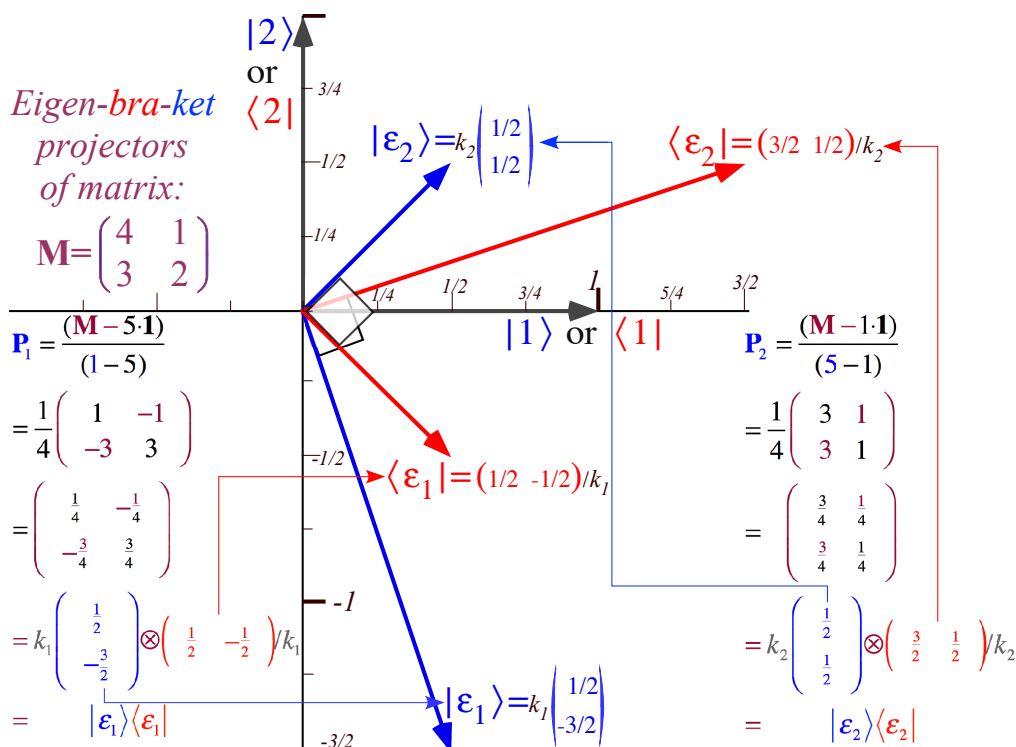

**QM
for
AMOP**
W. G. Harter

Chapter 3

Operator Eigensolutions



The concept of an operator’s “own-states” or *eigenstates* is introduced first through physical processes of analyzer filters, then visualized geometrically, and finally analyzed algebraically. The physical axioms 1-4 stated in Chapter 2 are related to four powerful *theorems* about the spectral decomposition of matrices. Applications of spectral decomposition to transformation and transfer matrices are shown.

Chapter 3 Introduction to Operator Eigensolutions

- 3.1 Operator Eigensolutions and Projection Operators3**
- Visualizing Real Symmetric Matrices and Real Eigenvectors4
- (a) Eigenvalue equations 5
 - (1) Secular equations 6
 - (2) Hamilton-Cayley equations 7
- (b) Eigenvector projectors (Distinct eigenvalues) 8
 - (1) Projector normalization 9
 - Matrix products and eigensolutions for polarizer-counter arrangements11
 - (2) Projector completeness and spectral decomposition 12
 - Eigensolutions are stationary or extreme-value solutions14
 - (3) Diagonalizing transformations from projectors 15
 - Matrix products and eigensolutions for active analyzers16
- (c) Eigenvector projectors (Degenerate eigenvalues) 17
 - (1) Minimal equation and diagonalizability criterion 17
 - (2) Nilpotent operators ("Bad" degeneracy) 18
 - (3) Multiple diagonalization ("Good" degeneracy) 19
 - Gram-Schmidt orthogonalization20
- (d) Projector splitting: A key to algebraic reduction 20
- (e) Why symmetry groups are useful 23
 - Quadratic surfaces help to visualize matrix operations24
- 3.2 Approximate Eigensolutions by Perturbation Techniques25**
- (a) Secular determinantal expansion 25
- (b) Perturbation approximations 26
- (c) Testing perturbation approximation with exact 2x2 eigenvalues 28
- Appendix 3.A Matrix Determinants, Adjuncts, and Inverses 1
- Appendix 3.B Classification of Permutations 4
- UNIT. 1 REVIEW TOPICS AND FORMULAS1**

Problems for Chapter 3.

3.1 Operator Eigensolutions and Projection Operators

Many quantum processes and analyzers can be represented by complex matrix *transfer* operators \mathbf{T} that act on an input state ket $|\Psi_{IN}\rangle$ to give the resulting output state kets $|\Psi_{OUT}\rangle$ as follows.

$$|\Psi_{OUT}\rangle = \mathbf{T}|\Psi_{IN}\rangle \tag{3.1.1}$$

(Recall discussion around (1.3.2).) In this way, matrix products predict the effect of the corresponding T-analyzer or a whole chain of analyzers. Generally, the effect of an analyzer is to change a state $|\Psi\rangle$ to one whose output vector $\mathbf{T}|\Psi\rangle$ is rotated or otherwise transformed as shown in Fig. 3.1.1 below. A transfer operator \mathbf{T} that is unitary ($\mathbf{T}^\dagger = \mathbf{T}^{-1}$) is also a *transformation* operator and satisfies Axioms 1-4.

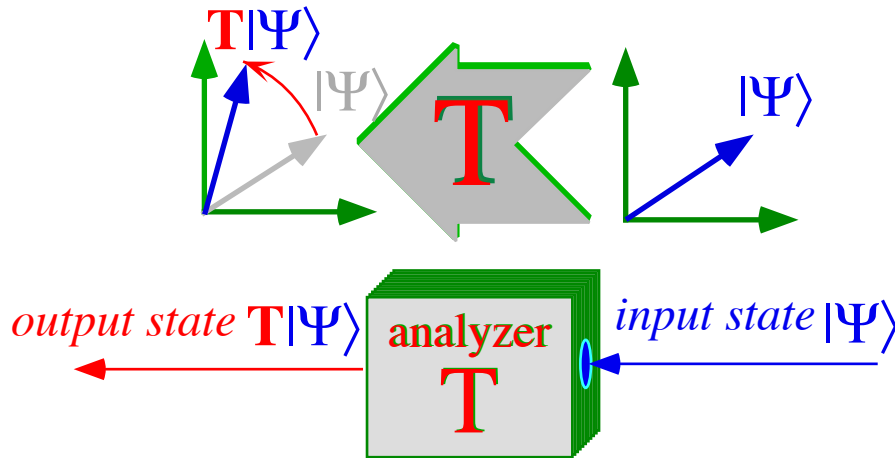


Fig. 3.1.1 Effect of analyzer represented by ket vector transformation of $|\Psi\rangle$ to new vector $\mathbf{T}|\Psi\rangle$.

However, most analyzers have certain of their *own* states whose kets $|e_j\rangle$ lie along certain "magic" directions that do not change when \mathbf{T} acts on them, that is, the input ket $|e_j\rangle$ just gets multiplied by a phase factor or other number ϵ_j as in

$$\mathbf{T}|e_j\rangle = \epsilon_j |e_j\rangle, \tag{3.1.2}$$

but the vector $|e_j\rangle$ remains pointing in the same direction as shown in Fig. 3.1.2 below.

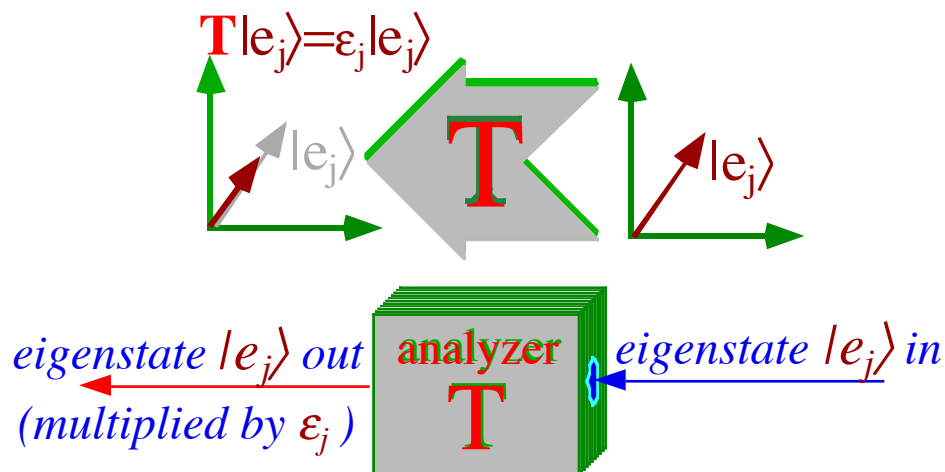
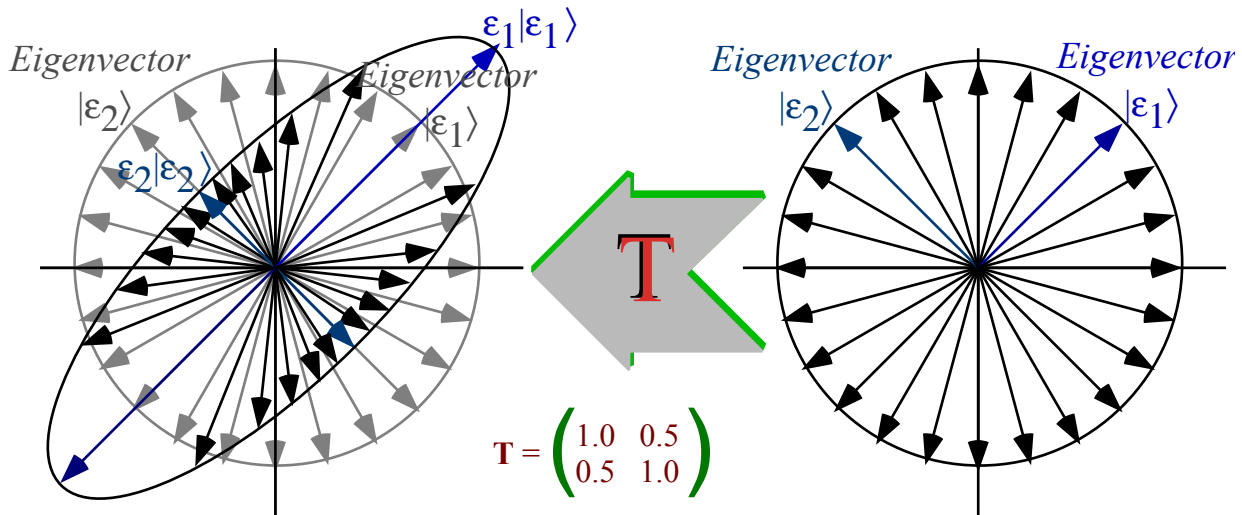


Fig. 3.1.2 Effect of analyzer on eigenket $|e_j\rangle$ is to simply multiply by eigenvalue ϵ_j ($\mathbf{T}|e_j\rangle = \epsilon_j |e_j\rangle$).

Visualizing Real Symmetric Matrices and Real Eigenvectors

You can learn something about a real matrix operator or transformation \mathbf{T} by applying it to a circular array of unit vectors \mathbf{c} . As shown below a matrix $\mathbf{T} = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}$ maps a circular array into an elliptical one



Only two vectors in the upper half plane survive the transformation \mathbf{T} without changing their directions. These lucky vectors are the *eigenvectors*

$$|\epsilon_1\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} / \sqrt{2}, \quad \text{and} \quad |\epsilon_2\rangle = \begin{pmatrix} -1 \\ 1 \end{pmatrix} / \sqrt{2}$$

which transform as follows: $\mathbf{T}|\epsilon_1\rangle = \epsilon_1|\epsilon_1\rangle = 1.5|\epsilon_1\rangle$, and $\mathbf{T}|\epsilon_2\rangle = \epsilon_2|\epsilon_2\rangle = 0.5|\epsilon_2\rangle$ by only suffering a length change given by *eigenvalues* $\epsilon_1 = 1.5$ and $\epsilon_2 = 0.5$, respectively. Obviously, the negatives $-|\epsilon_1\rangle$ or $-|\epsilon_2\rangle$ of eigenvectors are eigenvectors, too, as is $17|\epsilon_1\rangle$ or $-29|\epsilon_2\rangle, \dots$ etc. *Normalization* ($\langle \mathbf{c} | \mathbf{c} \rangle = 1$) is a separate condition that we generally require of eigenvectors, too.

Each vector $|\mathbf{r}\rangle$ on the left hand ellipse maps back to a vector $|\mathbf{c}\rangle = \mathbf{T}^{-1}|\mathbf{r}\rangle$ on the right hand unit circle, Each $|\mathbf{c}\rangle$ has unit length: $\langle \mathbf{c} | \mathbf{c} \rangle = 1 = \langle \mathbf{r} | \mathbf{T}^{-1} \mathbf{T}^{-1} | \mathbf{r} \rangle = \langle \mathbf{r} | \mathbf{T}^{-2} | \mathbf{r} \rangle$. (\mathbf{T} is real-symmetric: $\mathbf{T}^\dagger = \mathbf{T} = \mathbf{T}^T$.)

$$\mathbf{c} \cdot \mathbf{c} = 1 = \mathbf{r} \cdot \mathbf{T}^{-2} \cdot \mathbf{r} = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} T_{xx} & T_{xy} \\ T_{yx} & T_{yy} \end{pmatrix}^{-2} \begin{pmatrix} x \\ y \end{pmatrix}$$

This simplifies if rewritten in a coordinate system (x_1, x_2) of eigenvectors $|\epsilon_1\rangle$ and $|\epsilon_2\rangle$ where $\mathbf{T}^{-2}|\epsilon_1\rangle = \epsilon_1^{-2}|\epsilon_1\rangle$ and $\mathbf{T}^{-2}|\epsilon_2\rangle = \epsilon_2^{-2}|\epsilon_2\rangle$, that is, \mathbf{T} , \mathbf{T}^{-1} , and \mathbf{T}^{-2} are each represented by a diagonal matrix.

$$\begin{pmatrix} \langle \epsilon_1 | \mathbf{T} | \epsilon_1 \rangle & \langle \epsilon_1 | \mathbf{T} | \epsilon_2 \rangle \\ \langle \epsilon_2 | \mathbf{T} | \epsilon_1 \rangle & \langle \epsilon_2 | \mathbf{T} | \epsilon_2 \rangle \end{pmatrix} = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} \langle \epsilon_1 | \mathbf{T}^{-2} | \epsilon_1 \rangle & \langle \epsilon_1 | \mathbf{T}^{-2} | \epsilon_2 \rangle \\ \langle \epsilon_2 | \mathbf{T}^{-2} | \epsilon_1 \rangle & \langle \epsilon_2 | \mathbf{T}^{-2} | \epsilon_2 \rangle \end{pmatrix}^{-2} = \begin{pmatrix} \epsilon_1^{-2} & 0 \\ 0 & \epsilon_2^{-2} \end{pmatrix}$$

So, the matrix equation simplifies to an elementary ellipse equation of the form $(x/a)^2 + (y/b)^2 = 1$.

$$\mathbf{c} \cdot \mathbf{c} = 1 = \begin{pmatrix} x_1 & x_2 \end{pmatrix} \begin{pmatrix} \epsilon_1^{-2} & 0 \\ 0 & \epsilon_2^{-2} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \left(\frac{x_1}{\epsilon_1}\right)^2 + \left(\frac{x_2}{\epsilon_2}\right)^2$$

The ellipse semi-major-minor axes are eigenvalues $\epsilon_1 = 1.5$ and $\epsilon_2 = 0.5$. The axes are tilted as shown above. Such a \mathbf{T} operation is a *tensor* operation. \mathbf{T} anisotropically stretches and squeezes the space.

(a) Eigenvalue equations

The equation (3.1.2) is called an *eigenvalue equation* $\mathbf{T} |\epsilon_j\rangle = \epsilon_j |\epsilon_j\rangle$ and the kets $|\epsilon_j\rangle$ are called ket eigenvectors or simply *eigenkets* $|\epsilon_j\rangle$ and the scalar numbers are called *eigenvalues* ϵ_j of operator \mathbf{T} . For analyzers described by unitary operators ($\mathbf{T}^\dagger = \mathbf{T}^{-1}$) the eigenvalues are simply phase factors

$$\epsilon_j = e^{i\phi}, \tag{3.1.3}$$

so eigenkets stay the same magnitude. If the analyzer has a counter or particle sources then it may decrease (as in the Fig. 3.1.2) or increase the magnitude (and probability) of an eigenket vector.

The prefix "eigen" means "own" in German. The eigenvectors of a single analyzer-T are its own vectors, literally. We would call them "ownvectors" if we had to purge German from English. The eigenvectors $\{ |\epsilon_1\rangle, |\epsilon_2\rangle, \dots \}$ correspond to the *eigenstates* that get sorted out inside an analyzer as in Fig. 1.3.1 or Fig. 1.3.8. If a T-analyzer is set to a filter configuration like Fig. 1.3.4 then it can produce a beam that is made purely of one or another of its own eigenstates $|\epsilon_j\rangle$. (Excuse the bilingual redundancy.) Then another T-analyzer in the "do-nothing" mode would pass each of the resulting $|\epsilon_j\rangle$ particles 100% unchanged (except maybe for an overall phase) according to axiom-3. That would be an example of an eigen-equation $\mathbf{T} |\epsilon_j\rangle = \epsilon_j |\epsilon_j\rangle$ in its purest form.

If the \mathbf{T} -operator is represented in its own eigenbasis (Sorry, another bilingual redundancy.) then its matrix representation takes has a very simple *diagonal* form according to axiom-3.

$$\langle \epsilon_i | \mathbf{T} | \epsilon_j \rangle = \epsilon_j \langle \epsilon_i | \epsilon_j \rangle = \epsilon_j \delta_{ij} \tag{3.1.4a}$$

The diagonal matrix for an n-state system is

$$\begin{pmatrix} \langle \epsilon_1 | \mathbf{T} | \epsilon_1 \rangle & \langle \epsilon_1 | \mathbf{T} | \epsilon_2 \rangle & \dots & \langle \epsilon_1 | \mathbf{T} | \epsilon_n \rangle \\ \langle \epsilon_2 | \mathbf{T} | \epsilon_1 \rangle & \langle \epsilon_2 | \mathbf{T} | \epsilon_2 \rangle & \dots & \langle \epsilon_2 | \mathbf{T} | \epsilon_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \epsilon_n | \mathbf{T} | \epsilon_1 \rangle & \langle \epsilon_n | \mathbf{T} | \epsilon_2 \rangle & \dots & \langle \epsilon_n | \mathbf{T} | \epsilon_n \rangle \end{pmatrix} = \begin{pmatrix} \epsilon_1 & 0 & \dots & 0 \\ 0 & \epsilon_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \epsilon_n \end{pmatrix} \tag{3.1.4b}$$

However, we are usually given the \mathbf{T} -operator in someone else's basis $\{ |1\rangle, |2\rangle, \dots, |n\rangle \}$ as in

$$\begin{pmatrix} \langle 1 | \mathbf{T} | 1 \rangle & \langle 1 | \mathbf{T} | 2 \rangle & \dots & \langle 1 | \mathbf{T} | n \rangle \\ \langle 2 | \mathbf{T} | 1 \rangle & \langle 2 | \mathbf{T} | 2 \rangle & \dots & \langle 2 | \mathbf{T} | n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N | \mathbf{T} | 1 \rangle & \langle N | \mathbf{T} | 2 \rangle & \dots & \langle N | \mathbf{T} | n \rangle \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{nn} \end{pmatrix} \tag{3.1.4c}$$

Then the problem is one of *diagonalization* which consists of using n^2 matrix T_{ij} numbers to solve the following problems:

(Problem A) Find \mathbf{T} 's eigenvalues $\{ \epsilon_1, \epsilon_2, \dots, \epsilon_n \}$ (Find n numbers ϵ_j)

(Problem B) Find \mathbf{T} 's eigenket basis $\{ |\epsilon_1\rangle, |\epsilon_2\rangle, \dots, |\epsilon_n\rangle \}$ (Find n^2 numbers $\langle i | \epsilon_j \rangle$)

The lions share of work and information (particularly for large n) is in the n^2 components $\langle i | \epsilon_j \rangle$ of the *diagonalization transformation (d-tran) matrix* which will reduce (3.1.4c) to diagonal form (3.1.4b). The d-tran matrix $\langle i | \epsilon_j \rangle$ has in its columns the desired eigenkets $\{ |\epsilon_1\rangle, |\epsilon_2\rangle, \dots, |\epsilon_n\rangle \}$. (Recall (2.1.8).)

(1) Secular equations

The eigenvalue equations (3.1.2) for a general matrix operator \mathbf{M} can be written as follows

$$\mathbf{M}|\varepsilon_k\rangle = \varepsilon_k|\varepsilon_k\rangle, \text{ or: } (\mathbf{M} - \varepsilon_k\mathbf{1})|\varepsilon_k\rangle = \mathbf{0} \quad (3.1.5a)$$

and represented by

$$\begin{pmatrix} \langle 1|\mathbf{M}|1\rangle & \langle 1|\mathbf{M}|2\rangle & \cdots & \langle 1|\mathbf{M}|N\rangle \\ \langle 2|\mathbf{M}|1\rangle & \langle 2|\mathbf{M}|2\rangle & \cdots & \langle 2|\mathbf{M}|N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N|\mathbf{M}|1\rangle & \langle N|\mathbf{M}|2\rangle & \cdots & \langle N|\mathbf{M}|N\rangle \end{pmatrix} \begin{pmatrix} \langle 1|\varepsilon_j\rangle \\ \langle 2|\varepsilon_j\rangle \\ \vdots \\ \langle N|\varepsilon_j\rangle \end{pmatrix} = \varepsilon_j \begin{pmatrix} \langle 1|\varepsilon_j\rangle \\ \langle 2|\varepsilon_j\rangle \\ \vdots \\ \langle N|\varepsilon_j\rangle \end{pmatrix} \quad (3.1.5b)$$

or

$$\begin{pmatrix} \langle 1|\mathbf{M}|1\rangle - \varepsilon_j & \langle 1|\mathbf{M}|2\rangle & \cdots & \langle 1|\mathbf{M}|N\rangle \\ \langle 2|\mathbf{M}|1\rangle & \langle 2|\mathbf{M}|2\rangle - \varepsilon_j & \cdots & \langle 2|\mathbf{M}|N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N|\mathbf{M}|1\rangle & \langle N|\mathbf{M}|2\rangle & \cdots & \langle N|\mathbf{M}|N\rangle - \varepsilon_j \end{pmatrix} \begin{pmatrix} \langle 1|\varepsilon_j\rangle \\ \langle 2|\varepsilon_j\rangle \\ \vdots \\ \langle N|\varepsilon_j\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (3.1.5c)$$

These amount to n equations for each of n eigenvalues $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n\}$ or n^2 equations in all. The eigenvalues may be found by demanding that the determinant of the matrix in (3.1.5c) be zero. This is called the *secular equation*

$$\det|\mathbf{M} - \varepsilon\mathbf{1}| = 0 = (-1)^n (\varepsilon^n + a_1\varepsilon^{n-1} + a_2\varepsilon^{n-2} + \dots + a_{n-1}\varepsilon + a_n) \quad (3.1.5d)$$

where the polynomial coefficients are

$$a_1 = -\text{Trace}\mathbf{M}, \dots, a_k = (-1)^k \sum \text{diagonal k-by-k minors of } \mathbf{M}, \dots, a_n = (-1)^n \det|\mathbf{M}| \quad (3.1.5e)$$

The secular equation has n -factors, one for each eigenvalue.

$$\det|\mathbf{M} - \varepsilon\mathbf{1}| = 0 = (-1)^n (\varepsilon - \varepsilon_1)(\varepsilon - \varepsilon_2) \cdots (\varepsilon - \varepsilon_n) \quad (3.1.5f)$$

It may help to see some examples. For a two-by-two matrix \mathbf{H} ($n=2$) diagonalization is comparatively simple. The ($n=2$) secular equation is:

$$0 = \det \begin{vmatrix} H_{11} - \varepsilon & H_{12} \\ H_{21} & H_{22} - \varepsilon \end{vmatrix} = \varepsilon^2 - (H_{11} + H_{22})\varepsilon + (H_{11}H_{22} - H_{12}H_{21}) \quad (3.1.5)_{\text{example}}$$

and the polynomial coefficients are just related to matrix trace and determinant.

$$\begin{aligned} a_1 &= -(H_{11} + H_{22}) = -\text{Trace}H \\ a_2 &= H_{11}H_{22} - H_{12}H_{21} = \det H \end{aligned} \quad (3.1.5e)_{\text{example}}$$

Had we done this with a diagonal matrix then the coefficients in terms of eigenvalues would be

$$\begin{aligned} a_1 &= -(H_{11} + H_{22}) = -(\varepsilon_1 + \varepsilon_2) \\ a_2 &= H_{11}H_{22} - 0 = \varepsilon_1\varepsilon_2 \end{aligned} \quad (3.1.5e)_{\text{example}}$$

The preceding two equations must give the same numbers because the secular equation and its roots must not depend on the basis used to represent the abstract operator. Trace, determinant, and a_j are *invariant*.

For numerical examples, let us use two different matrices given below. One is Hermitian (self-conjugate) and one is not. (You might call them "good-cop" and "bad-cop", respectively.)

$$\mathbf{H} = \begin{pmatrix} 4 & -i\sqrt{3} \\ i\sqrt{3} & 2 \end{pmatrix} = \mathbf{H}^\dagger \tag{3.1.6a}$$

$$\mathbf{K} = \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \neq \mathbf{K}^\dagger \tag{3.1.6b}$$

They both have the same secular equation:

$$\begin{aligned} 0 &= S(\epsilon) = \epsilon^2 - 6\epsilon + 5 \\ 0 &= (\epsilon - 1)(\epsilon - 5) \end{aligned} \tag{3.1.7}$$

and same roots or eigenvalues ($\epsilon_1 = 1$ and $\epsilon_2 = 5$). However, the "bad-cop" matrix \mathbf{K} is not one that you are likely to see in quantum theory since it is neither unitary nor Hermitian. Still, it is instructive to see what the diagonalization formalism does with a pathological case such as this one. The "good-cop" matrix is not unitary, so it won't represent ideal analyzers, but because it is Hermitian, it could show up in other roles such as density operator or Hamiltonian matrices. (To be discussed later)

(2) Hamilton-Cayley equations

If each variable ϵ in the secular equation (3.1.5f) is replaced by the matrix operator \mathbf{M} and each ϵ_k by $\epsilon_k \mathbf{1}$ then the following matrix equation results.

$$\mathbf{0} = (\mathbf{M} - \epsilon_1 \mathbf{1})(\mathbf{M} - \epsilon_2 \mathbf{1}) \cdots (\mathbf{M} - \epsilon_n \mathbf{1}) \tag{3.1.8}$$

This operator equation is known as the *Hamilton-Cayley (HC) equation* or *Hamilton-Cayley theorem*.

The HC-equation is obviously true if \mathbf{M} has the diagonal form of (3.1.4b). But, that is circular logic since one needs to *prove* the diagonal form is possible first. We shall arrive at this proof in a roundabout way. For now a quick check of the HC-equation for the "bad-cop" \mathbf{K} -matrix (3.1.6b) is done below.

$$\begin{aligned} \mathbf{K}^2 - 6\mathbf{K} + 5\mathbf{1} &= \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix}^2 - 6 \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} + 5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 19 & 6 \\ 18 & 7 \end{pmatrix} - \begin{pmatrix} 24 & 6 \\ 18 & 12 \end{pmatrix} + \begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ &= \left[\begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} - 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \left[\begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} - 5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = \left[\begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} \right] \left[\begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix} \right] \end{aligned} \tag{3.1.8}_{\text{example}}$$

The HC-equation works fine in this case, as it does for all matrices.

(b) Eigenvector projectors (Distinct eigenvalues)

To obtain eigenvectors we construct *projection operators* \mathbf{p}_k by replacing k -th factor $(\mathbf{M} - \epsilon_k \mathbf{1})$ from HC eq.(3.1.8) by unit matrix $(\mathbf{1})$ as follows. (We assume distinct eigenvalues $\epsilon_1 \neq \epsilon_2 \neq \dots$ here.)

$$\begin{aligned} \mathbf{p}_1 &= (\mathbf{1}) (\mathbf{M} - \epsilon_2 \mathbf{1}) \cdots (\mathbf{M} - \epsilon_n \mathbf{1}) \\ \mathbf{p}_2 &= (\mathbf{M} - \epsilon_1 \mathbf{1}) (\mathbf{1}) \cdots (\mathbf{M} - \epsilon_n \mathbf{1}) \quad \text{or: } \mathbf{p}_k = \prod_{j \neq k} (\mathbf{M} - \epsilon_j \mathbf{1}) \\ &\vdots \\ \mathbf{p}_n &= (\mathbf{M} - \epsilon_1 \mathbf{1}) (\mathbf{M} - \epsilon_2 \mathbf{1}) \cdots (\mathbf{1}) \end{aligned} \tag{3.1.9}$$

Each operator \mathbf{p}_k has a delightful property. The \mathbf{p}_k solve the original eigenvector equation (3.1.5a).

$$(\mathbf{M} - \epsilon_k \mathbf{1}) \mathbf{p}_k = \mathbf{0} \quad \text{or:} \quad \mathbf{M} \mathbf{p}_k = \epsilon_k \mathbf{p}_k \tag{3.1.10a}$$

$$\mathbf{p}_k (\mathbf{M} - \epsilon_k \mathbf{1}) = \mathbf{0} \quad \text{or:} \quad \mathbf{p}_k \mathbf{M} = \epsilon_k \mathbf{p}_k \tag{3.1.10b}$$

This is true because putting back the k -th factor $(\mathbf{M} - \epsilon_k \mathbf{1})$ restores the original HC-equation and gives zero. Relation $\mathbf{M} \mathbf{p}_k = \epsilon_k \mathbf{p}_k$ implies that \mathbf{p}_k contains ket eigenvectors $|\epsilon_j\rangle$ in its columns and $\mathbf{p}_k \mathbf{M} = \epsilon_k \mathbf{p}_k$ implies that bra eigenvectors $\langle \epsilon_j|$ in its rows. (The "soft-bra-ket" notation $(|$ or $|)$ denotes un-normalized left or right eigenvectors.) Consider the "bad cop" example again. First, here are its projectors worked out.

$$\mathbf{K} - 5 \cdot \mathbf{1} = \left[\begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} - 5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = \begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix} = \mathbf{p}_1, \quad \mathbf{K} - 1 \cdot \mathbf{1} = \left[\begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} - 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = \begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} = \mathbf{p}_2. \tag{3.1.9} \text{example}$$

Note that matrix \mathbf{K} eigenvector relations are satisfied many ways by the \mathbf{p}_j 's. Here are the "right handed" un-normalized $|\epsilon_j\rangle$ -ket solutions.

$$\begin{aligned} \mathbf{K} \cdot \mathbf{p}_1 &= 1 \cdot \mathbf{p}_1, & \mathbf{K} \cdot \mathbf{p}_2 &= 5 \cdot \mathbf{p}_2, \\ \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix} &= 1 \cdot \begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix}, & \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} &= 5 \cdot \begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} \\ \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} -1 \\ 3 \end{pmatrix} &= 1 \cdot \begin{pmatrix} -1 \\ 3 \end{pmatrix}, & \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} 3 \\ 3 \end{pmatrix} &= 5 \cdot \begin{pmatrix} 3 \\ 3 \end{pmatrix} \end{aligned} \tag{3.1.10a} \text{example}$$

Here are the "left handed" or $\langle \epsilon_j|$ -bra solutions.

$$\begin{aligned} \mathbf{p}_1 \cdot \mathbf{K} &= 1 \cdot \mathbf{p}_1, & \mathbf{p}_2 \cdot \mathbf{K} &= 5 \cdot \mathbf{p}_2, \\ \begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix} \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} &= 1 \cdot \begin{pmatrix} -1 & 1 \\ 3 & -3 \end{pmatrix}, & \begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} &= 5 \cdot \begin{pmatrix} 3 & 1 \\ 3 & 1 \end{pmatrix} \\ \begin{pmatrix} -1 & 1 \end{pmatrix} \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} &= 1 \cdot \begin{pmatrix} -1 & 1 \end{pmatrix}, & \begin{pmatrix} 3 & 1 \end{pmatrix} \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} &= 5 \cdot \begin{pmatrix} 3 & 1 \end{pmatrix} \end{aligned} \tag{3.1.10b} \text{example}$$

This is a powerful way to calculate eigenbras and eigenkets. But, there is much more power hidden in this approach. We're just getting started! Read on.

(1) Projector normalization

We may normalize \mathbf{p}_k operators to make the *idempotent projection operators* \mathbf{P}_k defined by

$$\mathbf{P}_k = \frac{\prod_{j \neq k} (\mathbf{M} - \varepsilon_j \mathbf{1})}{\prod_{j \neq k} (\varepsilon_k - \varepsilon_j)} \tag{3.1.11}$$

The *normalized* projectors are denoted by upper case \mathbf{P} and satisfy \mathbf{p} -eigen-equations (3.1.10), too.

$$\mathbf{M} \mathbf{P}_k = \varepsilon_k \mathbf{P}_k, \quad (\mathbf{M})^2 \mathbf{P}_k = (\varepsilon_k)^2 \mathbf{P}_k \dots \tag{3.1.12a}$$

$$\mathbf{P}_k \mathbf{M} = \varepsilon_k \mathbf{P}_k, \quad \mathbf{P}_k (\mathbf{M})^2 = (\varepsilon_k)^2 \mathbf{P}_k \dots \text{ etc.} \tag{3.1.12b}$$

This normalization make \mathbf{P} 's *idempotent* ($\mathbf{P}^2 = \mathbf{P}$) as follows using: $f(\mathbf{M})\mathbf{P}_k = f(\varepsilon_k)\mathbf{P}_k$.

$$\mathbf{P}_k \mathbf{P}_k = \frac{\prod_{j \neq k} (\mathbf{M} - \varepsilon_j \mathbf{1})}{\prod_{j \neq k} (\varepsilon_k - \varepsilon_j)} \mathbf{P}_k = \frac{\prod_{j \neq k} (\varepsilon_k - \varepsilon_j)}{\prod_{j \neq k} (\varepsilon_k - \varepsilon_j)} \mathbf{P}_k = \mathbf{P}_k \tag{3.1.13a}$$

A *projector orthonormalization relation* follows since projectors, normalized or not, are mutually orthogonal.

$$\mathbf{p}_j \mathbf{p}_k = \mathbf{0} \text{ for } j \neq k \quad \text{or:} \quad \mathbf{P}_j \mathbf{P}_k = \delta_{jk} \mathbf{P}_k \tag{3.3.13b}$$

Consider a "bad cop" example after (3.1.10) to begin seeing what power \mathbf{P}_k -normalization relations give.

$$\mathbf{P}_1 = \frac{\begin{pmatrix} -1 & 1 \\ 3 & -3 \\ 1 & -5 \end{pmatrix}}{(1-5)} = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} \quad \mathbf{P}_2 = \frac{\begin{pmatrix} 3 & 1 \\ 3 & 1 \\ 5 & -1 \end{pmatrix}}{(5-1)} = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} \tag{3.1.11} \text{example}$$

Idempotence implies 4 ready-made sets of scalar products between 2 rows (bras) and 2 columns (kets).

$$\mathbf{P}_1 = \mathbf{P}_1 \mathbf{P}_1 = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix}, \quad \mathbf{P}_2 = \mathbf{P}_2 \mathbf{P}_2 = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} \tag{3.1.13} \text{examples}$$

For example, (1st row)·(1st column) dot product $(\varepsilon_k | \varepsilon_k)$ is already given by \mathbf{P}_k -matrix element $(\mathbf{P}_k)_{11}$.

$$(\varepsilon_1 | \varepsilon_1) = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \end{pmatrix} \begin{pmatrix} \frac{1}{4} \\ -\frac{3}{4} \end{pmatrix} = \frac{1}{4} = (\mathbf{P}_1)_{11}, \quad (\varepsilon_2 | \varepsilon_2) = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix} \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4} \end{pmatrix} = \frac{3}{4} = (\mathbf{P}_2)_{11}.$$

One way to get a *normalized bra* $\langle \varepsilon_k |$ or *ket* $|\varepsilon_k\rangle$ is to divide un-normal row- $(\varepsilon_k |$ or column- $|\varepsilon_j)$ by $\sqrt{(\mathbf{P}_k)_{11}}$.

$$|\varepsilon_1\rangle = \frac{|\varepsilon_1\rangle}{\sqrt{(\mathbf{P}_1)_{11}}} = \frac{1}{\sqrt{\frac{1}{4}}} \begin{pmatrix} \frac{1}{4} \\ -\frac{3}{4} \end{pmatrix}, \quad \langle \varepsilon_1| = \frac{\langle \varepsilon_1|}{\sqrt{(\mathbf{P}_1)_{11}}} = \frac{\begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \end{pmatrix}}{\sqrt{\frac{1}{4}}}, \quad |\varepsilon_2\rangle = \frac{|\varepsilon_2\rangle}{\sqrt{(\mathbf{P}_2)_{11}}} = \frac{1}{\sqrt{\frac{3}{4}}} \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4} \end{pmatrix}, \quad \langle \varepsilon_2| = \frac{\langle \varepsilon_2|}{\sqrt{(\mathbf{P}_2)_{11}}} = \frac{\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \end{pmatrix}}{\sqrt{\frac{3}{4}}}.$$

A more elegant way is to \otimes -factor (Recall (2.1.22)) each \mathbf{P}_j -matrix as shown here or in Fig. 3.1.3 below.

$$\mathbf{P}_1 = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} = k_1 \begin{pmatrix} \frac{1}{2} \\ -\frac{3}{2} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \end{pmatrix} / k_1 \tag{3.1.14a} \quad \mathbf{P}_2 = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} = k_2 \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \otimes \begin{pmatrix} \frac{3}{2} & \frac{1}{2} \end{pmatrix} / k_2 \tag{3.1.14b}$$

$$= |\varepsilon_1\rangle \langle \varepsilon_1| \quad = |\varepsilon_2\rangle \langle \varepsilon_2|$$

This way shows you may shift magnitude and phase between a ket-factor $|\varepsilon_j\rangle$ and its companion bra-factor $\langle \varepsilon_j|$ by varying a *gauge adjustment constant* k_j to any non-zero value, real or complex. All the projection algebra discussed below is invariant to k_j . (The first way above has $(k_1=1, k_2=1/\sqrt{3})$. Figure 3.1.3 has $k_1=1=k_2$.)

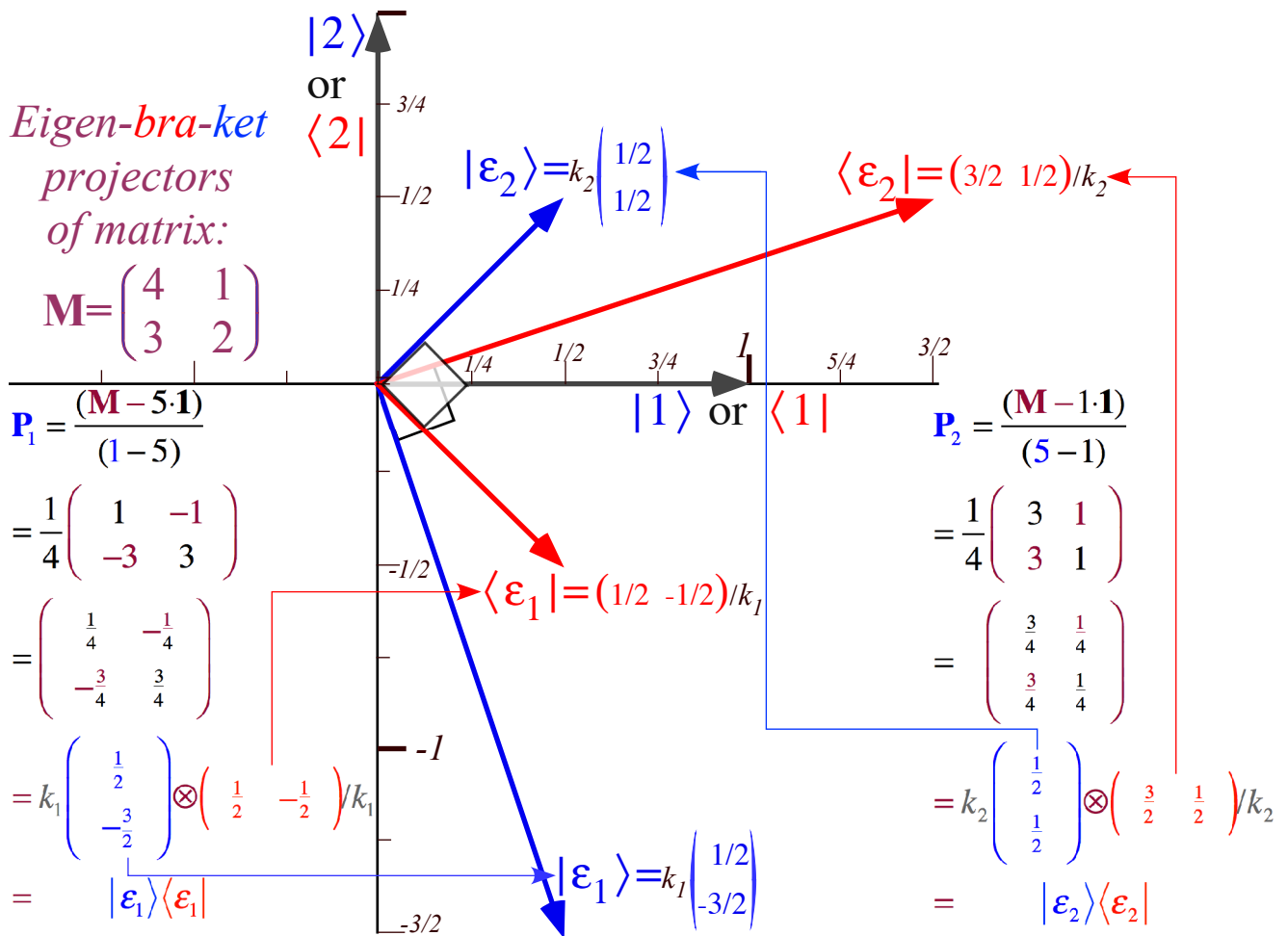


Fig. 3.1.3 Normalized eigenbras and eigenkets for asymmetric "bad cop" matrix K. (Here $k_1=1=k_2$.)

The first thing to notice is that the "bad cop" eigenvectors do not satisfy quantum conjugation relations associated with axiom-2, that is eigenbra $\langle \epsilon_j|$ is NOT equal to Hermitian conjugate $|\epsilon_j\rangle^\dagger$ of eigenket $|\epsilon_j\rangle$. Still, they are orthonormal and satisfy axiom-3. (They satisfy the "letter of the law" but not the intent, just like a "bad cop" would!) Each $\langle \epsilon_j|$ is 90° from $|\epsilon_{k \neq j}\rangle$ in Fig. 3.1.3 and normalized as per (3.1.13b) regardless of k_j .

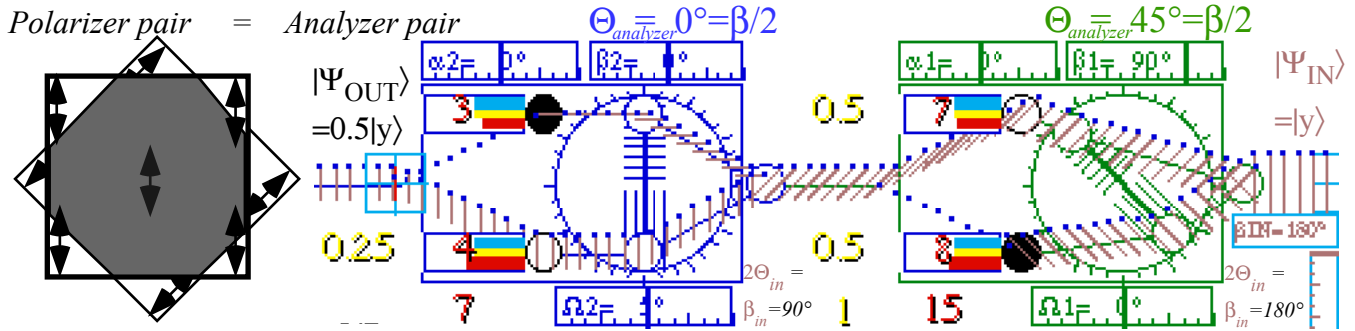
$$\langle \epsilon_1 | \epsilon_2 \rangle = 0 = \langle \epsilon_2 | \epsilon_1 \rangle \qquad \langle \epsilon_1 | \epsilon_1 \rangle = 1 = \langle \epsilon_2 | \epsilon_2 \rangle .$$

If you want to double the length of the first ket $|\epsilon_1\rangle$ in Fig. 3.1.3, you may increase k_1 from 1 to 2. Note this will halve the length of the first bra $\langle \epsilon_1|$ so the scalar products and projectors do not change. It is remarkable that you may then vary the second ket $|\epsilon_2\rangle$ and bra $\langle \epsilon_2|$ similarly and independently of the first. These are simple examples of *gauge transformations* that revise length or wave amplitude standards for plots like Fig. 3.1.3.

You should calculate **P**-matrices for the complex ("good cop") matrix **H** in (3.1.6a), and show that their eigenbra-kets also satisfy both the full quantum orthonormality and conjugation relations. The correct name for a "good cop" matrix is a *normal* matrix **N**, which simply means it commutes with its †-conjugate: $\mathbf{N}^\dagger \mathbf{N} = \mathbf{N} \mathbf{N}^\dagger$. Quantum theory is mainly concerned with normal matrices of which Hermitian ($\mathbf{H}^\dagger = \mathbf{H}$) and unitary ($\mathbf{U}^\dagger = \mathbf{U}^{-1}$) matrices are the most common. However, we need to learn to deal with the "abnormal" matrices, as well.

Matrix products and eigensolutions for polarizer-counter arrangements

Consider a 45° tilted ($\theta_1 = \beta_1/2 = \pi/4$ or $\beta_1 = 90^\circ$) sheet of polarizer lying below a y-sheet, that is, a $\beta_1 = 90^\circ$ (45° -polarized) filter followed by a $\beta_2 = 0^\circ$ filter with bottom path open which is like a y-polarized sheet.



(The $\beta_2 = 0^\circ$ filter with bottom path open is the same as a $\beta_2 = 180^\circ$ filter with top path open.) The transfer matrices for these filters are those of projection operators for the states they let pass. (Recall (2.1.22).)

$$T(2) = |y\rangle\langle y| = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad T(1) = |x'\rangle\langle x'| = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad (\text{for } |x'\rangle: \theta_2 = \beta_2/2 = 45^\circ)$$

Their matrix product is the transfer matrix for the total system of two filters.

$$T(\text{total}) = T(2) \cdot T(1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

The product's eigenvectors determine the eigenstates or "own-states" that may pass with only a change of overall magnitude or phase. The secular equation yields two eigenvalues and two projectors.

$$\lambda^2 - \frac{1}{2}\lambda + 0 = 0, \text{ or: } \lambda = 0, \frac{1}{2}, \text{ gives projectors } P_0 = \begin{pmatrix} \frac{-1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} - \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \quad P_{1/2} = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} - 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$$

The first eigenket is the non-zero column of P_0 , namely, $|0\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ with zero eigenvalue, that is, zero transfer.

The second eigenket is the non-zero column $|\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ of $P_{1/2}$ with eigenvalue $1/2$, giving 50% amplitude. The

figure above shows the latter eigenstate, namely y-polarization ($\beta_{IN} = 180^\circ$), entering on the right then emerging on the left with its amplitude cut in half and the probability cut by $(1/2)^2 = 1/4$ or 25%, according to

$T(\text{total})|\frac{1}{2}\rangle = \frac{1}{2}|\frac{1}{2}\rangle$. The eigenbras, namely $\langle 0| = (1 \ 0)$ and $\langle \frac{1}{2}| = (1 \ 1)$ describe what gets through going the

opposite way, that is, left-to-right, according to equations $\langle 0|T(\text{total}) = 0$ and $\langle \frac{1}{2}|T(\text{total}) = \frac{1}{2}\langle \frac{1}{2}|$. These equations

say that x-polarization gets stopped from going in the left end while 45° polarization would have a 50% transfer. The matrices $T(\beta = 180^\circ)$ and $T(\beta = 90^\circ)$ do not commute. Reversing their order gives a different product and a different set of eigensolutions. In this case, since the factor matrices are Hermitian, reversal would simply interchange the eigenbras with the eigenkets, that is, a \dagger -operation.

(2) Projector completeness and spectral decomposition

The normalized projection operators derive from matrix operator \mathbf{M} and its eigenvalues ϵ_k .

$$\mathbf{P}_k = \frac{\prod_{j \neq k} (\mathbf{M} - \epsilon_j \mathbf{1})}{\prod_{j \neq k} (\epsilon_k - \epsilon_j)} \tag{3.1.15a}$$

The projectors \mathbf{P}_k have been shown to be *eigenoperators* for \mathbf{M} .

$$\mathbf{P}_k \mathbf{M} = \mathbf{M} \mathbf{P}_k = \epsilon_k \mathbf{P}_k \tag{3.1.15b}$$

They have also been shown to satisfy *projector orthonormality and idempotency*.

$$\mathbf{P}_j \mathbf{P}_k = \delta_{jk} \mathbf{P}_k \tag{3.1.15c}$$

Now we will demonstrate that they also satisfy a *projector completeness relation*

$$\mathbf{1} = \mathbf{P}_1 + \mathbf{P}_2 + \dots + \mathbf{P}_n \tag{3.1.15d}$$

and a very powerful relation called *spectral decomposition of an operator M*.

$$\mathbf{M} = \epsilon_1 \mathbf{P}_1 + \epsilon_2 \mathbf{P}_2 + \dots + \epsilon_n \mathbf{P}_n \tag{3.1.15e}$$

The completeness relation (3.1.15d) resembles the abstraction (2.1.20) of *axiom-4* repeated here.

$$\mathbf{1} = \sum_{k=1}^n \mathbf{P}_k = \sum_{k=1}^n |k\rangle\langle k| \tag{3.1.16}$$

The similarity is no accident, but there is a logical difference between (3.1.15d) and (3.1.16). The latter is a *physical axiom* of *quantum wave path completeness*, while the former is a *algebraic theorem* being proved here. The spectral decomposition relation (3.1.15e) follows by operating on the completeness relation (3.1.15d) with the matrix \mathbf{M} using its eigen-operator relation (3.1.15b) that is an algebraic result.

First, let us check that (3.1.15d) and (3.1.16) are correct for examples (3.1.14) expressed in terms of an *outer* or *Kronecker tensor* (\otimes) *product* of eigen-bras and kets from "bad cop" matrix \mathbf{K} .

$$\mathbf{P}_1 = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} = k_1 \begin{pmatrix} \frac{1}{2} \\ -\frac{3}{2} \end{pmatrix} \otimes \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \end{pmatrix} / k_1 = |\epsilon_1\rangle\langle\epsilon_1|, \quad \mathbf{P}_2 = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} = k_2 \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \otimes \begin{pmatrix} \frac{3}{2} & \frac{1}{2} \end{pmatrix} / k_2 = |\epsilon_2\rangle\langle\epsilon_2|, \tag{3.1.14}_{repeat}$$

This agrees with the original results in (3.1.11)_{example}. Furthermore, they sum up to $\mathbf{1}$ as required. More importantly, they provide the following spectral decomposition (3.1.15e) of \mathbf{K} .

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} + \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} \tag{3.1.15d}_{example} \quad \mathbf{K} = \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} = 1 \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} + 5 \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} \tag{3.1.15e}_{example}$$

Spectral decomposition quickly finds the 100th power \mathbf{K}^{100} of \mathbf{K} using (3.1.15e).

$$\mathbf{K}^{100} = \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix}^{100} = 1^{100} \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{3}{4} & \frac{3}{4} \end{pmatrix} + 5^{100} \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1+3 \cdot 5^{100} & 5^{100}-1 \\ -3+3 \cdot 5^{100} & 5^{100}+3 \end{pmatrix}$$

Idempotence and orthonormality (3.1.15c) kills all cross terms so a function $f(\mathbf{M})$ of a matrix \mathbf{M} reduces to a sum of projectors weighted with the function evaluated at \mathbf{M} -eigenvalues ϵ_k .

$$f(\mathbf{M}) = f(\epsilon_1) \mathbf{P}_1 + f(\epsilon_2) \mathbf{P}_2 + \dots + f(\epsilon_n) \mathbf{P}_n \tag{3.1.17}$$

This is a *functional spectral decomposition of an operator M*. (Try \mathbf{K}^{-1} , or $\sqrt{\mathbf{K}}$ to test this technique.)

Now to prove the matrix completeness relation (3.1.15d) we will appeal to the numerical analysis lore. The formula (3.1.17) for functional spectral decomposition resembles the terms in the famous *Lagrange interpolation formula* of a function $f(x)$ approximated by its value at N discrete points.

$$L(f(x)) = \sum_{m=1}^N f(x_m) \cdot P_m(x) \quad \text{where: } P_m(x) = \frac{\prod_{j \neq m}^N (x - x_j)}{\prod_{j \neq m}^N (x_m - x_j)} \tag{3.1.18}$$

Lagrange’s formula fits a polynomial of degree $N - 1$ to N arbitrary points $\{x_1, x_2, \dots, x_n\}$ on a function curve $y = f(x)$. Note that each polynomial term $P_m(x)$ has zeros at each point $x = x_j$ *except* $x = x_m$ where $P_m(x_m) = 1$. So at each of these points x_m this L-approximation becomes exact: $L(f(x_m)) = f(x_m)$.

If $f(x)$ happens to be a polynomial of degree $N - 1$ or less, then the L-approximation is exact everywhere, that is, $L(f(x)) = f(x)$ for *all* points x . This is true since one point determines a constant, two points uniquely determine a line, three points uniquely determine a parabola, and N points uniquely determine an $(N - 1)^{th}$ degree curve. Hence if $(N > 1)$ the following special cases of a constant ($f(x) = 1$) and a line ($f(x) = x$) are exactly determined by $L(f(x)) = f(x)$ for *all* points x .

$$1 = \sum_{m=1}^N P_m(x), \qquad x = \sum_{m=1}^N x_m P_m(x)$$

The first corresponds to matrix completeness (3.1.15d) and the second one to spectral decomposition (3.1.15e).

Now a matrix \mathbf{M} and its powers \mathbf{M}^n obey the same algebra as a simple variable x and its powers x^n . So completeness relation is proved. Furthermore, it is true *for all distinct values of the eigenvalue parameters* $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n\}$. Completeness relation (3.1.15d) seems to be *more than true!* This is easily seen for $N = 2$.

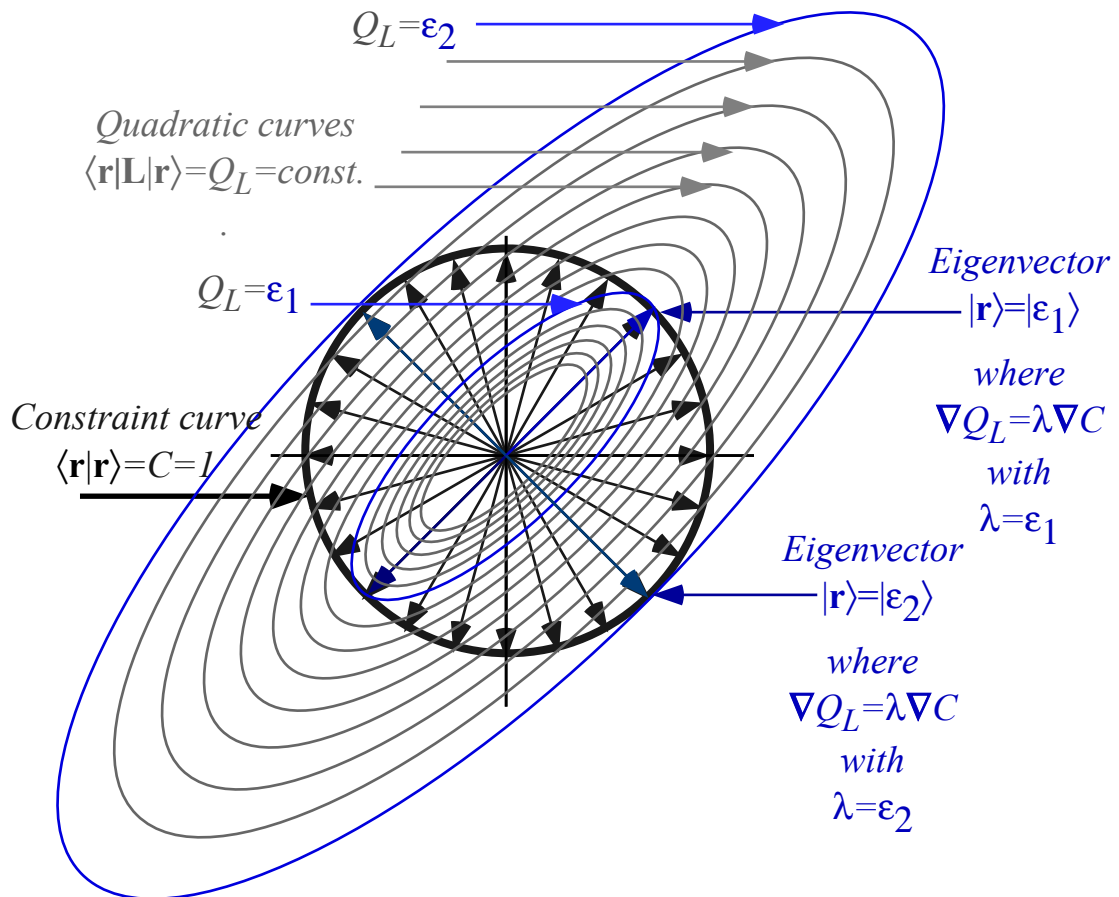
$$\mathbf{P}_1 + \mathbf{P}_2 = \frac{\prod_{j \neq 1} (\mathbf{M} - \varepsilon_j \mathbf{1})}{\prod_{j \neq 1} (\varepsilon_1 - \varepsilon_j)} + \frac{\prod_{j \neq 2} (\mathbf{M} - \varepsilon_j \mathbf{1})}{\prod_{j \neq 2} (\varepsilon_2 - \varepsilon_j)} = \frac{(\mathbf{M} - \varepsilon_2 \mathbf{1})}{(\varepsilon_1 - \varepsilon_2)} + \frac{(\mathbf{M} - \varepsilon_1 \mathbf{1})}{(\varepsilon_2 - \varepsilon_1)} = \frac{(\mathbf{M} - \varepsilon_2 \mathbf{1}) - (\mathbf{M} - \varepsilon_1 \mathbf{1})}{(\varepsilon_1 - \varepsilon_2)} = \frac{-\varepsilon_2 \mathbf{1} + \varepsilon_1 \mathbf{1}}{(\varepsilon_1 - \varepsilon_2)} = \mathbf{1} \quad (\text{for all } \varepsilon_j)$$

Direct algebraic verification of universal identity of completeness (3.1.15d) grows algebraically laborious for larger $N = 3, 4, \dots$, so it is nice that the Lagrangian analogy shows its ε_k independence for all N .

However, the ε_k are required to be the correct eigenvalues ε_k of matrix \mathbf{M} for the other relations in (3.1.15) such as orthogonality and spectral theorems.

Eigensolutions are stationary or extreme-value solutions

Eigenvalues λ of a matrix \mathbf{L} can be viewed as stationary-values of its quadratic form $Q_{\mathbf{L}}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{L} | \mathbf{r} \rangle$, that is, the min-max values of the function $Q(\mathbf{r})$ subject to the constraint of unit norm: $C(\mathbf{r}) = \langle \mathbf{r} | \mathbf{r} \rangle = 1$. Multi-dimensional constrained min-max problems may be solved using *Lagrange multiplier theory* as we will sketch here. The idea is to find those values of $Q_{\mathbf{L}}$ and vector \mathbf{r} for which the $Q_{\mathbf{L}}(\mathbf{r}) = \text{const.}$ ellipses is tangent to the constraint circle $C(\mathbf{r}) = 1$. Stated another way, imagine walking around the constraint circle $C(\mathbf{r}) = \langle \mathbf{r} | \mathbf{r} \rangle = 1$ in the figure below and looking for those places where one of the $Q_{\mathbf{L}}(\mathbf{r}) = \text{const.}$ ellipses is tangent to the unit circle $C(\mathbf{r}) = 1$. Lagrange pointed out that such points would have the gradient $\nabla Q_{\mathbf{L}}$ pointing in the same direction as ∇C , that is, the two gradient vectors $\nabla Q_{\mathbf{L}}$ and ∇C would be proportional to each. In honor of Lagrange, the proportionality constant is taken to be λ in $\nabla Q_{\mathbf{L}} = \lambda \nabla C$, where λ is called a *Lagrange Multiplier*.



The fact that λ symbolizes both the eigenvalue and a Lagrange multiplier is no coincidence; they are equal here. The gradients $\nabla Q_{\mathbf{L}} = \langle \mathbf{r} | \mathbf{L} + \mathbf{L} | \mathbf{r} \rangle$ and $\nabla C = \langle \mathbf{r} | + | \mathbf{r} \rangle$ in Lagrange equation give eigenvalue equations.

$$\mathbf{L} | \mathbf{r} \rangle = \lambda | \mathbf{r} \rangle \text{ and } \langle \mathbf{r} | \mathbf{L} = \langle \mathbf{r} | \lambda$$

On the eigen-directions the Lagrange multiplier is also the value of the quadratic form: $\lambda = Q_{\mathbf{L}}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{L} | \mathbf{r} \rangle$

for: $| \mathbf{r} \rangle = | \epsilon_1 \rangle$, $Q_{\mathbf{L}}(\mathbf{r}) = \langle \epsilon_1 | \mathbf{L} | \epsilon_1 \rangle = \epsilon_1$, and for: $| \mathbf{r} \rangle = | \epsilon_2 \rangle$, $Q_{\mathbf{L}}(\mathbf{r}) = \langle \epsilon_2 | \mathbf{L} | \epsilon_2 \rangle = \epsilon_2$.

$\langle \mathbf{r} | \mathbf{L} | \mathbf{r} \rangle$ is called an *expectation value* of matrix \mathbf{L} at \mathbf{r} . Eigenvalues are extreme expectation values.

(3) Diagonalizing transformations from projectors

The real goal of many quantum problems is to find a *d-tran matrix*, the transformation matrix that diagonalizes some quantum analyzer matrix **T** or other types of matrices not yet discussed like a scattering matrix **S** or a Hamiltonian matrix **H**. If all (meaning a complete set) of the projection matrices **P_k** are known for a given matrix **M** then the *diagonalization transformation (d-tran)* matrix is easy to get.

Here's how. First you use the columns of the **P_k** matrices to give a set of normalized eigenket vectors. This was described in the preceding section using an asymmetric ("bad cop") matrix **K** as an example and will be discussed further in the following sections. Then you load these columns into the d-tran matrix in whatever order you find convenient. That's all there is to it.

Consider that old "bad cop" matrix **K** again. Since it is asymmetric it requires an extra step you won't need for quantum matrices, but it's instructive to see this, too, given our eigenvectors (3.1.14) in Fig. 3.1.3.

$$\left\{ \langle \varepsilon_1 | = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \langle \varepsilon_2 | = \begin{pmatrix} \frac{3}{2} & \frac{1}{2} \end{pmatrix} \right\}, \left\{ | \varepsilon_1 \rangle = \begin{pmatrix} \frac{1}{2} \\ -\frac{3}{2} \end{pmatrix}, | \varepsilon_2 \rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\}$$

$(\varepsilon_1, \varepsilon_2) \leftarrow (1,2)$ *d-Tran matrix* $(1,2) \leftarrow (\varepsilon_1, \varepsilon_2)$ *INVERSE d-Tran matrix*

$$\begin{pmatrix} \langle \varepsilon_1 | 1 \rangle & \langle \varepsilon_1 | 2 \rangle \\ \langle \varepsilon_2 | 1 \rangle & \langle \varepsilon_2 | 2 \rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{3}{2} & \frac{1}{2} \end{pmatrix}, \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle & \langle 1 | \varepsilon_2 \rangle \\ \langle 2 | \varepsilon_1 \rangle & \langle 2 | \varepsilon_2 \rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2} & \frac{1}{2} \end{pmatrix}$$

Load distinct bras $\langle \varepsilon_1 |$ and $\langle \varepsilon_2 |$ into d-tran **rows**, and load kets $| \varepsilon_1 \rangle$ and $| \varepsilon_2 \rangle$ into inverse d-tran **columns**. It helps to use *Dirac labeling for all components* so actual transformation is done correctly as shown below.

$$\begin{pmatrix} \langle \varepsilon_1 | 1 \rangle & \langle \varepsilon_1 | 2 \rangle \\ \langle \varepsilon_2 | 1 \rangle & \langle \varepsilon_2 | 2 \rangle \end{pmatrix} \cdot \begin{pmatrix} \langle 1 | \mathbf{K} | 1 \rangle & \langle 1 | \mathbf{K} | 2 \rangle \\ \langle 2 | \mathbf{K} | 1 \rangle & \langle 2 | \mathbf{K} | 2 \rangle \end{pmatrix} \cdot \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle & \langle 1 | \varepsilon_2 \rangle \\ \langle 2 | \varepsilon_1 \rangle & \langle 2 | \varepsilon_2 \rangle \end{pmatrix} = \begin{pmatrix} \langle \varepsilon_1 | \mathbf{K} | \varepsilon_1 \rangle & \langle \varepsilon_1 | \mathbf{K} | \varepsilon_2 \rangle \\ \langle \varepsilon_2 | \mathbf{K} | \varepsilon_1 \rangle & \langle \varepsilon_2 | \mathbf{K} | \varepsilon_2 \rangle \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{3}{2} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 5 \end{pmatrix}$$

It is a good idea to check that your inverse-d-tran is really the inverse of your d-tran.

$$\begin{pmatrix} \langle \varepsilon_1 | 1 \rangle & \langle \varepsilon_1 | 2 \rangle \\ \langle \varepsilon_2 | 1 \rangle & \langle \varepsilon_2 | 2 \rangle \end{pmatrix} \cdot \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle & \langle 1 | \varepsilon_2 \rangle \\ \langle 2 | \varepsilon_1 \rangle & \langle 2 | \varepsilon_2 \rangle \end{pmatrix} = \begin{pmatrix} \langle \varepsilon_1 | \mathbf{1} | \varepsilon_1 \rangle & \langle \varepsilon_1 | \mathbf{1} | \varepsilon_2 \rangle \\ \langle \varepsilon_2 | \mathbf{1} | \varepsilon_1 \rangle & \langle \varepsilon_2 | \mathbf{1} | \varepsilon_2 \rangle \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{3}{2} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

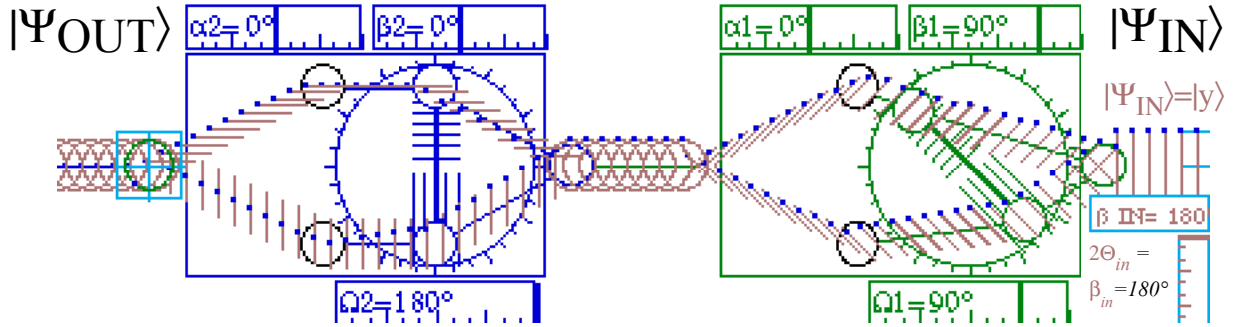
In standard quantum matrices, inverse of a d-tran matrix is its Hermitian conjugate (\dagger). (Not so above!)

$$\begin{pmatrix} \langle \varepsilon_1 | 1 \rangle & \langle \varepsilon_1 | 2 \rangle \\ \langle \varepsilon_2 | 1 \rangle & \langle \varepsilon_2 | 2 \rangle \end{pmatrix} = \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle & \langle 1 | \varepsilon_2 \rangle \\ \langle 2 | \varepsilon_1 \rangle & \langle 2 | \varepsilon_2 \rangle \end{pmatrix}^\dagger = \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle^* & \langle 2 | \varepsilon_1 \rangle^* \\ \langle 1 | \varepsilon_2 \rangle^* & \langle 2 | \varepsilon_2 \rangle^* \end{pmatrix} = \begin{pmatrix} \langle 1 | \varepsilon_1 \rangle & \langle 1 | \varepsilon_2 \rangle \\ \langle 2 | \varepsilon_1 \rangle & \langle 2 | \varepsilon_2 \rangle \end{pmatrix}^{-1}$$

The outer matrices are equal in all cases, even for "bad cop" matrix **K**. The inner matrix definition of (\dagger) can be set equal to the outer ones for unitary or Hermitian matrices like the "good cop" example **H**.

Matrix products and eigensolutions for active analyzers

Consider a 45° tilted ($\theta_1 = \beta_1/2 = \pi/4$ or $\beta_1 = 90^\circ$) analyzer followed by a untilted ($\beta_2 = 0$) analyzer shown below. Active analyzers have both paths open and a phase shift $e^{-i\Omega}$ between each path as in the examples introduced in Fig. 1.3.5. Here the first analyzer has $\Omega_1 = 90^\circ$. The second has $\Omega_2 = 180^\circ$.



The transfer matrix for each analyzer is a sum of projection operators for each open path multiplied by the phase factor that is active at that path. Here we will simply apply the entire phase factor $e^{-i\Omega_1} = e^{-i\pi/2}$ to the top path in the first analyzer and the factor $e^{-i\Omega_2} = e^{-i\pi}$ to the top path in the second analyzer.

$$T(2) = e^{-i\pi} |x\rangle\langle x| + |y\rangle\langle y| = \begin{pmatrix} e^{-i\pi} & 0 \\ 0 & 1 \end{pmatrix} \quad T(1) = e^{-i\pi/2} |x'\rangle\langle x'| + |y'\rangle\langle y'| = e^{-i\pi/2} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} \\ -\frac{1-i}{2} & \frac{1-i}{2} \end{pmatrix}$$

The matrix product $T(total) = T(2)T(1)$ relates input states $|\Psi_{IN}\rangle$ to output states: $|\Psi_{OUT}\rangle = T(total)|\Psi_{IN}\rangle$

$$T(total) = T(2)T(1) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} \\ -\frac{1-i}{2} & \frac{1-i}{2} \end{pmatrix} = \begin{pmatrix} \frac{-1+i}{2} & \frac{1+i}{2} \\ -\frac{1-i}{2} & \frac{1-i}{2} \end{pmatrix} = e^{-i\pi/4} \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \sim \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

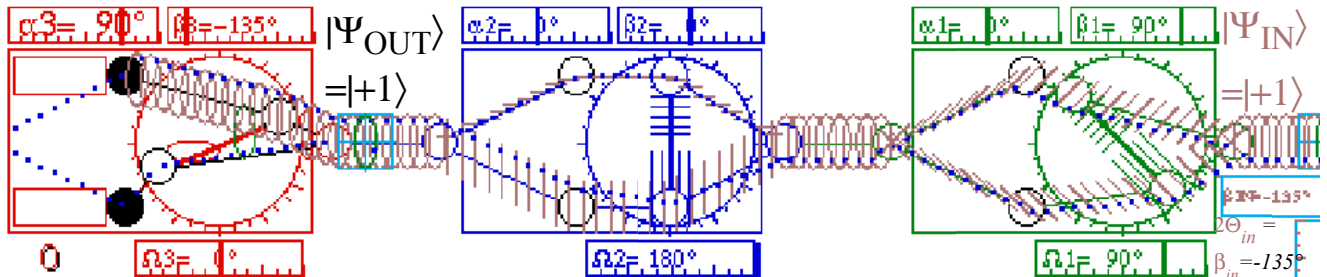
We drop the overall phase $e^{-i\pi/4}$ since it is unobservable. $T(total)$ yields two eigenvalues and projectors.

$$\lambda^2 - 0\lambda - 1 = 0, \text{ or: } \lambda = +1, -1$$

, gives projectors

$$P_{+1} = \frac{\begin{pmatrix} \frac{-1}{\sqrt{2}} + 1 & \frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} + 1 \end{pmatrix}}{1 - (-1)} = \frac{\begin{pmatrix} -1 + \sqrt{2} & i \\ -i & 1 + \sqrt{2} \end{pmatrix}}{2\sqrt{2}}, \quad P_{-1} = \frac{\begin{pmatrix} 1 + \sqrt{2} & -i \\ i & -1 + \sqrt{2} \end{pmatrix}}{2\sqrt{2}}$$

The first eigenvector $|+1\rangle = \begin{pmatrix} -1 + \sqrt{2} \\ -i \end{pmatrix} = \begin{pmatrix} 0.414 \\ -i \end{pmatrix}$ is a vertical left-handed ellipse with ratio $x:y = 0.414:1$. This eigen-ellipse must exit analyzer-2 as the same ellipse. Analyzer-3 yields $\alpha_3 = 90^\circ$ and $\beta_3 = -135^\circ$.



The other eigenvector $|-1\rangle$ is horizontal right-handed ellipse with inverse ratio $x:y = 1:2.414$ and angles $\alpha_3 = 90^\circ$ and $\beta_3 = 45^\circ$. The meaning of the electron spin angles α and β is described in section 2.10.

(c) Eigenvector projectors (Degenerate eigenvalues)

We have just shown that any matrix with distinct eigenvalues can be spectrally decomposed, i.e., diagonalized. What if the secular equation (3.1.5d) of an N -by- N matrix \mathbf{H} has some degenerate eigenvalues $\epsilon_1 = \epsilon_2 \dots = \epsilon_{\ell_1}$? If so, it is possible that \mathbf{H} cannot be completely diagonalized, though this is rarely the case. It all depends upon whether or not the HC equation (3.1.8) really needs its repeated factors. Suppose each eigenvalue ϵ_j is ℓ_j -fold degenerate so the secular equation factors as follows:

$$S(\epsilon) = 0 = (-1)^N (\epsilon - \epsilon_1)^{\ell_1} (\epsilon - \epsilon_2)^{\ell_2} \dots (\epsilon - \epsilon_p)^{\ell_p} \tag{3.1.19a}$$

where $\ell_1 + \ell_2 + \dots + \ell_p = N$. Then the N -th degree HC equation is:

$$\mathbf{0} = (-1)^N (\mathbf{H} - \epsilon_1 \mathbf{1})^{\ell_1} (\mathbf{H} - \epsilon_2 \mathbf{1})^{\ell_2} \dots (\mathbf{H} - \epsilon_p \mathbf{1})^{\ell_p} \tag{3.1.19b}$$

Each eigenvalue ϵ_j is repeated ℓ_j times as is each factor $(\mathbf{H} - \epsilon_j \mathbf{1})$ in the HC equation. The number ℓ_j is called the *degree of degeneracy* of eigenvalue ϵ_j .

Suppose, now you find that only *one* of each distinct factor is needed to give a *matrix* zero, that is, the following p -th degree equation holds.

$$\mathbf{0} = (\mathbf{H} - \epsilon_1 \mathbf{1})(\mathbf{H} - \epsilon_2 \mathbf{1}) \dots (\mathbf{H} - \epsilon_p \mathbf{1}) \tag{3.1.20}$$

This is just like the distinct eigenvalue situation in equation (3.1.8), so the matrix \mathbf{H} is completely diagonalizable and spectrally decomposable using the same techniques described previously.

(1) Minimal equation and diagonalizability criterion

Otherwise, if \mathbf{H} does not satisfy a non-degenerate equation then it is not diagonalizable. The lowest degree polynomial equation a matrix \mathbf{H} can satisfy is called its *minimal* equation. (If all roots are distinct, that is $p=N$, then the HC-equation is the minimal equation.)

When only one of each of p distinct factors $(\mathbf{H} - \epsilon_j \mathbf{1})$ in the minimal polynomial is needed to give zero, then removing that factor gives p non-zero $(p-1)$ -th degree operators $\{\mathbf{P}_1, \mathbf{P}_2, \dots, \mathbf{P}_p\}$ following (3.1.15a). They are idempotent ($\mathbf{P}_j^2 = \mathbf{P}_j$), orthogonal ($\mathbf{P}_i \mathbf{P}_j = \mathbf{0}$ if $i \neq j$) and complete ($\sum_{j=1}^p \mathbf{P}_j = \mathbf{1}$) just as in the case of no repeated roots. Here is the key *diagonalizability criterion*.

In general, an orthogonal and complete set of \mathbf{P}_j 's is possible, if and only if, the \mathbf{H} minimal equation has no repeated factors. Then and only then is matrix \mathbf{H} diagonalizable.

(2) Nilpotent operators ("Bad" degeneracy)

Repeated $(\mathbf{H} - \epsilon_j \mathbf{1})$ factors in the minimal equation are always fatal for the process of building a complete set of idempotents \mathbf{P}_j . Even one repeat is fatal, suppose:

$$\mathbf{0} = (\mathbf{H} - \epsilon_1 \mathbf{1})^2 (\mathbf{H} - \epsilon_2 \mathbf{1}) \dots, \text{ but: } \mathbf{N} = (\mathbf{H} - \epsilon_1 \mathbf{1})(\mathbf{H} - \epsilon_2 \mathbf{1}) \dots \neq \mathbf{0} \tag{3.1.21}$$

Removal of one repeat gives a non-zero operator \mathbf{N} whose square has the missing $(\mathbf{H} - \epsilon_1 \mathbf{1})$ that gives zero.

$$\mathbf{N}^2 = (\mathbf{H} - \epsilon_1 \mathbf{1})^2 (\mathbf{H} - \epsilon_2 \mathbf{1})^2 \dots = \mathbf{0}$$

(The presence of additional commuting factors $(\mathbf{H} - \varepsilon_2 \mathbf{1}) \dots$ does not save it.) Such an operator is called a *nilpotent operator* or, simply a nilpotent. A nilpotent is a troublesome and 'unwanted beast' for the basic diagonalization process but an essential feature of Non-Abelian symmetry analysis.

For example, consider a 'bad' degenerate matrix. (This is not just a "bad cop" but a real "crook"!)

$$\mathbf{B} = \begin{pmatrix} b & 1 \\ 0 & b \end{pmatrix}$$

Its secular equation has two equal roots ($\varepsilon = b$ twice).

$$S(\varepsilon) = \varepsilon^2 - 2b\varepsilon + b^2 = (\varepsilon - b)^2 = 0$$

The HC equation is then as follows.

$$S(\mathbf{B}) = \mathbf{B}^2 - 2b\mathbf{B} + b^2\mathbf{1} = (\mathbf{B} - b\mathbf{1})^2 = \mathbf{0}$$

The matrix factor

$$\mathbf{N} = \mathbf{B} - b\mathbf{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad (3.1.22)$$

is an example of nilpotent eigen-projector which satisfies

$$\mathbf{N}^2 = \mathbf{0} \text{ (but } \mathbf{N} \neq \mathbf{0} \text{) and: } \mathbf{BN} = b\mathbf{N} = \mathbf{NB}. \quad (3.1.23)$$

The nilpotent contains only one non-zero eigenket and one eigenbra.

$$|b\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \langle b| = (0 \ 1) \quad (3.1.24)$$

Also, they are orthogonal to each other! ($\langle b|b\rangle = 0$) There can be no completeness, orthonormality, spectral decomposition or diagonalization for this 'bad' degenerate matrix in the ordinary sense of (3.1.17).

Let us not give the impression that nilpotents or other "bad" matrices are not valuable for general quantum theory. In fact the operator described in (3.1.22) is an example of an *elementary operator* \mathbf{e}_{ab}

$$\mathbf{e}_{12} = |1\rangle\langle 2|$$

Along with its partners it makes up a 4-dimensional (recall Sec. 2.2d) *U(2) unit tensor operator space*

$$U(2) \text{ op-space} = \{\mathbf{e}_{11} = |1\rangle\langle 1|, \mathbf{e}_{12} = |1\rangle\langle 2|, \mathbf{e}_{21} = |2\rangle\langle 1|, \mathbf{e}_{22} = |2\rangle\langle 2|\} \quad (3.1.25a)$$

out of which all *U(2)* operators are made by linear combination. They obey a *simple matrix algebra*

$$\mathbf{e}_{ij} \mathbf{e}_{km} = \delta_{jk} \mathbf{e}_{im} \quad (3.1.25b)$$

This is very useful stuff later on. Just be aware you cannot diagonalize an \mathbf{e}_{ab} for $a \neq b$!

(3) Multiple diagonalization ("Good" degeneracy)

An example of a 'good' degenerate (but still diagonalizable) matrix is the anti-diagonal "gamma" matrix \mathbf{G} which Dirac used to generate Lorentz transformations.

$$\mathbf{G} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad (3.1.26)$$

It has a 4th degree secular equation.

$$S(\varepsilon) = 0 = \varepsilon^4 - 2\varepsilon^2 + 1 = (\varepsilon - 1)^2 (\varepsilon + 1)^2$$

There are two pairs of degenerate roots ($\varepsilon = \pm 1$, twice), but \mathbf{G} satisfies only a second degree minimal equation. (Check this!)

$$\mathbf{0} = (\mathbf{G} - \mathbf{1})(\mathbf{G} + \mathbf{1}) \quad (3.1.27)$$

This allows us to use theory based on projection formula (3.1.15) to derive two projection operators.

$$\mathbf{P}_1^G = \frac{\mathbf{G} - (-1)\mathbf{1}}{1 - (-1)} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad (3.1.28a)$$

$$\mathbf{P}_{-1}^G = \frac{\mathbf{G} - (1)\mathbf{1}}{-1 - (1)} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \quad (3.1.28b)$$

These satisfy all orthonormality and completeness or spectral decomposition relations (3.1.15a-d).

The main difference here is that each of these projectors contains two linearly independent ket vectors: from the first and second columns of \mathbf{P}_1 we get $|1_1\rangle$ and $|1_2\rangle$, and from \mathbf{P}_{-1} we get $|-1_1\rangle$ and $|-1_2\rangle$. (Recall that we showed in (3.1.20)_{example H} that each \mathbf{P}_j contains all the scalar products and normalization constants of its bra-rows and ket-columns.)

$$|1_1\rangle = \frac{|1_1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad |1_2\rangle = \frac{|1_2\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \quad |-1_1\rangle = \frac{|-1_1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \quad |-1_2\rangle = \frac{|-1_2\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \quad (3.1.29)$$

This example is particularly convenient since the $(1|2)$ components $(\mathbf{P}_j)_{12}$ happen to be zero, and therefore first and second rows are already orthogonal ($(j_1|j_2) = 0$). Otherwise we would need to orthogonalize to get a second orthonormal eigenket. Such a process is called *Gram-Schmidt orthogonalization* which is described below.

Gram-Schmidt orthogonalization

Suppose a non-zero scalar product $(\langle j_1 | j_2 \rangle \neq 0)$ exists between two vectors. Then we would need to orthogonalize to get a second orthonormal eigenket

$$|j_{\text{normal } 2}\rangle = N_1 |j_1\rangle + N_2 |j_2\rangle \quad (3.1.30a)$$

such that

$$\begin{aligned} \langle j_1 | j_{\text{normal } 2} \rangle &= 0 = N_1 \langle 1|1 \rangle + N_2 \langle 1|2 \rangle \\ \langle j_{\text{normal } 2} | j_{\text{normal } 2} \rangle &= 1 = N_1^2 \langle 1|1 \rangle + N_1 N_2 (\langle 1|2 \rangle + \langle 2|1 \rangle) + N_2^2 \langle 2|2 \rangle \end{aligned}$$

As we noted the a-row and b-column scalar product matrix is just the \mathbf{P}_j matrix, itself.

$$(a|b) = (\mathbf{P}_j)_{ab}$$

$(a|b)$ is sometimes called a *Grammian* matrix. Solving for (3.1.30a) coefficients gives

$$N_1 = -N_2 \frac{\langle 1|2 \rangle}{\langle 1|1 \rangle} \quad \text{where } N_2 = \sqrt{\frac{1}{\langle 2|2 \rangle - \frac{\langle 1|2 \rangle \langle 2|1 \rangle}{\langle 1|1 \rangle}}} \quad (3.1.30b)$$

This Gram Schmidt orthonormalization (3.1.30) is not a unique solution since any linear combination of degenerate eigenvectors is still an eigenvector. To help sort this out we consider below a more elegant procedure using spectral decomposition.

(d) Projector splitting: A key to algebraic reduction

Dirac notation for the \mathbf{G} example completeness relation using eigenvectors (3.1.29) is the following:

$$1 = \mathbf{P}_1^G + \mathbf{P}_{-1}^G = |1_1\rangle\langle 1_1| + |1_2\rangle\langle 1_2| + |-1_1\rangle\langle -1_1| + |-1_2\rangle\langle -1_2| \quad (3.1.31a)$$

$$= \mathbf{P}_{1_1} + \mathbf{P}_{1_2} + \mathbf{P}_{-1_1} + \mathbf{P}_{-1_2} \quad (3.1.32b)$$

Here the original projection operators (3.1.28) have each been “split” in two.

$$\begin{aligned} \mathbf{P}_1^G = \mathbf{P}_{1_1} + \mathbf{P}_{1_2} &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= |1_1\rangle\langle 1_1| + |1_2\rangle\langle 1_2| \end{aligned} \quad (3.1.32c)$$

$$\begin{aligned} \mathbf{P}_{-1}^G = \mathbf{P}_{-1_1} + \mathbf{P}_{-1_2} &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= |-1_1\rangle\langle -1_1| + |-1_2\rangle\langle -1_2| \end{aligned} \quad (3.1.32d)$$

Idempotent *projector splitting*, such as (3.1.32c-d), is an important process in the application of symmetry groups to quantum theory. Our first examples are the completeness splitting of the unit operator $\mathbf{1}$. Let us now see the power of splitting algebra and an important technique in symmetry analysis.

Suppose we are given two mutually commuting matrix operators: the \mathbf{G} from (3.1.26) before, and another operator \mathbf{H} .

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix} \tag{3.1.33}$$

(First, it is important to verify that they do, in fact, commute.)

$$\mathbf{GH} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \mathbf{HG} \tag{3.1.34}$$

This implies that the projection \mathbf{P}_g^G operators (3.1.28) of \mathbf{G} commute with any new projection operators \mathbf{P}_k^H generated by \mathbf{H} . This will lead to a combined set \mathbf{P}^{GH} which simultaneously spectrally decomposes both \mathbf{G} and \mathbf{H} . The new \mathbf{P}_k^H operators follow from the secular and minimal equations for \mathbf{H} .

$$\begin{aligned} \mathbf{P}_2^H &= \frac{(\mathbf{H} - (-2)\mathbf{1})}{2 - (-2)} & \mathbf{P}_{-2}^H &= \frac{(\mathbf{H} - (2)\mathbf{1})}{-2 - (2)} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} & & = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix} \end{aligned} \tag{3.1.35a}$$

These obey the following completeness relations and spectral decomposition for \mathbf{G} and \mathbf{H} , separately.

$$\mathbf{1} = \mathbf{P}_1^G + \mathbf{P}_{-1}^G \qquad \mathbf{1} = \mathbf{P}_2^H + \mathbf{P}_{-2}^H \tag{3.1.35b}$$

$$\mathbf{G} = (1)\mathbf{P}_1^G + (-1)\mathbf{P}_{-1}^G \qquad \mathbf{H} = (2)\mathbf{P}_2^H + (-2)\mathbf{P}_{-2}^H \tag{3.1.35c}$$

The old "1=1·1 trick"

By multiplying the two completeness relations one obtains a set of projectors that, together, satisfy orthonormality (because $\mathbf{P}_j^G \mathbf{P}_k^H = \mathbf{P}_k^H \mathbf{P}_j^G$) and completeness (because $\mathbf{1} = \mathbf{1} \cdot \mathbf{1}$).

$$\mathbf{1} = \mathbf{1} \cdot \mathbf{1} = (\mathbf{P}_1^G + \mathbf{P}_{-1}^G)(\mathbf{P}_2^H + \mathbf{P}_{-2}^H) \tag{3.1.36a}$$

$$\mathbf{1} = (\mathbf{P}_1^G \mathbf{P}_2^H + \mathbf{P}_1^G \mathbf{P}_{-2}^H + \mathbf{P}_{-1}^G \mathbf{P}_2^H + \mathbf{P}_{-1}^G \mathbf{P}_{-2}^H) \tag{3.1.36b}$$

(We call this the *'the old one-equals-one-times-one'* trick!) Matrix multiplication gives four new operators which in this case are orthonormal and complete projectors.

$$\begin{aligned}
\mathbf{P}_{1,2}^{GH} \equiv \mathbf{P}_1^G \mathbf{P}_2^H = & \quad \mathbf{P}_{1,-2}^{GH} \equiv \mathbf{P}_1^G \mathbf{P}_{-2}^H = & \quad \mathbf{P}_{-1,2}^{GH} \equiv \mathbf{P}_{-1}^G \mathbf{P}_2^H = & \quad \mathbf{P}_{-1,-2}^{GH} \equiv \mathbf{P}_{-1}^G \mathbf{P}_{-2}^H = \\
\frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} & \quad \frac{1}{4} \begin{pmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} & \quad \frac{1}{4} \begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix} & \quad \frac{1}{4} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}
\end{aligned}
\tag{3.1.37a}$$

(This isn't the way it always works out. Some may come out zero, but the ones that are not zero must be orthonormal idempotent projectors.) Each is automatically an eigen-operator of both \mathbf{G} and \mathbf{H} . (Note: \mathbf{H} commutivity is needed!)

$$\mathbf{G}\mathbf{P}_{g,h}^{GH} = \mathbf{G}\mathbf{P}_g^G \mathbf{P}_h^H = \varepsilon_g^G \mathbf{P}_{g,h}^{GH}
\tag{3.1.37b}$$

$$\mathbf{H}\mathbf{P}_{g,h}^{GH} = \mathbf{H}\mathbf{P}_g^G \mathbf{P}_h^H = \mathbf{P}_g^G \mathbf{H}\mathbf{P}_h^H = \varepsilon_h^H \mathbf{P}_{g,h}^{GH}
\tag{3.1.37c}$$

Thus, the $\mathbf{P}_{j,k}^{GH}$ spectrally decompose both \mathbf{G} and \mathbf{H} , simultaneously.

$$\mathbf{G} = (1)\mathbf{P}_{1,2}^{GH} + (1)\mathbf{P}_{1,-2}^{GH} + (-1)\mathbf{P}_{-1,2}^{GH} + (-1)\mathbf{P}_{-1,-2}^{GH}
\tag{3.1.37d}$$

$$\mathbf{H} = (2)\mathbf{P}_{1,2}^{GH} + (-2)\mathbf{P}_{1,-2}^{GH} + (2)\mathbf{P}_{-1,2}^{GH} + (-2)\mathbf{P}_{-1,-2}^{GH}
\tag{3.1.37e}$$

So, by simple matrix multiplication we have accomplished an idempotent splitting like that in (3.1.32) without needing to Gram-Schmidt orthogonalize bra-kets. (Yes!)

$$\mathbf{P}_1^G = \mathbf{P}_{1,2}^{GH} + \mathbf{P}_{1,-2}^{GH}
\tag{3.1.38a}$$

$$\mathbf{P}_{-1}^G = \mathbf{P}_{-1,2}^{GH} + \mathbf{P}_{-1,-2}^{GH}
\tag{3.1.38b}$$

Most important, the splitting is “just right” for the new \mathbf{H} matrix; finding the “right” Gram-Schmidt combination (3.1.30) to diagonalize both \mathbf{H} and \mathbf{G} at once, would require even more calculation.

In this case, no further idempotent splitting of (3.1.36b) is possible. For N -by- N matrix operators there can have no more than N linearly independent eigenvectors and no more than N orthonormal projectors. Each $\mathbf{P}_{g,h}^{GH}$ in (1.2.50c) has in its columns and rows one and only one independent eigenvector. Such an ‘unsplittable’ projector is called an *irreducible* idempotent or projector.

You can tell how many irreducible projectors are "hiding" inside a given idempotent projector \mathbf{P} (*reducible*) matrix by taking its trace. This *splitting number* is equal to the trace.

$$\text{Splitting number} = \text{Trace}\mathbf{P}(\text{reducible}) = \text{Number of irreducible projectors in } \mathbf{P}
\tag{3.1.39}$$

Irreducible projectors have unit trace!

$$\text{Trace}\mathbf{P}(\text{irreducible}) = 1
\tag{3.1.40}$$

Each of (3.1.37c) projectors have a unit trace as they should.

Note that such a complete splitting as we saw in (3.1.37) was not guaranteed. It depends on what \mathbf{H} operator we chose to do the splitting. It could have happened that one or more of the $\mathbf{P}_g^G \mathbf{P}_h^H = \mathbf{P}_{g,h}^{GH}$ products in (3.1.37b) came out to be zero. Then some of the non-zero $\mathbf{P}_{g,h}^{GH}$ will not be irreducible. Suppose, for example, we chose $\mathbf{H} = 2\mathbf{G}$: then $\mathbf{P}_{1,-2}^{GH}$ and $\mathbf{P}_{-1,2}^{GH}$ are zero while $\mathbf{P}_{1,2}^{GH} = \mathbf{P}_1^G$ and $\mathbf{P}_{-1,-2}^{GH} = \mathbf{P}_{-1}^G$ remain reducible.

Having a set of N irreducible \mathbf{G} and \mathbf{H} projectors like (3.1.37) is useful since any N -by- N operator \mathbf{K} which commutes with \mathbf{G} and \mathbf{H} must share exactly the same N projectors no matter what is the form of \mathbf{K} 's individual completeness relation.

$$\mathbf{1} = \sum_{k=1}^n \mathbf{P}_k^K \quad (n \leq N)$$

To see this note that a product of \mathbf{K} completeness relation by $\mathbf{P}_{g,h}^{GH}$ must have one *and only one* non-zero term.

$$\mathbf{P}_{gh}^{GH} = \sum_{k=1}^N \mathbf{P}_{g,h}^{GH} \mathbf{P}_k^K = \mathbf{P}_{g,h}^{GH} \mathbf{P}_k^K \quad (3.1.41)$$

Since $\mathbf{P}_{g,h}^{GH}$ is irreducible it cannot split into new orthogonal idempotent projectors, and this implies that each $\mathbf{P}_{g,h}^{GH}$ is already an eigen-operator for \mathbf{K} .

$$\mathbf{K} \mathbf{P}_{g,h}^{GH} = \mathbf{P}_{g,h}^{GH} \mathbf{K} \mathbf{P}_{k'}^K = \left(\epsilon_{k'}^K \right) \mathbf{P}_{g,h}^{GH} \quad (3.1.42)$$

We will then have diagonalized \mathbf{K} with less mathematical labor than the old Gram-Schmidt methods.

(e) Why symmetry groups are useful

The results ending with (3.1.42) illustrate an important symmetry technique. Imagine you wanted to diagonalize a complicated matrix \mathbf{K} and knew that it commutes with some other operators \mathbf{G} and \mathbf{H} for which irreducible projectors are more easily found. Then you don't have to bother with the secular equation of \mathbf{K} and may just multiply \mathbf{K} by the projectors provided by \mathbf{G} and \mathbf{H} as in (3.1.42) above.

In later chapters we will see how having a group of operators $\{ \mathbf{G}, \mathbf{H}, \dots \}$ that commute with a big system matrix \mathbf{K} helps to reduce its secular equation and sometimes solve it completely. When transformation operators $\mathbf{G}, \mathbf{H}, \dots$ (like rotations) commute with an analyzer matrix $\mathbf{T}=\mathbf{K}$ (or other type of quantum system matrix \mathbf{K}) it means that

$$\mathbf{K} \mathbf{G} = \mathbf{G} \mathbf{K} \quad \text{or} \quad \mathbf{G}^\dagger \mathbf{K} \mathbf{G} = \mathbf{K} \quad \text{or} \quad \mathbf{G} \mathbf{K} \mathbf{G}^\dagger = \mathbf{K} \quad (3.1.43)$$

which means \mathbf{K} is *invariant* to the transformation induced by \mathbf{G} . This is called a *symmetry* of the system \mathbf{K} stands for and it is often pretty easy to spot. The group of these operators is called a *symmetry group*.

Entire groups can be spectrally decomposed into irreducible projection operators, and then these can be used to decompose the system matrix \mathbf{K} into one set of \mathbf{P} 's made of \mathbf{G}, \mathbf{H} , symmetry operators.

More to the point, because \mathbf{K} is a spectral combination (3.1.15c) of \mathbf{P} 's and \mathbf{P} 's are in turn combinations (3.1.15a) or (3.1.37) of powers and products of $\mathbf{G}, \mathbf{H}, \dots$ it follows that \mathbf{K} is a *linear combination of its own group of symmetry operators*, including $\mathbf{G}, \mathbf{H}, \dots$ and their products. This is a very powerful idea! It will be useful in some problems and then be used extensively following Unit 3.

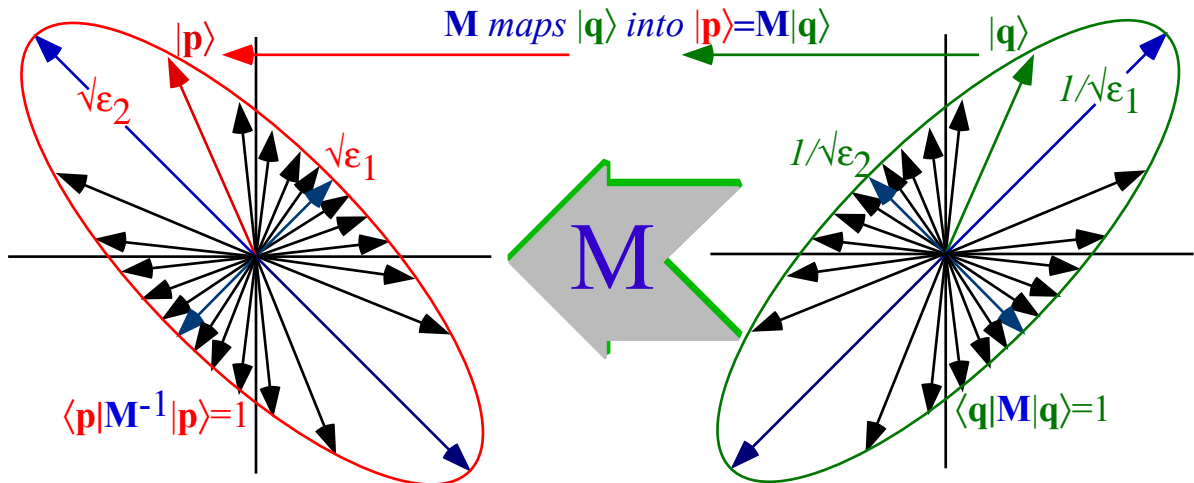
To summarize, we use the spectral decomposition of some easily "killed" operators to attack more difficult ones, much as a "killed" virus in a vaccine saves us from suffering troublesome or dangerous diseases.

Quadratic surfaces help to visualize matrix operations

The mapping $M|c\rangle=|r\rangle$ of a unit circle $\langle c|c\rangle=1$ by symmetric matrix M is an ellipse $I=\langle r|M^{-2}|r\rangle$ as shown in a previous sidebar. If, instead of mapping vectors $|c\rangle$ on a circle, we map vectors $|q\rangle$ on a surface corresponding to a unit constant *quadratic form* $I = \langle q|M|q\rangle$, the resulting vectors $|p\rangle = M|q\rangle$ of this mapping will lie on a related quadratic surface given by

$$I = \langle q|M|q\rangle = \langle q|p\rangle = \langle p|M^{-1}|p\rangle$$

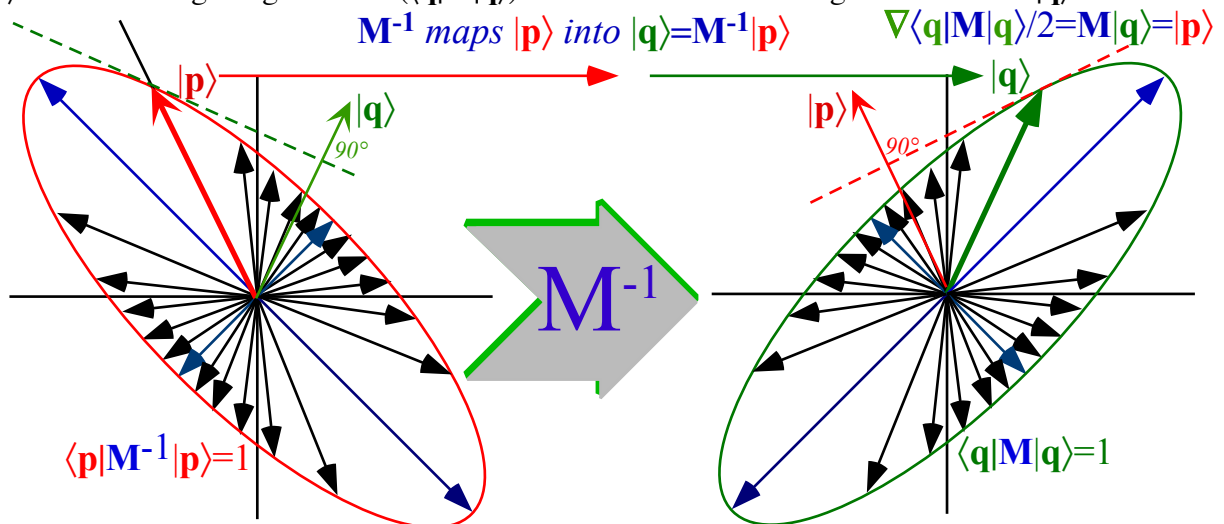
The surface $I = \langle p|M^{-1}|p\rangle$ defined by vectors $|p\rangle$ is called the conjugate or *inverse quadratic form*. An example of such a mapping is displayed in the figure below. The semi-axes of the $|p\rangle$ ellipse are square roots of eigenvalues $\sqrt{\epsilon_1}$ and $\sqrt{\epsilon_2}$ while $|q\rangle$ ellipse axes are inverse roots $1/\sqrt{\epsilon_1}$ and $1/\sqrt{\epsilon_2}$.



The precise geometry of this mapping is found by considering the gradient of the quadratic curves.

$$\nabla(\langle q|M|q\rangle)=\langle q|M + M|q\rangle = 2 M|q\rangle = 2 |p\rangle$$

Let matrix M be real symmetric so there is no distinction between bras and kets. This shows that the mapped vector $|p\rangle$ must lie along the gradient $\nabla(\langle q|M|q\rangle)$ that is normal to the tangent to curve at $|q\rangle$.



The inverse map works in the same way since $|q\rangle$ is normal to the tangent at mapped point $|p\rangle$. It should be noted that quadratic surfaces can be hyperbolic as well as elliptic if there are negative eigenvalues. Eigenvectors are any vectors that are in the same direction as quadratic curve gradient at their point.

3.2 Approximate Eigensolutions by Perturbation Techniques

One of the alternatives to numerical diagonalization or symmetry analysis techniques is called *perturbation analysis*. This often is a viable alternative for problems with little or no symmetry because such problems usually do not have resonances or degeneracies that often come with having symmetry. Then eigenvalues and vectors may change by only tiny amounts that can be approximated.

Perturbation techniques, like most "approximologies" are many and varied. Their use can be more art than a science. We discuss one here based upon analysis of the secular determinant (3.1.5d).

$$0 = \det|\mathbf{H} - \lambda\mathbf{1}| = \det \begin{vmatrix} H_{11} - \lambda & H_{12} & H_{13} & H_{14} & \cdots \\ H_{21} & H_{22} - \lambda & H_{23} & H_{24} & \cdots \\ H_{31} & H_{32} & H_{33} - \lambda & H_{34} & \cdots \\ H_{41} & H_{42} & H_{43} & H_{44} - \lambda & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} = \det \begin{vmatrix} D_{11} & D_{12} & D_{13} & D_{14} & \cdots \\ D_{21} & D_{22} & D_{23} & D_{24} & \cdots \\ D_{31} & D_{32} & D_{33} & D_{34} & \cdots \\ D_{41} & D_{42} & D_{43} & D_{44} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix}$$

where:

$$D_{\mu\nu} = \begin{cases} H_{\mu\mu} - \lambda & \text{if: } \mu=\nu \\ H_{\mu\nu} & \text{if: } \mu \neq \nu \end{cases} = H_{\mu\nu} - \delta_{\mu\nu}\lambda \quad (3.2.1)$$

(a) Secular determinantal expansion

The ϵ -tensor sum of permutations reviewed in Appendix 3.A-B. We do the sum class by class since each class of permutation is either all even (+) or all odd (-). We'll show only the terms for $N=4$.

$$0 = \det|\mathbf{H} - \lambda\mathbf{1}| = \sum_{perm} \epsilon_{\alpha\beta\gamma\delta} \dots D_{1\alpha} D_{2\beta} D_{3\gamma} D_{4\delta} \dots \quad (3.2.2)$$

First there is the "zero-flip" term corresponding to partition 1+1+1+1...

$$0 = \det|\mathbf{H} - \lambda\mathbf{1}| = D_{11} D_{22} D_{33} D_{44} \dots = (H_{11} - \lambda)(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda) \dots \quad (3.2.3a)$$

Then we subtract (odd) "one-flip" terms corresponding to partition 2+1+1... (There are $N(N-1)/2$ of these)

$$\begin{aligned} \dots - I(12) - I(13) - I(14) \dots &= \dots - H_{12} H_{21} D_{33} D_{44} - H_{13} D_{22} H_{31} D_{44} - H_{14} D_{22} D_{33} H_{41} \dots \\ - I(23) - I(24) \dots &\quad - D_{11} H_{23} H_{32} D_{44} - D_{11} H_{24} D_{33} H_{42} \dots \\ - I(34) \dots &\quad - D_{11} D_{22} H_{34} H_{43} \dots \end{aligned} \quad (3b)$$

Add the "two-flip" terms corresponding to partition 3+1... (There are $N(N-1)(N-2)/3$ of these.) Recall that (143) = (314) = (431) means, "1 goes where 4 was, 4 goes where 3 was, and 3 goes where 1 was," and the inverse is (143)⁻¹ = (134) = (341) = (413). It's called "two-flip" because (abc) = (ac)(bc) is two flips.

$$\begin{aligned} \dots + I(123) + I(124) + I(134) + I(234) \dots &= \dots + H_{13} H_{21} H_{32} D_{44} + H_{14} H_{21} D_{33} H_{42} + H_{14} D_{22} H_{31} H_{43} + D_{11} H_{24} H_{32} H_{43} \dots \\ \dots + I(132) + I(142) + I(143) + I(243) \dots &= \dots + H_{12} H_{23} H_{31} D_{44} + H_{12} H_{24} D_{33} H_{41} + H_{13} D_{22} H_{34} H_{41} + D_{11} H_{23} H_{34} H_{42} \dots \end{aligned} \quad (3c)$$

Add the "two-flip" terms corresponding to partition 2+2... (There are $N(N-1)(N-2)(N-3)/8$ of these.)

$$\dots + I(12)(34) + I(13)(24) + I(14)(23) \dots = \dots + H_{12} H_{21} H_{34} H_{43} + H_{13} H_{24} H_{31} H_{42} + H_{14} H_{23} H_{32} H_{41} + \dots \quad (3d)$$

Finally, (if N were really 4) subtract (odd) "three-flip" terms. (There are $N(N-1)(N-2)(N-3)/4$ of these.)

$$\begin{aligned} & \cdot - I(1234) - I(1324) - I(1423) \dots = \cdot - H_{14}H_{22}H_{32}H_{43} - H_{14}H_{23}H_{31}H_{42} - H_{13}H_{24}H_{32}H_{41} \dots \\ & \cdot - I(1432) - I(1423) - I(1324) \dots = \cdot - H_{12}H_{23}H_{34}H_{41} - H_{13}H_{24}H_{32}H_{41} - H_{14}H_{23}H_{31}H_{42} \dots \end{aligned} \quad (3e)$$

Collect these results and replace diagonal D_{mm} factors with $H_{mm}-\lambda$.

$$0 = (H_{11} - \lambda)(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda) \dots \quad (3.2.4a)$$

and include the $N(N-1)/2=6$ terms for "one-flip" partition 2+1+1...

$$\begin{aligned} \dots - H_{12}H_{21}(H_{33} - \lambda)(H_{44} - \lambda) - H_{13}(H_{22} - \lambda)H_{31}(H_{44} - \lambda) - H_{14}(H_{22} - \lambda)(H_{33} - \lambda)H_{41} \dots \\ - (H_{11} - \lambda)H_{23}H_{32}(H_{44} - \lambda) - (H_{11} - \lambda)H_{24}(H_{33} - \lambda)H_{42} \dots \\ - (H_{11} - \lambda)(H_{22} - \lambda)H_{34}H_{43} \dots \end{aligned} \quad (4b)$$

and the $N(N-1)(N-2)/3=8$ terms for "two-flip" partition 3+1...

$$\begin{aligned} \dots + H_{13}H_{21}H_{32}(H_{44} - \lambda) + H_{14}H_{21}(H_{33} - \lambda)H_{42} + H_{14}(H_{22} - \lambda)H_{31}H_{43} + (H_{11} - \lambda)H_{24}H_{32}H_{43} \dots \\ + H_{12}H_{23}H_{31}(H_{44} - \lambda) + H_{12}H_{24}(H_{33} - \lambda)H_{41} + H_{13}(H_{22} - \lambda)H_{34}H_{41} + (H_{11} - \lambda)H_{23}H_{34}H_{42} \dots \end{aligned} \quad (4c)$$

and the $N(N-1)(N-2)(N-4)/8=3$ terms for the other "two-flip" partition 2+2...

$$\dots + H_{12}H_{21}H_{34}H_{43} + H_{13}H_{24}H_{31}H_{42} + H_{14}H_{23}H_{32}H_{41} + \dots \quad (4.d)$$

and, finally the $N(N-1)(N-2)(N-4)/4=6$ terms (for $N=4$) "three-flip" partition 4...

$$\begin{aligned} \dots - H_{14}H_{22}H_{32}H_{43} - H_{14}H_{23}H_{31}H_{42} - H_{13}H_{24}H_{32}H_{41} \dots \\ - H_{12}H_{23}H_{34}H_{41} - H_{13}H_{24}H_{32}H_{41} - H_{14}H_{23}H_{31}H_{42} \dots \end{aligned} \quad (4.e)$$

(b) Perturbation approximations

Now we look at the art of approximation. Suppose we want to approximate the one unknown eigenvalue $\lambda = E_I$ closest to the known \mathbf{H} -matrix diagonal element H_{11} . Suppose further that all the other diagonal differences $|H_{11} - H_{22}|$, $|H_{22} - H_{33}|$, $|H_{33} - H_{44}|$, ... are larger than the magnitudes off-diagonal matrix elements H_{12} , H_{13} , ..., H_{24} , H_{34} , etc. Then we can divide the secular equation by the large factors $(H_{22} - \lambda)$ $(H_{33} - \lambda)$ $(H_{44} - \lambda)$ and leave behind the (supposedly) small factor $(H_{11} - \lambda)$. Then we collect terms on the right hand side $(H_{11} - \lambda)$ terms that can be discarded since they should be tiny.

$$\begin{aligned} 0 = (H_{11} - \lambda) & - \frac{H_{12}H_{21}}{(H_{22} - \lambda)} - \frac{H_{13}H_{31}}{(H_{33} - \lambda)} - \frac{H_{14}H_{41}}{(H_{44} - \lambda)} \dots & - \frac{(H_{11} - \lambda)H_{23}H_{32}}{(H_{22} - \lambda)(H_{33} - \lambda)} - \frac{(H_{11} - \lambda)H_{24}H_{42}}{(H_{22} - \lambda)(H_{44} - \lambda)} \\ & (\Updownarrow \text{"keepers"} \Updownarrow) & (\Updownarrow \text{"discards"} \Updownarrow) - \frac{(H_{11} - \lambda)H_{34}H_{43}}{(H_{33} - \lambda)(H_{44} - \lambda)} \\ \dots + \frac{H_{12}H_{23}H_{31} + H_{13}H_{32}H_{21}}{(H_{22} - \lambda)(H_{33} - \lambda)} & + \frac{H_{12}H_{24}H_{41} + H_{14}H_{42}H_{21}}{(H_{22} - \lambda)(H_{44} - \lambda)} \dots & + \frac{(H_{11} - \lambda)(H_{23}H_{34}H_{42} + H_{24}H_{43}H_{32})}{(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda)} \\ & + \frac{H_{13}H_{34}H_{41} + H_{14}H_{43}H_{31}}{(H_{33} - \lambda)(H_{44} - \lambda)} + \dots \\ \dots + \frac{H_{12}H_{21}H_{34}H_{43} + H_{13}H_{24}H_{31}H_{42} + H_{14}H_{23}H_{32}H_{41}}{(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda)} & + \dots \end{aligned}$$

$$\frac{-H_{14}H_{43}H_{32}H_{22} - H_{14}H_{42}H_{23}H_{31} - H_{13}H_{32}H_{24}H_{41}\dots}{(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda)}$$

$$\frac{-H_{12}H_{23}H_{34}H_{41} - H_{13}H_{32}H_{24}H_{41} - H_{14}H_{42}H_{23}H_{31}\dots}{(H_{22} - \lambda)(H_{33} - \lambda)(H_{44} - \lambda)}$$

Now we have an equation for the unknown perturbed eigenvalue λ with one more approximation, that is, to replace every λ in the "keeper" denominators by the approximate energy $\lambda \sim H_{11} = E_1^{(0)}$. (In fact, this substitution kills the "discard" terms.)

$$\lambda = H_{11} - \frac{H_{12}H_{21}}{(H_{22} - H_{11})} - \frac{H_{13}H_{31}}{(H_{33} - H_{11})} - \frac{H_{14}H_{41}}{(H_{44} - H_{11})} \dots$$

$$\dots + \frac{H_{12}H_{23}H_{31} + H_{13}H_{32}H_{21}}{(H_{22} - H_{11})(H_{33} - H_{11})} + \frac{H_{12}H_{24}H_{41} + H_{14}H_{42}H_{21}}{(H_{22} - H_{11})(H_{44} - H_{11})} + \frac{H_{13}H_{34}H_{41} + H_{14}H_{43}H_{31}}{(H_{33} - H_{11})(H_{44} - H_{11})} \dots$$

The terms that are fourth order in H_{mn} are left off above, but included below in the final result.

$$\lambda = E_1 + \sum_{j \neq 1}^N \frac{H_{1j}H_{j1}}{(E_1 - E_j)} + \sum_{j \neq 1}^N \sum_{k \neq 1, j}^N \frac{H_{1j}H_{jk}H_{k1}}{(E_1 - E_j)(E_1 - E_k)} + \sum_{j=1}^N \sum_{k \neq j}^N \sum_{\ell \neq j, k}^N \frac{H_{1j}H_{jk}H_{k\ell}H_{\ell 1}}{(E_1 - E_j)(E_1 - E_k)(E_1 - E_\ell)} \dots$$

(3.2.5a)

Here the diagonal terms are denoted as approximate eigenvalues:

$$E_m = H_{mm} \tag{3.2.5b}$$

A diagrammatic representation of this is given in Fig. 3.2.1. Note that the choice of the number-1 value is arbitrary. This approximation works just as well replacing 1 by 2, 3, ..., or N . The figure indicates number 1 as the lowest eigenvalue but that is not a necessary condition, either. Neither are all the terms in the order chosen for the figure; it shows only one of many combinations and permutations of the 3rd and 4th order terms.

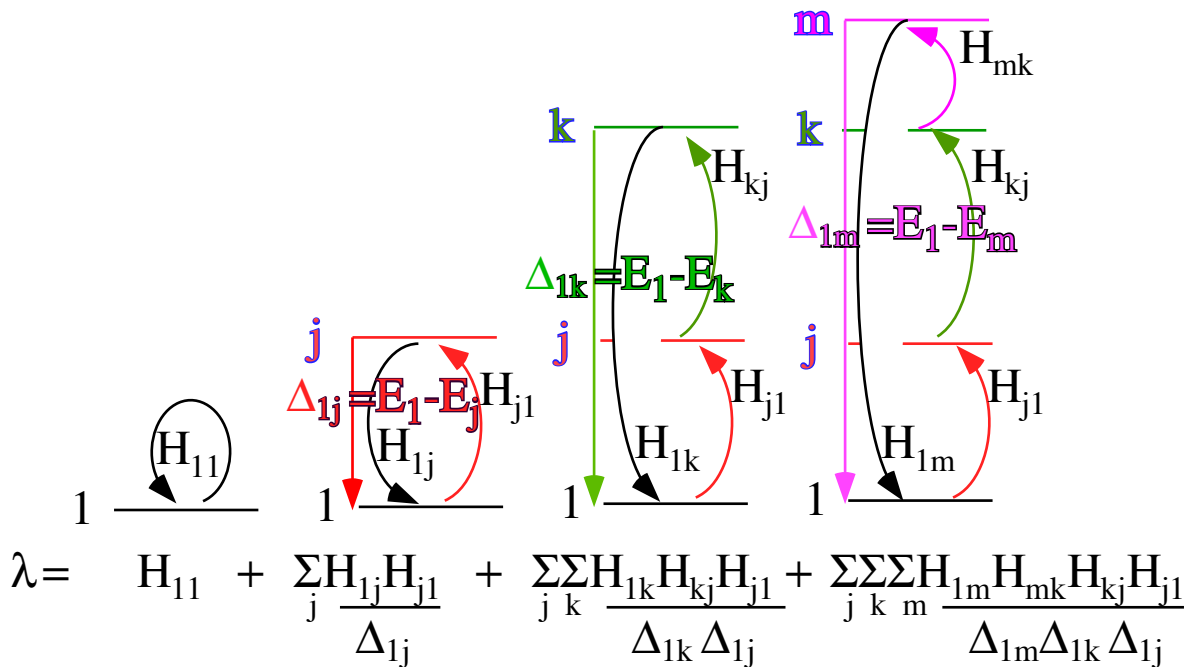


Fig. 3.2.1 Diagrammatic description of perturbation series

Later, in Chapter 9, we will show how the eigenvalues of the Hamiltonian energy matrix \mathbf{H} correspond to quantized energy levels E_j and energy eigenstates $|\epsilon_j\rangle$. According to this we interpret each perturbation term as tracing a path or circuit between the approximate eigenvalues $E_j = H_{jj}$ which correspond to, as yet, imprecisely defined energy states $|\epsilon_j\rangle$ which are initially nothing but the original base states $|\epsilon_j\rangle \sim |j\rangle$ for the problem.

Each path begins and ends on the level that one is interested in defining more precisely. (In Fig. 3.2.1 it is called level E_l .) The path visits a number of intermediate levels $E_m = H_{mm}$ once (and only once) and each one has what is called an *energy* or *resonance denominator*

$$\Delta_m = E_l - E_m = H_{ll} - H_{mm} \quad (3.2.6)$$

This determines, along with matrix element products $H_{km}H_{mj}$, a contributing factor $H_{km}H_{mj} / \Delta_m$ for the intermediate base state $|\epsilon_m\rangle \sim |m\rangle$ to the energy correction for that path. Obviously, a zero or near-zero energy denominator Δ_m would signal a major or infinite contribution of one path and one base state. Unfortunately, it would also signal the invalidity of the perturbation approximation.

(c) Testing perturbation approximation with exact 2x2 eigenvalues

In order to see how well perturbation theory works, it helps to compare its lowest order predictions with that of direct and exact diagonalization. By choosing a simple two-by-two matrix such as

$$\mathbf{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix}, \quad (3.2.7)$$

this test is easy to do. We choose off-diagonal V to be real to make it even easier.

First, do the perturbation calculation. (It's often the first thing to try!) Up to second order we have the following approximate eigenvalues using (3.2.5) to the second order term.

$$\begin{aligned} \lambda_1 &= E_1 + \frac{V^2}{E_1 - E_2}, \\ \lambda_2 &= E_2 + \frac{V^2}{E_2 - E_1}. \end{aligned} \quad (3.2.8)$$

Then the exact calculation starts with the secular equation (3.1.5).

$$\lambda^2 - (\text{Trace}\mathbf{H})\lambda + \det|\mathbf{H}| = 0 = \lambda^2 - (E_1 + E_2)\lambda + (E_1E_2 - V^2) \quad (3.2.9a)$$

The two roots are

$$\lambda_{1,2} = \frac{E_1 + E_2 \pm \sqrt{(E_1 + E_2)^2 - 4E_1E_2 + 4V^2}}{2} = \frac{E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4V^2}}{2}, \quad (3.2.9b)$$

The comparison is made by assuming (as in (3.2.5)) that V is small compared to $|E_1 - E_2|$. Then the binomial approximation $(a+b)^{1/2} \sim a^{1/2} + b/(2a^{1/2})$...gives

$$\lambda_{1,2} = 1/2 \left(E_1 + E_2 \pm (E_1 - E_2) \pm 4V^2 / (2(E_1 - E_2)) \right), \quad (3.2.9c)$$

which agrees perfectly with second order perturbation approximation (3.2.8).

The results are plotted in Fig. 3.2.2 below to show the differences. The 2nd order perturbation approximation fits a parabola to the exact hyperbola of each eigenvalue trace versus the off-diagonal element V . As expected, the perturbation approximation deviates as the off-diagonal matrix element V increases. However, it would improve with an increase in the difference $|E_1 - E_2|$, the two are related and it is a larger ratio of V to $|E_1 - E_2|$ that will make a perturbation approximation less accurate.

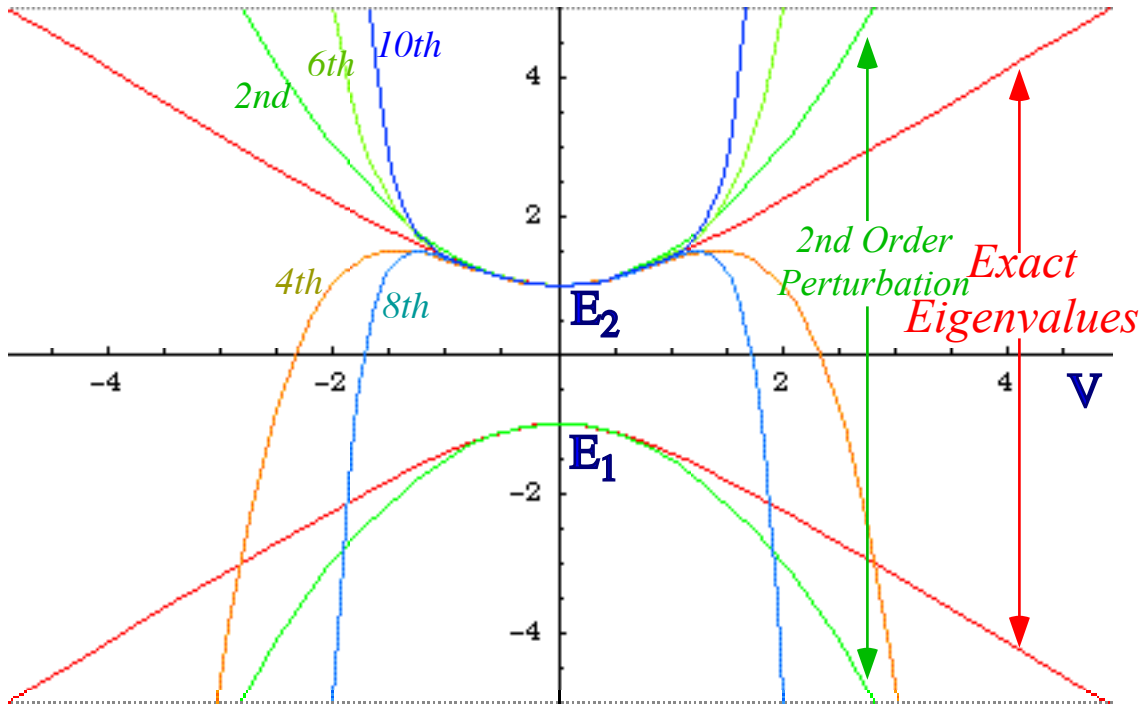


Fig. 3.2.2 Comparison of exact vs. 2nd-order thru 8th-order perturbation approximations

Second order perturbation formulas are simple, easy to apply, and, for this example, at least, quite an effective approximation for a range of V roughly equal to $|E_1 - E_2|$. The same cannot be said for higher order perturbation terms, particularly those of 6th or higher which seem to follow a law of diminishing returns. Even a 10th order formula only extends the range of validity a little in Fig. 3.2.2. Worse, a simple application of (3.2.5) to the two-level problem is wrong for 6th and higher orders. A direct application of (3.2.5) gives

$$E_2 = \frac{\Delta}{2} + \frac{V^2}{\Delta} - \frac{V^4}{\Delta^3} + \frac{V^6}{\Delta^5} - \frac{V^8}{\Delta^7} + \frac{V^{10}}{\Delta^9} \dots, \text{ where: } \Delta = |E_1 - E_2|$$

while the correct binomial expansion of the exact result (3.2.9) which is plotted in Fig. 3.2.2 is

$$E_2 = \frac{\Delta}{2} + \frac{V^2}{\Delta} - \frac{V^4}{\Delta^3} + \frac{2V^6}{\Delta^5} - \frac{5V^8}{\Delta^7} + \frac{14V^{10}}{\Delta^9} \dots$$

But, even the corrected polynomials are miserable approximations to the hyperbola approaching its asymptote. Also, the series is divergent. Similar problems exist for 3, 4, ..., or N-level systems.

The problem is that eigenvalues are generally more like oscillatory (sinusoidal) or exponential and hyperbolic functions and do not take kindly to being represented by polynomials. Check this out by comparing a sine wave to its Taylor series polynomial approximation. How many orders do you need to approximate one full oscillation to 1% or better? And, note what happens outside that range of validity!