Chapter 6 Theory, part 3

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Normalization

- From where we last were, we had the matrix form of the eigenvalue equation:
  - $\bar{\bar{\mathbf{V}}}\bar{\bar{\mathbf{A}}} = \bar{\bar{\boldsymbol{\lambda}}}\bar{\bar{\mathbf{T}}}\bar{\bar{\mathbf{A}}}$

- We want to normalize the eigenvectors such that:
  - $\bar{\bar{\mathbf{A}}}^{\mathsf{T}}\,\bar{\bar{\mathbf{T}}}\,\bar{\bar{\mathbf{A}}} = \bar{\bar{\mathbf{I}}}$ (eqn 6.23) and
  - $\bar{\bar{\mathbf{A}}}^{\mathsf{T}}\,\bar{\bar{\mathbf{V}}}\,\bar{\bar{\mathbf{A}}} = \bar{\bar{\boldsymbol{\lambda}}}$ (eqn 6.26)

- Taking a matrix $\bar{\bar{V}}$ to $\bar{\bar{\lambda}}$ in the form of the transformation $\bar{\bar{\lambda}} = \bar{\bar{A}}^T\bar{\bar{V}}\,\bar{\bar{A}}$ is called a congruence transformation so that it becomes a diagonal matrix with eigenvalues λ_i

The λ matrix

- For the iith element of the **λ** matrix, the equation is:
  - $\lambda_{ii} = \sum_{k,l} (a^t)_{ik} V_{kl} a_{li}$
- But we also know that:
  - $\lambda_{ij} = \lambda_{ii} \delta_{ij}$
  - $V^*_{kl} = V_{kl} = V_{lk}$
- Therefore we can write λ_{ii} as
  - $\lambda_{ii} = \sum_{k,l} v_{kl} (a^*_{kl} a_{li}) = \sum_k v_{kk} |a_{ki}|^2 + \sum_k \sum_{l \neq k} v_{kl} (a_{ki} a_{li})$

The λ_{ii} element

- Consider

$$S = \sum_{k \neq l} a^{*}{}_{ki}\, a_{li}\, v_{kl} = \sum_{k \neq l} \frac{v_{kl}}{2} (a_{lk}{}^{*} a_{li} + aki\, a_{li}{}^{*})$$

$$= \sum_{k \neq l} \frac{v_{kl}}{2} (|a_{ki} + a_{li}|^2 - |a_{ki}|^2 - |a_{li}|^2)$$

- Looking at the second form of the equation of S one can easily see that the equation will always be positive. Therefore $S \geq 0$ which also causes $\lambda_{ii} \geq 0$

Recap of the problem

- Basically we want to be able to solve the equation
  - $\bar{\bar{T}}\ddot{\bar{q}} = -\bar{\bar{V}}\bar{q}$
  - If we let $\bar{q} = \bar{\bar{A}}\bar{Q}$ then the equation becomes
    $$\bar{\bar{T}}\bar{\bar{A}}\ddot{\bar{Q}} = -\bar{\bar{V}}\bar{\bar{A}}\bar{Q}$$
  - Which then can become:
    $\bar{\bar{A}}^{\mathrm{T}}\bar{\bar{T}}\bar{\bar{A}}\ddot{\bar{Q}} = -\bar{\bar{A}}^{\mathrm{T}}\bar{\bar{V}}\bar{\bar{A}}\bar{Q}$
  - And if you substitute in eqns 6.23 and 6.26, you get:
    $\bar{\bar{I}}\,\ddot{\bar{Q}} = \bar{\bar{\lambda}}\,\bar{Q}$

Form of $\ddot{Q}_i$

- Usually we write $\bar{\bar{I}}\,\ddot{\bar{Q}} = -\bar{\bar{\lambda}}\,\bar{Q}$ as $\bar{\bar{I}}\,\ddot{\bar{Q}} = -\bar{\bar{\omega}}^2\bar{Q}$ for oscillators

  – since we showed that $\lambda_{ii} \geq 0$, lets write $\lambda_{ii} = \omega_i^2$

- Making our equation look like $\ddot{Q}_i = -\omega_i^2\, Qi$

Solutions to the equation

- The generic solution to this equation is the form of either $Q_i(t) = A_i \sin \omega_i t + B_i \cos \omega_i t$, or

  $Q_i(t) = A_i e^{-i\omega_i t} + B_i\, e^{i\omega_i t}$, where A and B are the constants of integration

- One of the particular solutions is a form of $Q_i = C_i \cos(w_i t + \ \phi_i)$, where both C_i and ϕ_I are the constants of integration

Solution part 2

- Let $\bar{Q}(t) = \bar{E}(t)$, where $E_i \equiv C_i \cos(\omega_i t + \phi_i)$

- This becomes $\bar{\bar{A}}\bar{Q}(t) = \bar{\bar{A}}\bar{E}(t)$, and earlier substituted $\bar{q} = \bar{\bar{A}}\bar{Q}$, therefore $\bar{q} = \bar{\bar{A}}\bar{E}$

- So we now have a solution to the Lagrangian that we started out with since we now know our q's

Lagrangian

- Our Lagrangian now becomes once again

- $L = \frac{1}{2}(\dot{\bar{q}}^{\mathsf{T}}\ \bar{\bar{T}}\ \dot{\bar{q}}\ -\ \bar{q}^{T}\ \bar{\bar{V}}\ \bar{q})$

Assumptions we made to get this

- All $\lambda_i \equiv \lambda_{ii}$ were different
- We used $\bar{\bar{T}}\bar{\bar{A}} = -\bar{\bar{V}}\bar{\bar{A}}\,\bar{\bar{\lambda}}^{-1}$ to get $\det\left|\bar{\bar{V}} - \bar{\bar{\lambda}}\,\bar{\bar{T}}\right| = 0$
  - The determinant gave us n distinct λi's which we used to determine n-1 of the n and (a_{i1},… a_{in}) numbers
  - We then proved that those λi's were real and also chose to make all of the aij elements real such that $\bar{\bar{A}}^* = \bar{\bar{A}}$

The Degenerate Case

- If not all of the λ_i's are not distinct solutions to the eigenvalue problem then we get the degenerate case where for example $\lambda_1=\lambda_2$.

- Like in quantum mechanics we still need to have a complete orthogonal basis set so have to form an $\bar{a}_1$, $\bar{a}_2$ out of the same λ equation, beyond that follow the same logic as before

Normal Coordinates

- The $\bar{Q}_i$'s are also called the normal coordinates since each behave like SHOs, and are decoupled from all the other $\bar{Q}_i$'s.

The Basic Algorithm

- Step 1: Choose an origin and a generalized coordinate system (follow steps 1-8 on our guide to solving Lagrangian Problems)
- Step 2: Find out what T and V are in the problem (step 9 in our guide to solving)

Basic Algorithm Part 2

- Step 3: Write out the Lagrangian, L, in matrix form: $L = \frac{1}{2}(\dot{\bar{q}}^T \bar{\bar{T}} \dot{\bar{q}} - \ \bar{q}^T \bar{\bar{V}} \bar{q})$. **Make sure not to forget the ½ in L!**

- Step 4: Write and Identify what $\bar{\bar{T}}$ and $\bar{\bar{V}}$ are

- Step 5: Solve det$\left|\bar{\bar{V}} - \omega^2 \bar{\bar{T}}\right| = 0$, for all ω^2's

Basic Algorithm Part 3

- Step 6: If the ω^2's are degenerate then use the orthonormality relations of the $\bar{a}$ vectors to from a complete set of vectors.
- Step 7: Write the solution to the problem for a future time, step 12 in our guide to solving Lagrangian problems

Basic Algorithm Part 4

- Step 8: Let $\bar{q} = \bar{\bar{A}}\bar{Q}$ be the general solution and that $\bar{Q}(t) = \bar{E}(t)$, has been solved.

- Step 9: Use initial conditions to solve for constants in $\bar{E}(t)$ (step 13 in the problem solving guide)

- Step 10: Make sure your answer makes sense.(step 14-18 in the problem solving guide)

Highlights of section 6.3: Fundamental Harmonics

- If the system is displaced barely from equilibrium and then is released to move, this system does small oscillations around the equilibrium position with frequencies $\omega_{1},\ldots,\omega_{n}$.

- These frequencies are called the free vibrations, resonant frequencies, or the fundamental harmonics of the system

Highlights of sect 6.3 continued

- These frequencies will not appear in the complete solution of the motion since they are by definition small oscillations around the equilibrium

- The solutions to the fundamental harmonics are usually a summation of simple harmonic oscillations over all ω's. One can transfer these coordinates to a new set of generalized coordinates called the normal coordinates

Highlights of section 6.3: Normal Coordinates

- Let $\bar{\bar{\eta}} = \bar{\bar{A}}\,\bar{\bar{\xi}}$ (eqn 6.41\`)
- $V = \frac{1}{2}\bar{\bar{\xi}}^T\bar{\bar{V}}\,\bar{\bar{\xi}},\ T = \frac{1}{2}\dot{\bar{\bar{\xi}}}^T\dot{\bar{\bar{\xi}}}$ (eqns 6.42 and 6.44 respectively
- $L = \frac{1}{2}(\dot{\xi}_k\dot{\xi}_k - \omega^2{}_k\xi^2)$ eqn 6.45.

Equation of motion with normal coordinates

- The Lagrange eqns of motion become with this Lagrangian:
  - $\ddot{\xi}_k + \omega^2{}_k \xi_k$ eqn 6.46
- Solutions to these equations we know the solution to, which happen to once again be of the form:
  - $\xi_k = Cke^{-i\omega_k t}$ eqn 6.47

Highlights of section 6.4

- This sections goes over an example of resonant frequencies and normal modes with the linear triatomic molecule

ω_1 frequency and equation

- For $\omega_1 = 0$, $a_{11}=a_{21}=a_{31}$
  - $a_{11}=1/\sqrt{2m+M}$

- This is the case for when the equation of motion is a linear function
  - $\ddot{q} = 0$

ω_2 frequency and equation

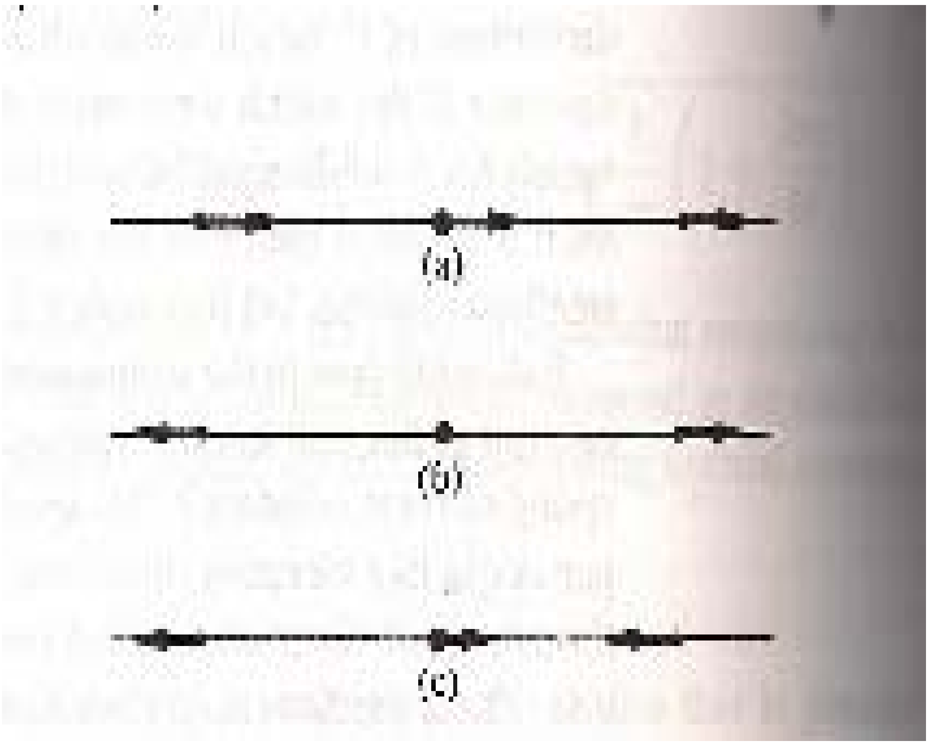
- For $\omega_2 = \sqrt{k/m}$ $a_{22}=0$, $a_{13}=-a_{32}$
  - $a_{12} = 1/\sqrt{2m}$, $a_{22}=0$, $a_{32} = -1/\sqrt{2m}$

ω_3 frequency and equation

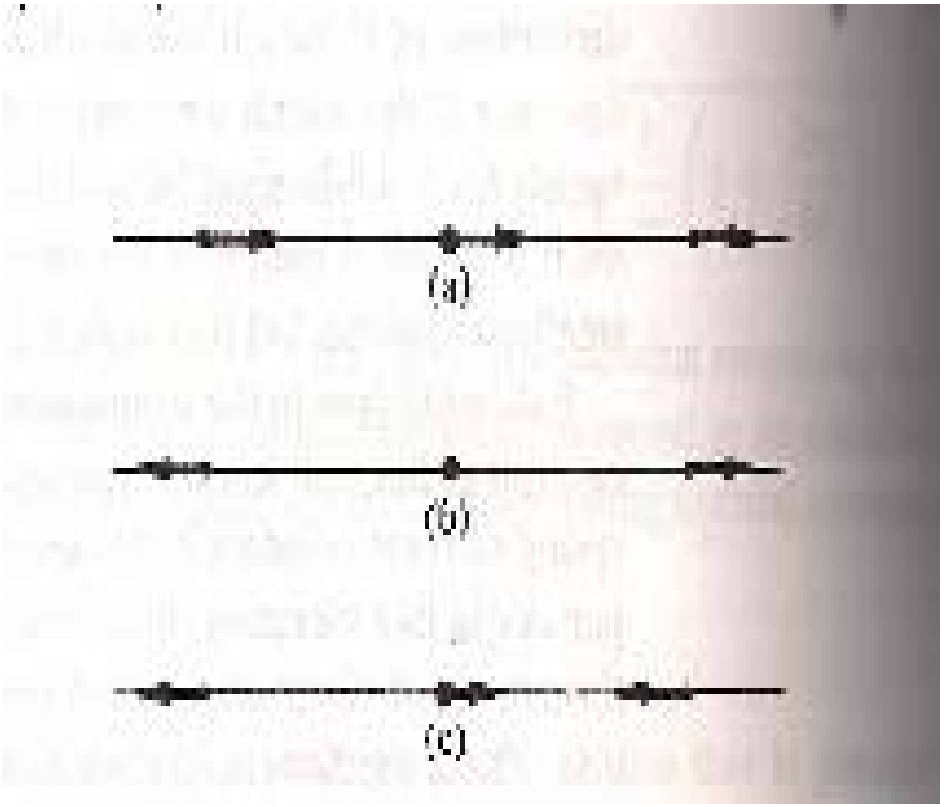
- For $\omega_3=\sqrt{\frac{k(1+\frac{2m}{M})}{m}}$, $a_{11}=a_{13}$

$-\ a_{23}= -2/\sqrt{2M(2+M/m}$, $a_{33}=1/\sqrt{2m(1+2m/M}$

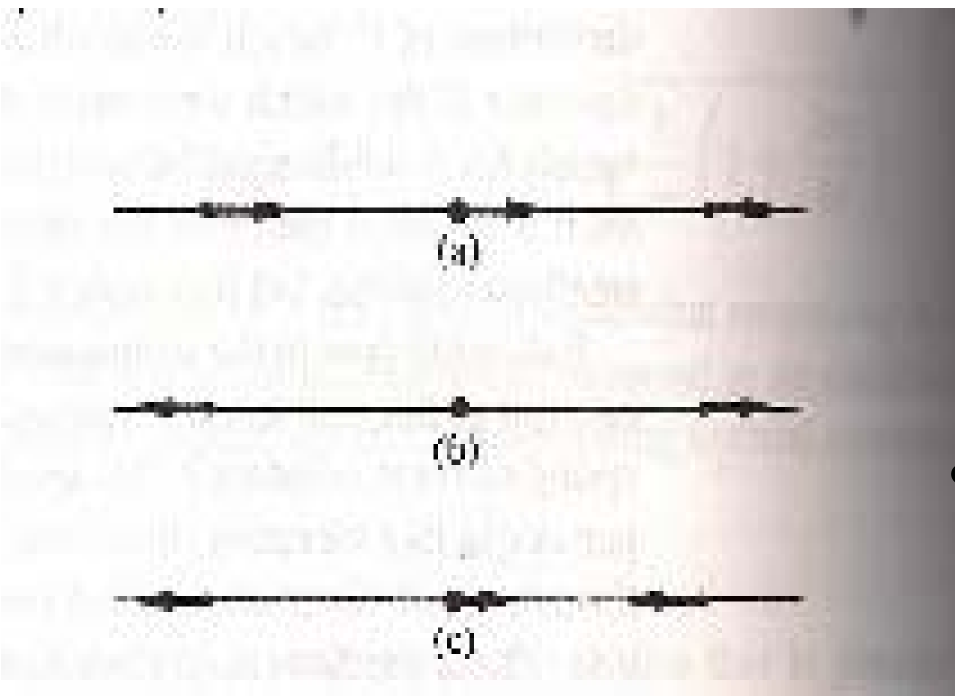
- In both cases of ω_2 and ω_3 if $\omega^2< 0$, then the solution becomes an exponential equation with a saddle point for the minimum of V



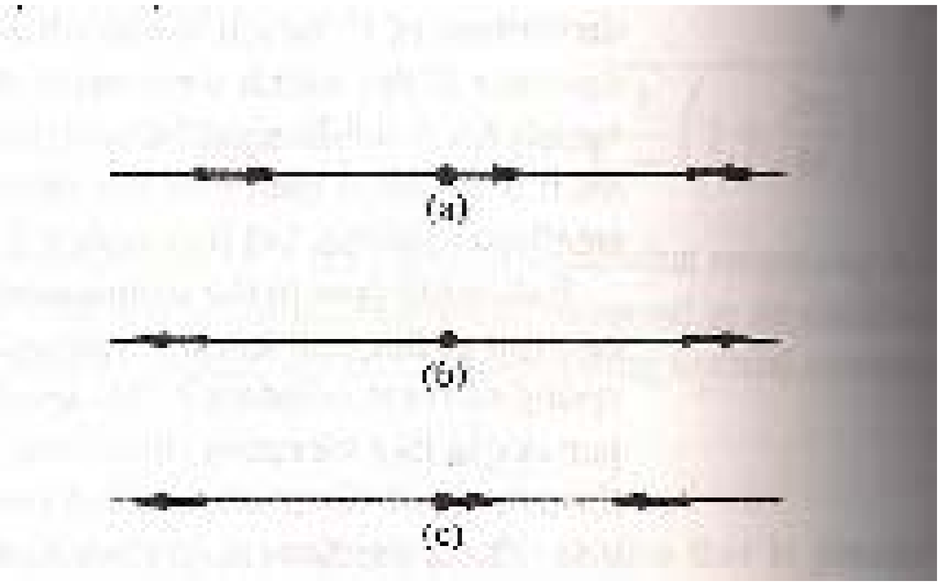
- Picture on the right is fig 6.4 from Goldstein
- This shows the normal modes of the linear symmetric triatomic molecule



- (a) shows the normal modes for ω_1, where the nodes are all equally spaced between and all point in same direction
- These are symmetric nodes



- (b) shows the normal modes for ω_2 where there are only two real nodes that do anything and point in opposite directions
- These are antisymmetric nodes



- (c) shows the normal modes for ω_3 where the modes are not evenly spaced and do not all point in the same direction