigenvalue Equation and the Principal Axis Transformation

Assume that solution will be $\eta_i = Ca_i e^{-i\omega t}$

$T_{ij}\ddot{\eta}_j + V_{ij}\eta_j = 0 \Longrightarrow -\omega^2 T_{ij}a_j + V_{ij}a_j = 0$ or
$\mathbf{Va} - \lambda\mathbf{Ta} = 0$ with $\lambda = \omega^2$

It's a slightly odd eigenvalue equation

Solution can be found by $|\mathbf{V} - \lambda\mathbf{T}| = 0$

n-th order polynomial of $\lambda \rightarrow$ Expect n solutions for λ

λ must be real and $\lambda = \omega^2 > 0$

Reality of Eigenvalues

Start from $\mathbf{Va} = \lambda\mathbf{Ta}$

Take adjoint (伴随，complex conjugate + transpose)

$$\Longrightarrow \mathbf{a}^\dagger\mathbf{V} = \lambda^*\mathbf{a}^\dagger\mathbf{T}$$

Multiplying by $\mathbf{a}^\dagger$ or $\mathbf{a}$ gives $\mathbf{a}^\dagger\mathbf{Va} = \lambda\mathbf{a}^\dagger\mathbf{Ta} = \lambda^*\mathbf{a}^\dagger\mathbf{Ta}$

$$\Longrightarrow (\lambda - \lambda^*)\,\mathbf{a}^\dagger\mathbf{Ta} = 0$$

Writing $\mathbf{a}$ as $\boldsymbol{\alpha} + i\boldsymbol{\beta}$ ($\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are real)

$$\mathbf{a}^\dagger\mathbf{Ta} = (\tilde{\boldsymbol{\alpha}} - i\tilde{\boldsymbol{\beta}})\mathbf{T}(\boldsymbol{\alpha} + i\boldsymbol{\beta}) = \tilde{\boldsymbol{\alpha}}\mathbf{T}\boldsymbol{\alpha} + \tilde{\boldsymbol{\beta}}\mathbf{T}\boldsymbol{\beta} + i(\tilde{\boldsymbol{\alpha}}\mathbf{T}\boldsymbol{\beta} - \tilde{\boldsymbol{\beta}}\mathbf{T}\boldsymbol{\alpha})$$

zero

Since $T = \frac{1}{2}\tilde{\dot{\boldsymbol{\eta}}}\mathbf{T}\dot{\boldsymbol{\eta}}$ is positive for any real $\dot{\boldsymbol{\eta}}$

$$\mathbf{a}^\dagger\mathbf{Ta} = \tilde{\boldsymbol{\alpha}}\mathbf{T}\boldsymbol{\alpha} + \tilde{\boldsymbol{\beta}}\mathbf{T}\boldsymbol{\beta} > 0 \Longrightarrow \lambda - \lambda^* = 0, \text{ i.e., } \lambda \text{ is real}$$

Reality of Eigenvalues

Now that we know λ is real

$$\mathbf{Va} = \lambda\mathbf{Ta} \Longrightarrow \mathbf{V}\boldsymbol{\alpha} + i\mathbf{V}\boldsymbol{\beta} = \lambda\mathbf{T}\boldsymbol{\alpha} + i\lambda\mathbf{T}\boldsymbol{\beta}$$

$\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ both satisfy the same eigenvalue equation

Suppose that the eigenvalues are not degenerate

$$|\mathbf{V} - \lambda\mathbf{T}| = 0 \Longrightarrow \lambda = \lambda_1, \lambda_2, \ldots, \lambda_n$$

Will worry about the degenerate case later...

Each eigenvalue corresponds to 1 eigenvector

$\rightarrow\alpha$ and β are proportional to each other

$\mathbf{a} = \boldsymbol{\alpha} + i\boldsymbol{\beta} = \gamma\boldsymbol{\alpha}$, where γ is a complex number

a can be made real by absorbing γ in C of $\eta_i = Ca_i e^{-i\omega t}$

Positive Definiteness

We now have an all-real equation $\tilde{\mathbf{a}}\mathbf{V}\mathbf{a} = \lambda\tilde{\mathbf{a}}\mathbf{T}\mathbf{a}$

$$\Longrightarrow \lambda = \frac{\tilde{\mathbf{a}}\mathbf{V}\mathbf{a}}{\tilde{\mathbf{a}}\mathbf{T}\mathbf{a}}$$

positive semi-definite because $V = \frac{1}{2}\tilde{\eta}\mathbf{V}\eta \geq 0$ for any real η if V is minimum at the equilibrium

Already shown to be positive

$\lambda = \omega^2$ is positive semi-definite

We now have a guarantee that each solution of the eigenvalue equation gives an oscillating solution

$\boldsymbol{\eta} = C\mathbf{a}e^{-i\omega t}$ with a definite frequency $\lambda = \omega^2$

Normalization

Eigenvector satisfying $\mathbf{Va} = \lambda \mathbf{Ta}$ has arbitrary scale

$\mathbf{a} \to C\mathbf{a}$ can absorb such scale as well as imaginary phase

We fix the normalization by declaring

$$\tilde{\mathbf{a}}\mathbf{Ta} = 1$$

Just the sign ($\pm$) remains ambiguous

This turns $\lambda = \dfrac{\tilde{\mathbf{a}}\mathbf{Va}}{\tilde{\mathbf{a}}\mathbf{Ta}} \Longrightarrow \lambda = \tilde{\mathbf{a}}\mathbf{Va}$

Principal Axis Transformation

There are n eigenvectors $\rightarrow$ Call them $\mathbf{a}_j$

$$\mathbf{V}\mathbf{a}_j = \lambda_j \mathbf{T}\mathbf{a}_j \quad j = 1,2,\ldots,n \quad \text{no sum over } j \text{ or } k$$

Take transpose $\rightarrow$ $\tilde{\mathbf{a}}_k \mathbf{V} = \lambda_k \tilde{\mathbf{a}}_k \mathbf{T} \Longrightarrow \left(\lambda_j - \lambda_k\right) \tilde{\mathbf{a}}_k \mathbf{T}\mathbf{a}_j = 0$

$$\Longrightarrow \tilde{\mathbf{a}}_k \mathbf{T}\mathbf{a}_j = \delta_{jk} \leftarrow \text{Assuming } \lambda_j \neq \lambda_k \text{ for } j \neq k$$

$$\tilde{\mathbf{a}}_k \mathbf{V}\mathbf{a}_j = \lambda_j \delta_{jk}$$

If we stack $\mathbf{a}_j$ to make $\mathbf{A} = \left[\mathbf{a}_1 \ \mathbf{a}_2 \ \cdots \ \mathbf{a}_n\right]$

$$\begin{cases} \tilde{\mathbf{A}}\mathbf{T}\mathbf{A} = \mathbf{1} \\ \tilde{\mathbf{A}}\mathbf{V}\mathbf{A} = \boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \end{cases}$$

T and V are diagonalized by the principal axis transformation

6.3 Frequencies of Free Vibration, and Normal Coordinates

Lagrangian was $L = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j - \frac{1}{2} V_{ij} \eta_i \eta_j = \frac{1}{2} \tilde{\boldsymbol{\eta}} \mathbf{T} \dot{\boldsymbol{\eta}} - \frac{1}{2} \tilde{\boldsymbol{\eta}} \mathbf{V} \boldsymbol{\eta}$

Once we have $\mathbf{A}$, we can switch to new coordinates

$\boldsymbol{\zeta} \equiv \mathbf{A}^{-1} \boldsymbol{\eta} \rightarrow$ Normal coordinates

$\mathbf{A}^{-1}$ does exist because $\tilde{\mathbf{A}} \mathbf{T} \mathbf{A} = \mathbf{1} \Longrightarrow |\mathbf{A}| \neq 0$

Lagrangian becomes

$$L = \frac{1}{2} \dot{\tilde{\boldsymbol{\xi}}} \tilde{\mathbf{A}} \mathbf{T} \mathbf{A} \dot{\boldsymbol{\xi}} - \frac{1}{2} \tilde{\boldsymbol{\xi}} \tilde{\mathbf{A}} \mathbf{V} \mathbf{A} \boldsymbol{\xi} = \frac{1}{2} \dot{\tilde{\boldsymbol{\xi}}} \dot{\boldsymbol{\xi}} - \frac{1}{2} \tilde{\boldsymbol{\xi}} \boldsymbol{\lambda} \boldsymbol{\xi} = \frac{1}{2} \sum_k \dot{\zeta}_k \dot{\zeta}_k - \frac{1}{2} \sum_k \lambda_k \zeta_k \zeta_k$$

No cross terms

Solutions are obvious

$$\ddot{\zeta}_k = -\lambda_k \zeta_k \Longrightarrow \zeta_k = C_k e^{-i\omega_k t} \quad \omega_k^2 = \lambda_k$$

Normal coordinates are independent simple harmonic oscillators

Initial Conditions

The coefficients C_k is fixed by the initial conditions

Suppose at $t = 0$ $\quad \boldsymbol{\eta} = \boldsymbol{\eta}(0) \quad \dot{\boldsymbol{\eta}} = \dot{\boldsymbol{\eta}}(0)$

$$\boldsymbol{\eta}(0) = \mathbf{A}\boldsymbol{\xi}(0) \Longrightarrow \eta_j(0) = a_{jk} \operatorname{Re} C_k$$

Remember: take the real part!

$$\dot{\boldsymbol{\eta}}(0) = \mathbf{A}\dot{\boldsymbol{\xi}}(0) \Longrightarrow \dot{\eta}_j(0) = a_{jk} \operatorname{Re}\left(-i\omega_k C_k\right) = a_{jk}\omega_k \operatorname{Im} C_k$$

Using $\tilde{\mathbf{A}}\mathbf{T}\mathbf{A} = \mathbf{1}$

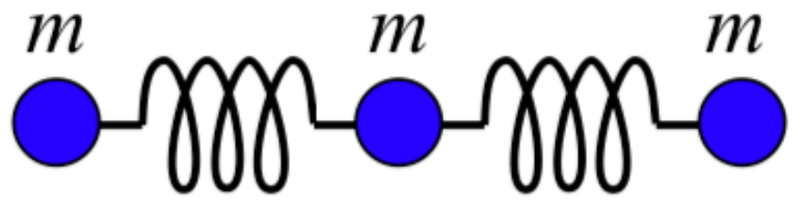
$$\operatorname{Re} C_k = a_{lk} T_{lj} \eta_j(0)$$

$$\operatorname{Im} C_k = \frac{1}{\omega_k} a_{lk} T_{lj} \dot{\eta}_j(0)$$

We need an example now...

6.4 Free Vibrations of a Linear Triatomic Molecule

Consider a molecule like CO_2



Consider only motion along the axis

$$T = \frac{m}{2}\left(\dot{\eta}_1^2 + \dot{\eta}_2^2 + \dot{\eta}_3^2\right) \quad V = \frac{k}{2}\left(\eta_2 - \eta_1\right)^2 + \frac{k}{2}\left(\eta_3 - \eta_2\right)^2$$

$$\mathbf{T} = \begin{bmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{bmatrix} \qquad \mathbf{V} = \begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix}$$

We want to solve eigenvalue equation $\left(\mathbf{V} - \omega^2\mathbf{T}\right)\mathbf{a} = 0$

Linear Triatomic Molecule

$$\left|\mathbf{V}-\omega^2\mathbf{T}\right| = \begin{vmatrix} k-\omega^2 m & -k & 0 \\ -k & 2k-\omega^2 m & -k \\ 0 & -k & k-\omega^2 m \end{vmatrix} = 0$$

$$\Longrightarrow \omega^2\left(k-\omega^2 m\right)\left(3k-\omega^2 m\right)=0$$

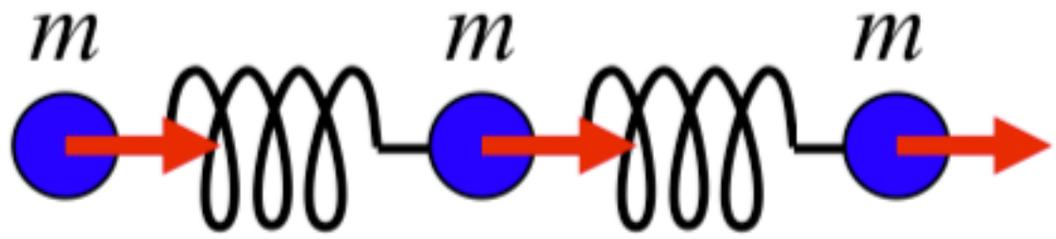
Solutions are $\omega_1 = 0 \quad \omega_2 = \sqrt{\frac{k}{m}} \quad \omega_3 = \sqrt{\frac{3k}{m}}$

$$\mathbf{a}_1 = \frac{1}{\sqrt{3m}}\begin{bmatrix}1\\1\\1\end{bmatrix} \quad \mathbf{a}_2 = \frac{1}{\sqrt{2m}}\begin{bmatrix}1\\0\\-1\end{bmatrix} \quad \mathbf{a}_3 = \frac{1}{\sqrt{6m}}\begin{bmatrix}1\\-2\\1\end{bmatrix}$$

Linear Triatomic Molecule

First solution is linear movement of the molecule

$$\omega_1 = 0 \quad \mathbf{a}_1 = \frac{1}{\sqrt{3m}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$



This is not an “oscillation”

Consider it as an oscillation with infinitely long period

Although V is minimum at the equilibrium, it does not increase when the whole molecule is shifted

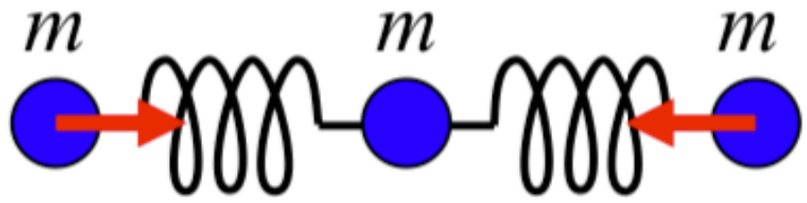
Position of the CoM is a cyclic coordinate

Total momentum is conserved

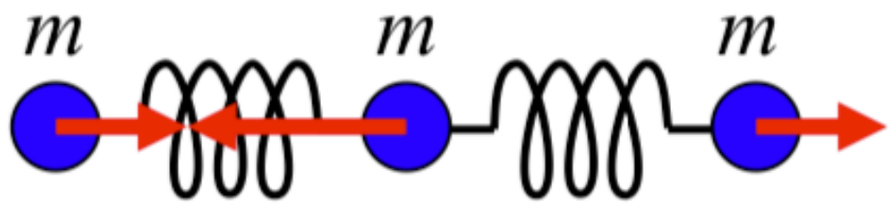
Linear Triatomic Molecule

Two “normal” oscillation modes exist

$$\omega_2 = \sqrt{\frac{k}{m}} \quad \mathbf{a}_2 = \frac{1}{\sqrt{2m}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$



$$\omega_3 = \sqrt{\frac{3k}{m}} \quad \mathbf{a}_3 = \frac{1}{\sqrt{6m}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$



CoM does not move→Orthogonal to the first solution

Linear Triatomic Molecule

Putting together $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$

$$\mathbf{A} = \frac{1}{\sqrt{6m}} \begin{bmatrix} \sqrt{2} & \sqrt{3} & 1 \\ \sqrt{2} & 0 & -2 \\ \sqrt{2} & -\sqrt{3} & 1 \end{bmatrix} \Longrightarrow \mathbf{A}^{-1} = \sqrt{\frac{m}{6}} \begin{bmatrix} \sqrt{2} & \sqrt{2} & \sqrt{2} \\ \sqrt{3} & 0 & -\sqrt{3} \\ 1 & -2 & 1 \end{bmatrix}$$

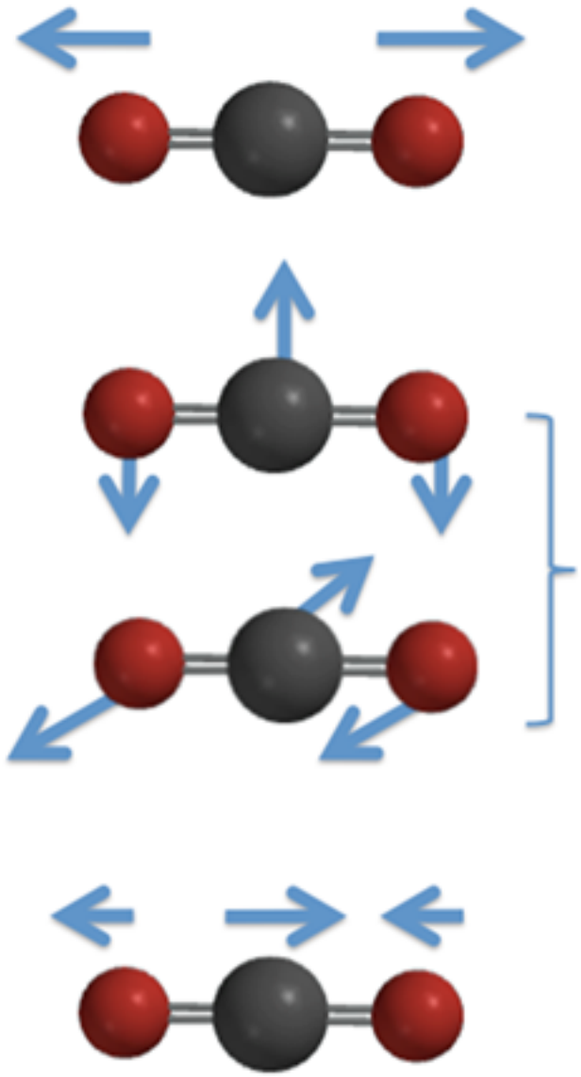
Normal coordinates are

$$\zeta_1 = \sqrt{\frac{m}{3}} (\eta_1 + \eta_2 + \eta_3) \quad \zeta_2 = \sqrt{\frac{m}{2}} (\eta_1 - \eta_3) \quad \zeta_3 = \sqrt{\frac{m}{6}} (\eta_1 - 2\eta_2 + \eta_3)$$

$$\Longrightarrow L = \frac{1}{2} \left(\dot{\zeta}_1^2 + \dot{\zeta}_2^2 + \dot{\zeta}_3^2 \right) - \frac{k}{2m} (\zeta_2^2 + 3\zeta_3^2)$$

ζ_1 is cyclic as we expect

Linear Triatomic Molecule



v_1 Symmetric C-O Stretch

1340 cm^{-1}

v_2 Bend

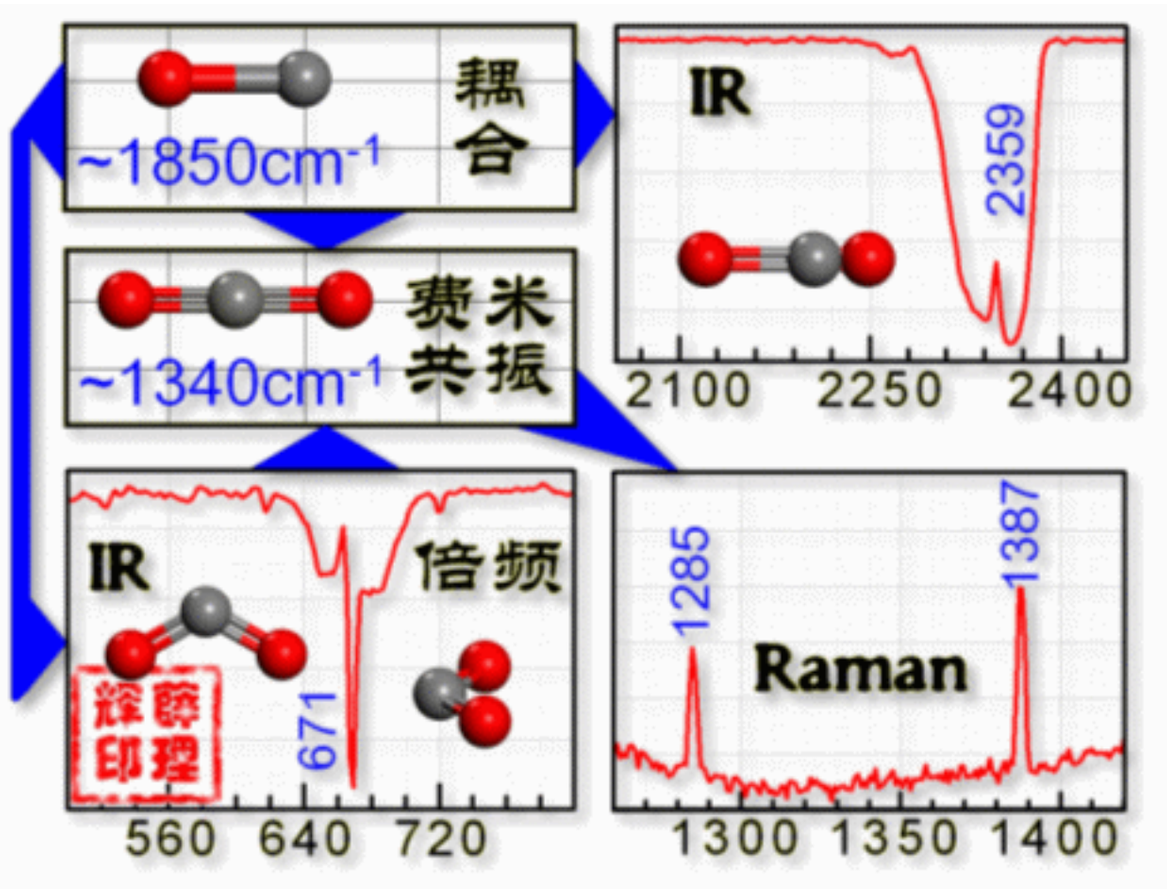
671 cm^{-1}

v_3 Asymmetric C-O stretch

2359 cm^{-1}

Fig. 1 Vibrational modes of CO_2

$$\left.\frac{v_3}{v_1}\right|_{\text{exp.}} \simeq \frac{2359}{1340} = 1.76$$



$$\left.\frac{v_3}{v_1}\right|_{\text{theo.}} = \sqrt{1 + 2\frac{m_O}{M_C}} = 1.91$$

Degenerate Solutions

We assumed $\lambda_j \neq \lambda_k$ for $j \neq k$

What if the eigenvalue equation has multiple roots?

Can we still achieve $\tilde{\mathbf{A}}\mathbf{T}\mathbf{A} = \mathbf{1}$?

Quick answer: Don't worry

Multiple root corresponds to multiple eigenvectors

$|\mathbf{V} - \lambda\mathbf{T}| = (\lambda - \kappa)^m f(\lambda) = 0 \leftarrow \lambda = k$ is an m-fold root

$\Longrightarrow (\mathbf{V} - \kappa\mathbf{T})\mathbf{a}_j = 0 \quad (j = 1,\ldots,m) \leftarrow m$ eigenvectors

Any linear combination $c_j\mathbf{a}_j$ is also an eigenvector

It is always possible to find a set of m orthogonal vectors

Gram–Schmidt process

Summary

Studied oscillation

Discussed general features of multi-dimensional oscillators

Equation of motion → Eigenvalue problem $\mathbf{Va} = \lambda\mathbf{Ta}$

Showed that oscillating solutions exist $\eta_i = Ca_i e^{-i\omega t}$

Eigenvalues ω^2 are positive semi-definite

Provide that V is minimum at the equilibrium

Principal axis transformation diagonalizes **T** and **V**

Normal coordinates behave as independent oscillators