Lecture September 17

Project 2

$$\left.\begin{array}{l} \dfrac{d^2 u(x)}{dx^2} = \lambda u(x) \\ u(0) = u(1) = 0 \\ x \in [0,1] \end{array}\right\} \to$$

$$T u = \lambda u$$

$$T = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & -1 & \ddots & \ddots & \\ 0 & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Jacobi's method

$$\boxed{S\, T \cdot S^T = D} = [\lambda_1\ \lambda_2\ \ldots\ \lambda_n]$$

$$S = \begin{bmatrix} 1 & & & 0 & \\ & 1 & & & \\ 0 & & \cos\theta & \sin\theta \ldots & \\ & & -\sin\theta & \cos\theta \ldots & 1 \end{bmatrix}$$

$$SS^T = S^T S = \mathbb{1}$$

$$S \cdot \left[\left(T \cdot \right) u = \lambda \cdot u \right]$$

$$S^T S$$

$$S T S^T \underbrace{S u} = \lambda \underbrace{S u}$$

eigenvector.

$$S_m S_{m-1} \ldots S_1 T S_1^T \ldots S_{m-1} S_m$$

$$= D$$

Final eigenvector:

$$v = \boxed{S_m S_{m-1} \ldots S_1} u$$

$u = ?$

complete orthogonal basis

u, defined for $i = 1, \ldots n$

$T \in \mathbb{R}^{n \times n}$ $\quad u_i \in \mathbb{R}^n$

Project 2a:

$$u_i^T u_j = \delta_{ij}$$

$$v_i^T v_j = u_i^T \underbrace{S^T S}_{1} u_j = \delta_{ij}$$

final basis also orthogonal.

<u>Unit test 1</u>: check that

$$v_i^T v_j = \delta_{ij} \text{ is satisfied.}$$

With a complete orthogonal basis u, we can express a new orthogonal basis v

$$v_j = \sum_{i=1}^{n} \boxed{s_{ji}} u_i$$

They are given by the Jacobi rotations

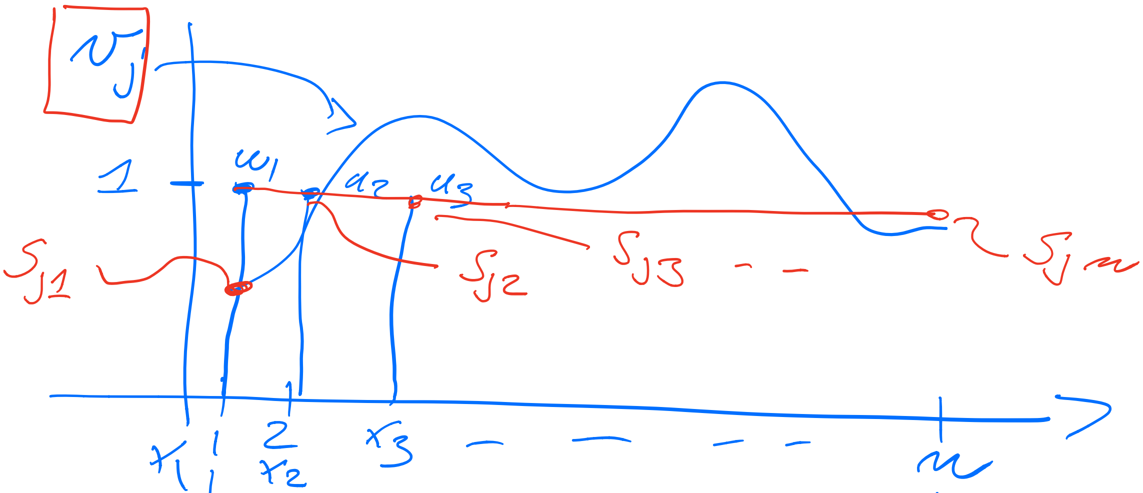
$$\boxed{S = S_m S_{m-1} \cdots S_1}$$

$$U = [u_1 \; u_2 \; \cdots \; u_n]$$

$$u_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad u_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \cdots$$

The final eigenvector v_j for eigenvalue λ_j will be a linear combination of all u_i, defined by the S_{ij}

We want the v_j to be a function we can plot



corresponds to a discrete coordinate x

With orthogonal transformations, eigenvalues are unchanged, but the eigenvectors change via $\boxed{Su}$

$$v_j = \begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix} u_i$$

Modifying of $\frac{d^2 u(x)}{dx^2} = -F\,u(x)$

to a different problem but with almost the same code.

Schrödinger's eq for one particle in 3-dim:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \boxed{V(\vec{r})}\right)\psi(\vec{r}) = E\psi(\vec{r})$$

$$\vec{r} = x\vec{e}_x + y\vec{e}_y + z\vec{e}_z$$

cartesian $\to$ spherical coordinates

3 decoupled differential eqs

one for $\phi \in [0, 2\pi]$

— " — $\theta \in [0, \pi]$

— " — $r \in [0, \infty)$

$x, y, z \in (-\infty, +\infty)$

$$\psi(\vec{r}) = \boxed{Y_{ml}(\theta, \varphi)}\, R(r)$$

We have

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} + \overset{l=0}{\frac{l(l+1)}{r^2}}\right)R(r)$$

$$+ V(r)R(r) = E R(r)$$

gives 2nd derivative +

1ST — l —

Problem $\quad \underline{R(0) = \text{const} = ?}$

$R(\infty) = 0$

Solve instead

$$u(r) = r R(r)$$

$$\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr}\left(\frac{u(r)}{r}\right)$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\boxed{\frac{d^2 u(r)}{dr^2}} + \boxed{V(r)}\, u(r)$$

$$= \boxed{E\, u(r)}$$

$R(0) = \text{const} \Rightarrow u(0) = 0$

$u(0) = 0 \quad \wedge \quad u(\infty) = 0$

original:

$$\gamma \boxed{\frac{d^2 u(x)}{dx^2}} = - F u(x)$$

$$V(r) = \frac{1}{2} m \omega^2 r^2$$

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + \frac{1}{2} m \omega^2 r^2 u(r)$$

$$= E\, u(r)$$

Scale the equations:

Dim-less variable $\rho = \boxed{\alpha} \cdot r$

dimension inverse length

$$-\frac{\hbar^2 \alpha^2}{2m} \frac{d^2 u}{d\rho^2} + \frac{1}{2} m \omega^2 \frac{\rho^2}{\alpha^2} u(\rho) = E\, u(\rho)$$

multiply with $\frac{2m}{\hbar^2 \alpha^2}$

$$-\frac{d^2 u}{d\rho^2} + \boxed{\frac{m^2 \omega^2}{\hbar^2 \alpha^4}} \rho^2 u = \lambda u$$

$$\lambda = \frac{E \cdot 2m}{\hbar^2 \alpha^2}$$

$$\frac{m^2 \omega^2}{\hbar^2 \alpha^4} = 1 \quad \Rightarrow$$

$$\alpha^2 = \sqrt{\frac{m^2 \omega^2}{\hbar^2}} \quad \Rightarrow$$

$$\alpha = \sqrt{\frac{m \cdot \omega}{\hbar}}$$

$$\sqrt{\frac{mc^2 \hbar\omega}{\hbar^2 c^2}}$$

(energy x length)^2

$$\sim \frac{1}{\text{length}}.$$

α = natural length scale.

$$-\frac{d^2u}{d\rho^2} + \rho^2 u = \lambda u$$

Discretized version

$$Tu = \lambda u$$

$$T = \begin{bmatrix} \frac{2}{h^2} + \rho_1^2 & -\frac{1}{h^2} & & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + \rho_2^2 & \ddots & -1/h^2 \\ & -\frac{1}{h^2} & \ddots & \\ 0 & & -\frac{1}{h^2} & \frac{2}{h^2} + \rho_n^2 \end{bmatrix}$$