In general we have

$$\begin{vmatrix} H_{11}-E & H_{12}-S_{12}E\cdots H_{1n}-S_{1n}E \\ H_{21}-S_{21}E & H_{22}-E \quad \cdots \quad H_{2n}-S_{2n}E \\ \vdots & \vdots \qquad\qquad \vdots \\ H_{n1}-S_{n1}E & H_{n2}-S_{n2}E\cdots H_{nn}-E \end{vmatrix} = 0$$

Example: particle in box problem

$$f_1 = x(\ell - x)$$
$$f_2 = x^2(\ell - x)^2$$
$$f_3 = x(\ell - x)\left(\frac{1}{2}\ell - x\right)$$

$$S_{13} = S_{31} = 0$$
$$S_{23} = S_{32} = 0$$
$$H_{13} = H_{31} = 0$$
$$H_{23} = H_{32} = 0$$

$$\begin{vmatrix} H_{11}-S_{11}E & H_{12}-S_{12}E & 0 \\ H_{21}-S_{21}E & H_{22}-S_{22}E & 0 \\ 0 & 0 & H_{33}-S_{33}E \end{vmatrix} = 0$$

Note: This is block diagonal by symmetry. S_{11}, S_{22}, S_{33} were included because the starting functions were not normalized.

The upper block is

$$\begin{vmatrix} \dfrac{\hbar^2 \ell^3}{6m} - \dfrac{\ell^5}{30} E & \dfrac{\hbar^2 \ell^5}{30m} - \dfrac{\ell^7}{140} E \\ \dfrac{\hbar^2 \ell^5}{30m} - \dfrac{\ell^7}{140} E & \dfrac{\hbar^2 \ell^7}{105m} - \dfrac{\ell^9}{630} E \end{vmatrix} = 0$$

$$E = 0.1250 \frac{h^2}{m\ell^2}, 1.293 \frac{h^2}{m\ell^2}$$

The exact values are $0.1250 \dfrac{h^2}{m\ell^2}, 1.125 \dfrac{h^2}{m\ell^2}$

System of linear equations

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

$$\mathbf{Ax} = \mathbf{b}$$

$$\mathbf{A}^{-1}\mathbf{Ax} = \mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$ If the inverse exists

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Energy eigenvalue problem

$\mathbf{Ac} = \boldsymbol{\lambda}\mathbf{c},$ Assuming basis is orthonormal.

$\det\left(A_{ij} - \lambda\delta_{ij}\right) = 0 \rightarrow$ characteristic eq.

Here **c** is an individual eigenvector

If $\mathbf{A}$ is diagonal, this determinant is diagonal

$$\det\left(\mathbf{A}\right) = \left(a_{11} - \lambda\right)\left(a_{22} - \lambda\right)\ldots\left(a_{nn} - \lambda\right)$$

Two vectors **b** and **c** are orthogonal if

$$\sum_{i=1}^{n} b_i * c_i = 0 \quad \Bigg| \quad \left(b_1 * b_2 * \cdots b_n *\right)\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = 0$$

$$\mathbf{H}\mathbf{c}^{(i)} = E_i \mathbf{c}^{(i)}, \quad i = 1, 2, \ldots n$$

$$\mathbf{HC} = \mathbf{CE}$$

$$\mathbf{E} = \begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n \end{pmatrix}$$

and $\mathbf{C} = \left(\mathbf{c}^{(1)} \quad \cdots \quad \mathbf{c}^{(n)}\right)$

If $\mathbf{C}$ has an inverse

$$\mathbf{C}^{-1}\mathbf{HC} = \mathbf{E}$$

The eigenvectors can be used to diagonalize $\mathbf{H}$

One can always normalize the eigenvectors

Transpose of $\mathbf{A}$ is $\mathbf{A}^{\mathrm{T}}$ interchanges rows and columns

Sometimes referred to as $\tilde{\mathbf{A}}$

For a symmetric matrix $\mathbf{m}, \quad \mathbf{m}^{\mathrm{T}} = \mathbf{m}$

Complex conjugate transpose of $\mathbf{A}$ is $(\mathbf{A}^*)^{\mathrm{T}} = \mathbf{A}^{\dagger}$

$$a_{ij}^{\dagger} = a_{ji}^{*}$$

Orthogonal matrix: $\mathbf{A}^{-1} = \mathbf{A}^{\mathrm{T}}$

Unitary matrix: $\mathbf{U}^{-1} = \mathbf{U}^{\dagger}$

$\mathbf{U}^{\dagger}\mathbf{U} = \mathbf{I}$ if $\mathbf{U}$ is in unitary

Columns of a unitary matrix are orthogonal to one another and normalized.

If the eigenvectors of a Hermitian matrix are chosen to be orthonormal, then the matrix $\mathbf{C}$ of these vectors is unitary.

$\mathbf{C}^{\dagger}\mathbf{H}\mathbf{C} = \mathbf{E}$, where $\mathbf{H}$ is Hermitian

if $\mathbf{H}$ is real, $\mathbf{C}$ is orthogonal and $\mathbf{C}^{\mathrm{T}}\mathbf{H}\mathbf{C} = \mathbf{E}$

Large eigenvalue problems are not solved the way we used in our examples

Generally, one starts with a guess of the eigenvector(s), and iteratively solves the problem