Eigenvalues, Eigenvectors, and the Discrete Variable Representation (DVR)

should have read CDTL pages 94-144

ψ in $\{\phi\}$ basis set

$$|\psi_{\mathrm{i}}\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}_{\psi} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \\ a_N \end{pmatrix}_{\phi}$$

$$a_j = {}_{\phi}\langle \phi_j | \psi_i \rangle_{\phi}$$

Last time:

a "*bra*" $\quad {}_{\phi}\langle \ \ | = \begin{pmatrix} a_1^* & \dots & a_N^* \end{pmatrix}_{\phi}$

a"*ket*" $\quad | \ \ \rangle_{\phi} = \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}_{\phi}$

$| \ \ \rangle\langle \ \ |$ an $N \times N$ matrix

$\langle \ \ | \ \ \rangle$ a $(\text{complex})\#$

$$\mathbb{1} = \begin{pmatrix} 1 & & & \\ & 1 & & 0 \\ & & 1 & \\ & 0 & & \ddots \end{pmatrix} = \sum_k |k\rangle\langle k|$$

The "unit" matrix

at end of lecture #10 we saw

$$\langle \phi_i | \mathbf{AB} | \phi_j \rangle = \sum_k \langle \phi_i | \mathbf{A} \underbrace{|\phi_k\rangle\langle \phi_k|}_{\mathbf{1}} \mathbf{B} | \phi_j \rangle$$

$$= \sum_k A_{ik} B_{kj} = (\mathbf{AB})_{ij}$$

updated 9/25/20 9:31 AM

What is the connection between the Schrödinger (wavefunction) and Heisenberg (matrix) representations?

$$\psi_i(x) = \langle x | \psi_i \rangle$$

$$|x_0\rangle = \delta(x, x_0)$$ eigenfunction of **x** with eigenvalue x_0

Using this formulation for $\psi_i(x)$, you can go freely (and rigorously) between the Schrödinger and Heisenberg representations.

Today: **eigenvalues** of a matrix – what are they? how do we get them? (secular equation). Why do we need them?

eigenvectors – how do we get them?

Arbitrary V(x) in Harmonic Oscillator Basis Set (Discrete Variable Representation)

The Schrödinger Equation is an eigenvalue equation

$$\hat{A}\psi = \underset{\text{an eigenvalue}}{a}\psi$$

$$\mathbf{A}|\psi_i\rangle = a_i|\psi_i\rangle$$

In matrix language:

$$A^{\phi} = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & a_N \end{pmatrix}_{\psi}$$

$$|1\rangle_{\psi} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad |2\rangle_{\psi} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

etc…

$$|n\rangle_{\psi} = \begin{pmatrix} \vdots \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$ n'th position

The ψ representation is special. We want to derive it from a computationally explicit starting point. We compute A^{ϕ} for a complete ortho-normal basis set $\{\phi\}$.

$$A^{\phi} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ \vdots & A_{22} & & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ A_{N1} & \cdots & \cdots & A_{NN} \end{pmatrix}_{\phi}$$

a non-diagonal matrix

The basis set that we choose can be the eigenfunctions for a simplified problem or they can be computationally convenient functions.

How do we find the eigenvalues and eigenfunctions of a non-diagonal $\mathbf{A}^{\phi}$?

I am using unconventional notation, ϕ or ψ subscripts or superscripts, which make the meaning of all symbols explicit. (They are like training wheels on a bicycle, discarded as soon as you learn to ride.

Some notation

$$|i\rangle_{\phi} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ j \end{pmatrix}_{\phi}$$

i'th position

$$\mathbf{T}|i\rangle_{\phi} = \begin{pmatrix} T_{1i} \\ \vdots \\ T_{Ni} \end{pmatrix}_{\phi}$$

the i'th column of **T**

Suppose we have a diagonal matrix, $\mathbf{A}^{\psi}$, an eigenvector of $\mathbf{A}^{\psi}$ is given by

$$\mathbf{A}^{\psi}\left|i\right\rangle_{\psi} = \mathbf{A}^{\psi}\begin{pmatrix}0\\ \vdots\\ 1\\ \vdots\\ 0\end{pmatrix} = \begin{pmatrix}0\\ 1\\ a_i\\ \vdots\\ 0\end{pmatrix} = a_i\begin{pmatrix}0\\ \vdots\\ 1\\ \vdots\\ 0\end{pmatrix}_i$$

The following **Non-Lecture** section is a derivation and discussion of the most important and useful equation in matrix mechanics.

$$\mathbf{S}^{\dagger}\mathbf{A}^{\phi}\mathbf{S}\left(\mathbf{S}^{\phi}\left|\ \right\rangle_{\phi}\right) = \mathbf{A}^{\psi}\left|\ \right\rangle_{\psi}$$

The eigenvectors are given by

$$\left(\mathbf{S}^{\dagger}\left|\ \right\rangle_{\phi}\right)$$

The i-th eigenvector is the i-th column or $\mathbf{S}^{\dagger}$

Sometimes, as for a time-dependent wavepacket, you want to know how a non-eigenvector is expressed as a linear combination of eigenkets. These are given by the columns of **S**.

$$\mathbf{S}\left|\ \right\rangle_{\psi} = \left|\ \right\rangle_{\phi}$$

Another very useful trick will be to evaluate the elements of **S** or $\mathbf{S}^{\dagger}$ using perturbation theory rather than diagonalization of the full matrix by a computer.

For the exact $\mathbf{H}$, we use perturbation theory, discussed in Lectures #14 – 17.

$$\mathbf{H} = \underbrace{\mathbf{H}^{(0)}}_{\substack{\text{exactly}\\\text{solved}\\\text{(diagonal)}}} + \underbrace{\mathbf{H}^{(1)}}_{\substack{\text{bad stuff}\\\text{(not diagonal)}}}$$

$$\left(\mathbf{S}^{\dagger}\mathbf{HS}\right)_{ii} = \mathbf{H}_{i}^{(0)} + \sum_{j \neq i} \frac{\left|\mathbf{H}_{ij}^{(1)}\right|^{2}}{E_{i}^{(0)} - E_{j}^{(0)}}$$

$$\mathbf{S}_{ij}^{\dagger} = \frac{\mathbf{H}_{ji}^{(1)}}{E_{j}^{(0)} - E_{i}^{(0)}}$$ which is the amount of $\left|i\right\rangle_{(0)}$ mixed into $\left|j\right\rangle$

where $E_{j}^{(0)}$ and $E_{i}^{(0)}$ are two eigen-energies of $\mathbf{H}^{(0)}$

The equation

$$\mathbf{S}^{\dagger}\mathbf{A}^{\phi}\mathbf{S}\mathbf{S}^{\dagger}\Big|\ \Big\rangle_{\phi} = \mathbf{A}^{\psi}\Big|\ \Big\rangle_{\psi}$$

is the most important equation in matrix mechanics

$\Big|\ \Big\rangle_{\phi}$ a complete, ortho-normal set of basis-kets

$\Big|\ \Big\rangle_{\psi}$ the complete set of eigen-kets of Hermitian operator **A**

$\mathbf{A}^{\phi}$ is the $N \times N$ (N can, in principle, be ∞) matrix representation of **A** where the elements of **A** are

$$A_{ij}^{\phi} = {}_{\phi}\langle i|\mathbf{A}|j\rangle_{\phi} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ A_{N1} & \cdots & \cdots & A_{NN} \end{pmatrix}_{\phi}$$

$\mathbf{A}^{\psi}$ is the diagonal matrix representation of **A** in the eigen-basis.

$$A^{\psi} = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & a_N \end{pmatrix}_{\psi}$$

A is Hermitian, which means that $\mathbf{A}^{\dagger} = \mathbf{A}$ where $A_{ij}^{\dagger} = A_{ji}^{*}$ and all the $\{a_i\}$ are real.

$\mathbf{S}$	is a unitary matrix
$\mathbf{S}^{\dagger} = \mathbf{S}^{-1}$	is the definition of a unitary matrix
$\mathbf{S}^{\dagger}\mathbf{S} = \mathbb{1}$	unit matrix
$\mathbf{S}^{\dagger}\mathbf{A}\mathbf{S}$	is a unitary transformation of **A**

We are interested in the unitary transformation that “diagonalizes” **A**

$$\mathbf{S}^{\dagger}\mathbf{A}^{\phi}\mathbf{S} = \mathbf{A}^{\psi}$$

and gives us the eigen-kets of **A**,

$$\mathbf{S}^{\dagger}\left|\ \right\rangle_{\phi} = \left|\ \right\rangle_{\psi}$$

This means that the j-th column of $\mathbf{S}^{\dagger}$ is the j-th eigenvector of $\mathbf{A}$.

$$\sum_i \mathbf{S}^{\dagger}_{ij}\left|i\right\rangle_{\phi} = \begin{pmatrix} S^{\dagger}_{1j} \\ \vdots \\ S^{\dagger}_{Nj} \end{pmatrix}_{\phi} = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}_{\psi}\begin{array}{l} \\ \\ \leftarrow \text{j-th} \\ \\ \\ \end{array} = \left|j\right\rangle_{\psi}$$

If $|\ \rangle_{\phi}$ is orthonormal, the unitary transformation preserves the orthonormality of $|\ \rangle_{\psi}$.

Efficient computer programs exist that diagonalize any Hermitian matrix. The diagonalization is done in sequence of 2×2 transformations $\{S_i^{\dagger}\}$, and the final diagonalizing matrices, $\mathbf{S}$, $\mathbf{S}^{\dagger}$, are expressed as a product of partial diagonalization steps

$$\mathbf{S}^{\dagger} = \prod_{i=1}^{N_{\max}} S_i^{\dagger}$$

which means that the computer gives us both the eigenvalues and the eigenvectors of $\mathbf{A}$.

Now where does this come from? Linear Algebra.

This is discussed in elegant detail in Merzbacher, Chapters 10.1 – 10.2, pages 207-212.

Eigenvalue Equation

$$\psi_j = \sum_i c_i^j \phi_i$$

completeness, an eigenstate is obtained from a linear combination of basis functions.

$$\mathbf{A}\sum_i c_i^j \phi_i = a_j \sum c_i^j \phi_i$$

left multiply by ϕ_k^* and integrate

$$\int \phi_k^* \mathbf{A} \phi_i \, d\tau = A_{ki}^{\phi}$$

$$\sum_i c_i^j A_{ki}^{\phi} - a_j c_k^j = 0$$

a linear homogeneous equation in unknown coefficients $\left\{c_k^j\right\}$

rearrange:

$$\sum_i \left[c_i^j A_{ki} - a_j \delta_{ki} c_i^j \right] = 0$$

$$\sum_i c_i^j \left(A_{ki} - a_j \delta_{ki} \right) = 0$$

left multiply by $\phi_{k'}^*$, and integrate, get another homoeneous linear equation.

The determinant of the unknown coefficients of the set of $\left\{c_i^j\right\}$ must be zero to yield a non-trivial solution: non-zero values of the c_i^j.

$$\left|\mathbf{A}^{\phi} - a\delta_{ki}\right| = 0$$

The vertical lines denote a determinant.

If we diagonalize $\mathbf{A}$, then we have an equation that satisfies the determinant of $|\mathbf{A}| = 0$ requirement.

$$\prod_{i=1}^{N}\left[A_{ii}^{\psi} - a\right] = 0 \quad \text{for each eigenvalue in the set } \left\{a_j\right\}$$

For each member of the set of eigenvalues $\{a_j\}$, we get one factor of the N-term product that is zero, which ensures that $|A^{\psi} - a| = 0$.

Two Useful Properties of Hermitian Matrices

Determinant Invariance

$$|\mathbf{ABC}| = |\mathbf{A}||\mathbf{B}||\mathbf{C}|$$

$$\text{This means } \left|\mathbf{S}^{\dagger}\mathbf{AS}\right| = \left|\mathbf{S}^{\dagger}\mathbf{S}\right||\mathbf{A}| = |\mathbf{A}|$$

$$\text{so } \left|A^{\phi}\right| = \left|A^{\psi}\right| = \prod_{i=1}^{N} a_i$$

Invariance of the product of eigenvalues

Trace Invariance

$$\sum_{i=1}^{N} A_{ii} = \sum_{i=1}^{N} a_i$$

Representation of the sum of eigenvalues

End of Non-Lecture

Can now solve many difficult appearing problems!

Start with a **matrix representation** of *any operator* that is expressable as a function of a matrix.

e.g. $\underset{\text{propagator}}{e^{-i\mathbf{H}(t-t_0)/\hbar}}$, $\underset{\text{potential curve}}{f(\mathbf{x})}$

prescription example

$$f(\mathbf{x}) = \mathbf{T}f\underbrace{\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right)}_{\substack{\text{diagonalize } \mathbf{x} \text{ – so } f(\,) \text{ is} \\ \text{applied to each diagonal} \\ \text{element}}}\mathbf{T}^{\dagger}$$

$$\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T} = \begin{pmatrix} x_1 & & & 0 \\ & x_2 & & \\ & & \ddots & \\ 0 & & & x_N \end{pmatrix}$$

$$f\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right) = \begin{pmatrix} f(x_1) & & & 0 \\ & f(x_2) & & \\ & & \ddots & \\ 0 & & & f(x_N) \end{pmatrix}$$

Then perform the inverse transformation, $\mathbf{T}$ f($\mathbf{T}^{\dagger}$ $\mathbf{x}$ $\mathbf{T}$)$\mathbf{T}^{\dagger}$ – undiagonalizes matrix, which gives matrix representation of the desired function of a matrix.

Show that this actually is valid for simple example

$$f(x) = \mathbf{x}^N$$

$$\underline{\underline{f\left(\mathbf{x}^N\right)}} = \mathbf{T}\Big[\underset{1}{\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right)}\underset{2}{\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right)}\cdots\underset{\mathrm{N}}{\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right)}\Big]\mathbf{T}^{\dagger} \qquad \text{apply prescription}$$

$$= \mathbf{T}\left[\mathbf{T}^{\dagger}\mathbf{x}^N\mathbf{T}\right]\mathbf{T}^{\dagger} = \mathbf{x}^N \qquad \text{get expected result}$$

general proof for arbitrary f($\mathbf{x}$) → expand in power series. Use previous result for each integer power.

John Light: Discrete Variable Representation (DVR)
General $V(x)$ evaluated in Harmonic Oscillator Basis Set.
we did not do H-O yet, but the general formula for all of the nonzero matrix elements of **x** in the harmonic oscillator basis set is:

$$\langle n|\mathbf{x}|n+1\rangle = \left[\frac{\hbar}{2\omega\mu}\right]^{1/2}(n+1)^{1/2} \qquad \omega = (k/\mu)^{1/2}$$

$$(\text{infinite dimension matrix}) \qquad \mathbf{x} = \left[\frac{\hbar}{2\omega\mu}\right]^{1/2}\begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & \cdots & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\ \vdots & \vdots & \sqrt{3} & 0 & \sqrt{4} \\ \vdots & \vdots & \vdots & \sqrt{4} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

[CARTOON]

$$\mathbf{x}^2 = \left[\frac{\hbar}{2\omega\mu}\right]\begin{array}{c c} \begin{array}{ccccccccc} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} & n= \\ \begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & \sqrt{6} & 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 5 & 0 & \sqrt{12} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 7 & 0 & & 0 & 0 & 0 \\ 0 & 0 & \sqrt{12} & 0 & 9 & 0 & & 0 & 0 \\ 0 & 0 & 0 & & 0 & 11 & 0 & & 0 \\ 0 & 0 & 0 & 0 & & 0 & 13 & 0 & \\ 0 & 0 & 0 & 0 & 0 & & 0 & 15 & \ddots \\ 0 & 0 & 0 & 0 & 0 & 0 & & \ddots & \ddots \end{pmatrix} & \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ \\ \\ \end{array} \end{array}$$

-two off-main diagonal $[n(n+1)]^{1/2}$

-main diagonal $|2n+1\rangle$

etc. matrix multiplication

to get matrix for f(**x**) diagonalize e.g., 1000 × 1000 (truncated) **x** matrix that was expressed in harmonic oscillator basis set.

$$\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T} = \begin{pmatrix} x_1 & 0 & 0 & 0 \\ 0 & x_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & x_{1000} \end{pmatrix}_x$$

diagonalized-**x** basis $\{x_i\}$ are eigenvalues. They have no obvious physical significance.

$$\mathbf{V}(x)_x = \begin{pmatrix} V(x_1) & 0 & 0 & 0 \\ 0 & V(x_2) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & V(x_{1000}) \end{pmatrix}_x$$

next transform back from x-basis to H-O basis set

$$\mathbf{V}(x)_{H-O} = \mathbf{T}\mathbf{V}(x)_x\mathbf{T}^{\dagger} = \begin{pmatrix} \\ \text{full} \\ \text{complicated} \\ \text{matrix} \\ \\ \end{pmatrix}_{\substack{1000 \times 1000 \\ H-O}}$$

T was determined when **x** was diagonalized

$$\mathbf{H} = \frac{\mathbf{p}^2}{2\mu} + V(x)$$

need matrix for $\mathbf{p}^2$, get it from $\mathbf{p}$ (the general formula for all non-zero matrix elements of $\mathbf{p}$)

$$\langle n|p|n+1\rangle = -i\left[\frac{\hbar(\omega\mu)}{2}\right]^{1/2}(n+1)^{1/2}$$

$$\mathbf{p} = -i\left[\frac{\hbar(\omega\mu)}{2}\right]^{1/2}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 \\ 0 & -\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots \\ 0 & 0 & \ddots & \ddots & \ddots \end{pmatrix}$$ same structure as $\mathbf{x}$

$$\mathbf{p^2} = -\left[\frac{\hbar(\omega\mu)}{2}\right]\begin{pmatrix} -1 & 0 & \sqrt{2} & 0 & 0 \\ 0 & -3 & 0 & \ddots & 0 \\ \sqrt{2} & 0 & -5 & 0 & \ddots \\ 0 & \ddots & \ddots & \ddots & \ddots \\ 0 & \ddots & \ddots & \ddots & \end{pmatrix}$$

if $\quad \mathrm{H} = \frac{p^2}{2\mu} + \frac{1}{2}kx^2 \qquad \left(\frac{1}{2}k = \frac{1}{2}\omega^2\mu\right)$

$$H = \frac{\hbar\omega}{4}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 14 \end{pmatrix} = \hbar\omega\begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 \\ 0 & 0 & 5/2 & 0 \\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

but for arbitrary V(x), express **H** in HO basis set,

$$\mathbf{H}_{HO} = \frac{\mathbf{p}_{HO}^2}{2\mu} + \underbrace{\mathbf{V}(\mathbf{x})_{HO}}_{\mathbf{TV}(\mathbf{x})_x\mathbf{T}^\dagger}$$

eigenvalues obtained by $\mathbf{S}^\dagger\mathbf{H}_{HO}\mathbf{S} = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & E_N \end{pmatrix}$

columns of $\mathbf{S}^\dagger$ are eigenvectors in HO basis set!

1. Express matrix of **x** in H-O basis (automatic; easy to program a computer to do this), get $\mathbf{x}_{\mathrm{HO}}$.
2. Diagonalize $\mathbf{x}_{\mathrm{HO}}$. Get $\mathbf{x}_{\mathrm{x}}$ and **T**.
3. Trivial to write $V(x)_x$ as $V(x_i) = \mathbf{V}(\mathbf{x})_x$ in **x** basis
4. Transform $\mathbf{V}(\mathbf{x})_x$ back to $\mathbf{V}(x)_{\mathrm{HO}}$
5. Diagonalize $\mathbf{H}_{\mathrm{HO}}$.

Solve many V(x) problems in this basis set.

1000×1000 **T** matrix diagonalizes $\mathbf{x} \Rightarrow 1000\ x_i$' s

Save the **T** and the $\{x_i\}$ for future use on *all* V(x) problems.

To verify convergence, repeat for new **x** matrix of dimension 1100×1100. There will be no obvious resemblance between

$$\{\mathbf{x}_i\}_{1000} \text{ and } \{\mathbf{x}_i\}_{1100}.$$

If the lowest energy eigenvalues of **H** (i.e. the ones you care about) do not change (by measurement accuracy), converged!

Next: Matrix Solution of Harmonic Oscillator (completely without wavefunctions, starting from the [**x**,**p**] commutation rule)

Then (at last) Perturbation Theory