PHONONS → DIAGONALIZATION ①

I) QUANT. MECH. & STAT MECH COUPLED N-ptcl SYSTEMS

OF COUPLED SYSTEM HAMILTONIAN

A) Refs. Reif: ch. 10 *

Hill: ch. 5 Einstein model

⇓

High freq liquids

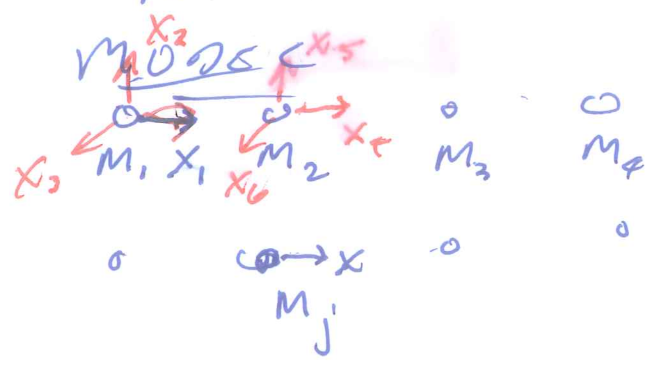
$\tau < 10^{-14}$ s

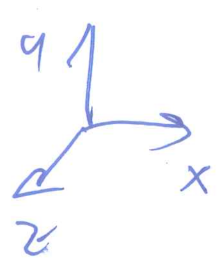
WILEY & BARRETT
ADV. ENGINEERING MATH
pg. 734

B) PHONON

- PHYSICS
- MATH
- REVIEW

C) MODEL





(4) cubic array of atoms in solid

D) Focus on QO to crazy

CONSERVATIVE DYNAMICS:

2^{x}

$$H_{sys} = \frac{1}{2}\sum m_i \dot{x}_i \dot{x}_i + V(x_1, x_2, x_3, \ldots, x_{3N-2}, x_{3N-1}, x_{3N})$$

E) Brief: Assume small oscillations

a) $V(x_1 \ldots x_{3N}) = V(x_{10}, x_{20}, x_{30} \ldots x_{3N0})$

V_0

x_{j0} = equil mag of x_j

$\frac{\partial V}{\partial x_j}$ = Force in x_j on ~~what~~ ptcl, ass'd all x_j

$$+ \sum_{j=1}^{3N} \frac{\partial V}{\partial x_j}\Bigg|_{x_{j0}\ \forall j} x_j$$

$\to 0$

$$+ \frac{1}{2}\sum_{i,j=1}^{3N} \left(\frac{\partial^2 V}{\partial x_i \partial x_j}\right)\Bigg|_{x_{i0}, x_{j0}} x_i x_j + O(x_j^3)$$

rel error

$$O\left(\frac{x_j^3}{x_j^2}\right) \sim O(x_j)$$

③

b) ∴ $$\boxed{V(\cdots) = V_0 + \frac{1}{2}\sum_{i,j} V_{ij}\, x_i x_j}$$

$$V_{ij} \equiv \left.\frac{\partial^2 V}{\partial x_i \partial x_j}\right|_{equil}$$

c) b) in matrix form ;

(3.1) $$\boxed{V(\cdots) = V_0 + \frac{1}{2}\underline{x}^T \underline{\underline{V}}\, \underline{x}}$$ ✱✱

d) ∴ $$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{3N} \end{bmatrix} \qquad \underline{x}^T = [x_1\, x_2 \cdots x_{3N}]$$

Note: $\underline{\underline{V}}$ is symmetric

why ? is $V_{ij} = V_{ji}$? calc

④

e) $KE_{sys} = \frac{1}{2} \sum_i m_i \dot{x}_i \dot{x}_i$

f) $KE_{sys} = \underbrace{\begin{bmatrix} \dot{x}_1 & \dot{x}_2 & \dot{x}_3 & \cdots & \dot{x}_{3N} \end{bmatrix}}_{\underline{\dot{x}}^T} \underbrace{\begin{bmatrix} M_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & M_1 & 0 & 0 & \cdots & \\ 0 & 0 & M_1 & 0 & \cdots & \\ \vdots & & & M_2 & & \\ \vdots & & & & M_2 & \\ \vdots & & & & & M_2 \\ & & & & & \ddots \\ \cdots & & & & & M_N \end{bmatrix}}_{\underline{M}\ (3N \times 3N)} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \vdots \\ \dot{x}_{3N} \end{bmatrix}$

$\frac{1}{2} [\dot{x}_1 \quad \cdots \quad \dot{x}_{3N}] \begin{bmatrix} M_1 \dot{x}_1 \\ M_1 \dot{x}_2 \\ M_1 \dot{x}_3 \\ M_2 \dot{x}_4 \\ \vdots \\ M_N \dot{x}_{3N} \end{bmatrix}$

g) $\therefore \boxed{KE_{sys} = \frac{1}{2} \underline{\dot{x}}^T \underline{M} \, \underline{\dot{x}}}$ (4,1)

⊕ $\underline{M}$ IS ALSO SYMMETRIC

$\frac{1}{2} [M_1 \dot{x}_1^2 + M_1 \dot{x}_2 + M_1 \dot{x}_3^2 + \cdots + M_N \dot{x}_{3N}^2]$

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∴ II) ∴ A)

$$\boxed{H_{sys} = \frac{1}{2}\dot{\underline{x}}^T \underline{\underline{M}}\,\dot{\underline{x}} + V_0 + \frac{1}{2}\underline{x}^T \underline{\underline{V}}\,\underline{x}} \quad (5.1)$$

B) FROM MILITARY MATH BOOK:

TMM

a) Let $\underline{\underline{M}}$ and $\underline{\underline{V}}$ BE 3N X 3N - SYMM. MATRICES

b) $\underline{\underline{V}}$ positive def

c) THEN FOR FOLLOWING EIGEN ~~VB~~ PROBLEM

eigenvalue, eigenvector

$$(5.1)\quad \boxed{[\underline{\underline{V}} - \lambda \underline{\underline{M}}]\,\underline{a} = \underline{0}}$$

i) Let $\underline{\underline{A}} \equiv [\underline{a}$

~~Va~~ d) (5.1) ⇒ characteristic eqn in λ:

$$\text{Det}\left|\underline{\underline{V}} - \lambda \underline{\underline{M}}\right| = 0$$

$$\Downarrow$$

has 3N real roots

$$\boxed{\lambda_1, \lambda_2, \lambda_3 \ldots \lambda_{3N}}$$

e) to get the j^{th} eigenvector $\underline{a}_j$:

$$\left[\underline{\underline{V}} - \lambda_j \underline{\underline{M}}\right] \underline{a}_j = \underline{0}$$

$$\downarrow$$

$$\boxed{\underline{a}_j} = \cancel{3N}\ 3N \times 1$$

Let

$$\boxed{\underline{\underline{A}} = \underbrace{\left[\underline{a}_1\ \underline{a}_2\ \underline{a}_3 \ldots \underline{a}_{3N}\right]}_{(3N \times 3N)}}$$

THM Result:

$$\underline{\underline{A}}^T \underline{\underline{V}}\,\underline{\underline{A}} = \underline{\underline{D}}$$

$$\underline{\underline{A}}^T \underline{\underline{M}}\,\underline{\underline{A}} = \underline{\underline{I}}$$

$$\underline{\underline{D}} = \begin{array}{r c} & \scriptstyle 3N \\ & \Downarrow \\ \scriptstyle 3N \rightarrow & \begin{bmatrix} \lambda_1 & 0 & & & \cdots & 0 \\ 0 & \lambda_2 & & & & \\ 0 & 0 & \lambda_3 & 0 & 0 & \\ \vdots & & & \ddots & & \\ 0 & \cdots & & & & \lambda_{3N} \end{bmatrix} \end{array}$$

$$\underline{\underline{I}} = \begin{bmatrix} 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ 0 & 0 & 1 & & & \\ & & & \ddots & & \\ & & & & \ddots & \\ & & & & & \ddots \end{bmatrix}$$

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III) Now,

A) Let $\boxed{\underline{x} = \underline{\underline{A}}\,\underline{x}'}$ (8.1)

uncoupled coords

$\Rightarrow \boxed{\underline{\dot{x}} = \underline{\underline{A}}\,\underline{\dot{x}}'}$ (8.2)

$$\Rightarrow \boxed{\begin{aligned} \underline{x}^T &= (\underline{\underline{A}}\,\underline{x}')^T \\ &= (\underline{x}')^T \underline{\underline{A}}^T \\ \underline{\dot{x}}^T &= (\underline{\underline{A}}\,\underline{\dot{x}}')^T \\ &= \underline{\dot{x}}'^T \underline{\underline{A}}^T \end{aligned}} \quad (8.3)$$

B) $H_{sys} = \frac{1}{2}\underline{\dot{x}}^T \underline{\underline{M}}\,\underline{\dot{x}} + \frac{1}{2}\underline{x}^T \underline{\underline{V}}\,\underline{x} + U_0$

$$H_{sys} = \frac{1}{2}\underline{\dot{x}}'^T \underbrace{\underline{\underline{A}}^T \underline{\underline{M}}\,\underline{\underline{A}}}_{\underline{\underline{I}}}\,\underline{\dot{x}}' + \frac{1}{2}\underline{x}'^T \underbrace{\underline{\underline{A}}^T \underline{\underline{V}}\,\underline{\underline{A}}}_{\underline{\underline{D}}}\,\underline{x}' + V_0$$

phonons

solid state phys

Great illustra of phrases

Prev NR 505 rule 4/10/23

1) $V_{sys} = V(x_1, x_2, x_3 \;\cdots\; x_{3N-2}, x_{3N-1}, x_{3N})$

2)

3 main steps

1) Figure out H_{sys} $\Rightarrow$ place in ~~form~~

2) Use NM $\Rightarrow$ H_{sys} in decoupling form form $\Rightarrow$ $\boxed{3N \text{ harmonic oscillators}}$

3) Diagnose : $\dfrac{\ell_{ptel}}{\lambda_{DB}}$

4) write down S.E. for single oscillator $\frac{p^2}{2m} + K\tilde{x}$

$$\boxed{\frac{p^2}{2m_i}\nabla_i^2 \psi_i - \omega^2 m \tilde{x}^2 \psi = E\psi}$$

$$\Downarrow$$

$$\boxed{E_\alpha^{(n)} = \left(n + \tfrac{1}{2}\right)\hbar\omega}$$

8

1) $H = V(\quad) + \frac{1}{2}\sum m_i \dot{x}_i^2$

2) $V(\quad) = V_0 + \frac{1}{2}\sum_{ij} V_{x_i x_j} x_i x_j$

$V_{ij} = V_{ji}$

3) $\cancel{KE = \frac{1}{2}[\dot{\underset{\sim}{x}}_1, \dot{\underset{\sim}{x}}_2, \dot{\underset{\sim}{x}}_3 \ldots \dot{x}_{3n}]}$ $\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & & \end{bmatrix}$

$\cancel{\underset{\sim}{X}_j = \sqrt{M_j}\, x_j}$

$\cancel{x_j = \frac{1}{\sqrt{M_j}} \underset{\sim}{x}_j}$

$\cancel{V_e}$

4) $\cancel{H = [\dot{\underset{\sim}{X}}^T][\underline{\underline{I}}][\dot{\underset{\sim}{X}}] + \frac{1}{2}}$

$= \frac{1}{2}\dot{\underline{X}}^T \underline{\underline{M}}\, \dot{\underline{X}} + V_0 + \frac{1}{2}\underline{X}^T \underline{\underline{V}}\, \underline{X}$

5) Then: $[\underline{\underline{M}} - \lambda \underline{\underline{V}}]\underline{a} = \underline{0}$ $\quad \underline{\underline{M}}, \underline{\underline{V}}$ symmetric and $\underline{\underline{V}}$ pos def

a) $\mathrm{Det}|\underline{\underline{M}} - \lambda\underline{\underline{V}}| = 0 \Rightarrow \lambda_1, \lambda_2, \lambda, \ldots \lambda_{3n}$

c) solve $[\quad]\underline{a} = \underline{0} \rightarrow \underline{a}_1, \underline{a}_2, a_3 \ldots$

d) $\underline{\underline{A}} = \left[\underline{a}_1 \ \underline{a}_2 \ \underline{a}_3 \ \cdots \ \underline{a}_{3N} \right]$

e) From

$$\boxed{\begin{aligned} \underline{\underline{A}}^T \underline{\underline{M}}\, \underline{\underline{A}} &= \underline{\underline{D}} \\ \underline{\underline{A}}^T \underline{\underline{M}}\, \underline{\underline{A}} &= \underline{\underline{I}} \end{aligned}}$$

$$\underline{\underline{D}} = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_{3N} \end{bmatrix}$$

6) Let $\cancel{\underline{X}' = \underline{\underline{A}}\, \underline{X}}$ $\quad \boxed{\underline{X} = \underline{\underline{A}}\, \underline{X}'}$

$\Rightarrow$ $\cancel{\underline{\dot{X}}' = \underline{\underline{A}}\, \underline{\dot{X}}}$ $\quad \underline{\dot{X}} = \underline{\underline{A}}\, \underline{\dot{X}}'$

7) $\therefore$ 4) $\Rightarrow \frac{1}{2} \underline{\dot{X}}^T \underline{\underline{M}}\, \underline{\dot{X}} + V_0 + \frac{1}{2} \underline{X}^T \underline{\underline{V}}\, \underline{X} = H_{sys}$

$\Rightarrow \frac{1}{2} (\underline{\underline{A}}\, \underline{\dot{X}}')^T \underline{\underline{M}}\, \underline{\underline{A}}\, \underline{\dot{X}}' + V_0 + \frac{1}{2} (\underline{\underline{A}}\, \underline{X}')^T \underline{\underline{V}}\, \underline{\underline{A}}\, \underline{X}' = H_s$

$\Rightarrow \frac{1}{2} (\underline{\dot{X}}')^T \underline{\underline{A}}^T \underline{\underline{M}}\, \underline{\underline{A}}\, \underline{\dot{X}}' + V_0 + \frac{1}{2} (\underline{X}')^T \underline{\underline{A}}^T \underline{\underline{V}}\, \underline{\underline{A}}\, \underline{X}' = H$

8) $H_{sys} = \frac{1}{2}(\dot{\underline{X}}')^T \underline{\underline{D}} \, \dot{\underline{X}}' + \frac{1}{2} \underline{X}'^T \underline{\underline{I}} \, \underline{X}' + V_0$

9) GO BACK ~~LAN~~ AND

SOLVE

$$\boxed{[\underline{\underline{V}} - \lambda \underline{\underline{M}}] \, \underline{a} = \underline{0}}$$

$\Rightarrow H_{sys} = \frac{1}{2} \dot{\underline{X}}'^T \cdot \dot{\underline{X}}' +$

$\Rightarrow [X_1' \; X_2' \ldots]^T \begin{bmatrix} \lambda_1 X_1' \\ \lambda_2 X_2' \end{bmatrix}$ $\qquad \frac{1}{2}(\underline{X}'^T) [\lambda_1 \underline{D} \, \underline{X}' + V_0$ λ_2

$$\boxed{H_{sys} = \frac{1}{2} \sum_{j=1}^{3N} \dot{x}_j' \dot{x}_j' + \cancel{\frac{1}{2} X_i \delta_{ij} \lambda_i X_j} \; \frac{1}{2} \sum_{j=1}^{3N} \lambda_j X_j'^2 + V_0}$$

$V_0 \to 3N\left(\frac{V_0}{3N}\right)$

$H_{sys} = H_{phonon_1} + H_{P_2} + H_{P_3} + \ldots H_{P_{3N}}$

(46) $$\boxed{H_{P_k} = \frac{1}{2} \dot{X}_k'^2 + \frac{\lambda_k X_k'^2}{2} + V_0'}$$

4a

to get ~~xx~~ into standard form

go back and

define $\tilde{x}_j = \sqrt{m}\, x'_j \Rightarrow \cancel{x'_j}$

$\Rightarrow x \qquad \Rightarrow \cancel{x'_j\, A}$

$\therefore \quad \dot{x}'_k \cdot \dot{x}'_k = m$

$\underline{x} = \underline{\underline{A}}\, \underline{x}'$

$\Updownarrow$

$\sqrt{m}\, \dfrac{\underline{x}_{\text{new}}}{\sqrt{m}} \Rightarrow \underline{x} = {}^{\sqrt{m}}\underline{\underline{A}} \cdot \underline{x}'$

$\therefore$

$\dot{\underline{x}}'^{T}\, \underline{\underline{A}}^{T}\, \underline{\underline{M}}\, \cancel{\underline{\underline{A}}}'\, \dot{\underline{x}}'$

$\underline{\underline{M}}$

d. magnose

$l_{pkcl} \sim 5\,\mathring{A}$

scale s.t. $\cancel{X_{SG}}$ a) $K\sigma_K \sim V_K \sim \cancel{E_K} \uparrow k_BT$

b) $\cancel{m v^2}$

$$\frac{p_K^2}{2m_K}\psi_K + V_K\psi = E_K\psi_K$$

$$\rightarrow \frac{-\hbar^2}{2m_K}\nabla^2 \cancel{\psi_K} \sim k_BT \cancel{\psi_K}$$

$$\frac{1}{X_{SG}^2}$$

$$\rightarrow \boxed{X_{SG} \sim \frac{\hbar}{\sqrt{2m_K k_BT}}}$$

$$X_{SG} \sim 10^{-34}\,\mathrm{J\,s}$$

$$m_K = \frac{63\,\mathrm{kg}}{10^{26}\,\mathrm{kg\,mol}} = 6(10^{-25})\,\mathrm{kg}$$

$$X_{SG} \sim \frac{10^{-34}\,\mathrm{J\,s}}{\sqrt{(12)(10^{-25})\,\mathrm{kg}\,(1.34)\frac{\mathrm{J}}{\mathrm{K}}\,300\,\mathrm{K}\,10^{-23}}} \quad \mathrm{kg\,m^2/s^2}$$

$$\sqrt{(50)\,10^{-46}}$$

$$\sim \frac{10^{-34}}{(7)\,10^{-23}} \sim 1.4(10^{-11})\,\mathrm{m}$$

$$\sim 0.15\,\mathring{A}$$