Matricies As Vectors

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Preface to the introduction

My recent publication on the NMR theories of spin relaxation, in Magnetic Resonance Ampere (MR-2-689-2021) engendered a request by one reader for more supplemental information, made available via some web site. I sent a copy of this to him and have now decided to put the same ups on "Research Gate".

Of course, they are rough notes, hand written no less (a lost art form for sure - look at this cursive!) This is because I am something of a "lazy dog".* It is alot of arcane work to type set equations in a document that may never be published!

One can find a more formal reference set in my MR Ampere article.

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* Minkowski's quip anent Einstein

Matrices as Vectors

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Introduction

These notes summerize aspects of the N^2 dimensional vector space of $N \times N$ matrices and in particular the applications to finite dimensional density matrix equations. I eschew the Dirac notation I find it unnecessarily verbose and often cryptic in meaning eg $A_{ij} \equiv \langle i | A | j \rangle$ which is 3 vs 7 in pencil strokes, as well as "big" even though it is "inline". In this preference I am not entirely alone, cf WEINberg's "Lectures on quantum Mechanics."

Doing so also allows me to avoid all kinds of contructions regarding operators and "super operators" and the manner inwhich they are symbolized, with various "hats" and "double hats" etc etc etc. after awhile various symbols get really beaten up with notational caveats. As much as possible, I avoid this.

The basic idea is this: Since matrices encode how vectors transform amoung themselves, the study of how matrices transform amoung themselves can be approached by turning a matrix into a vector.

An important class of transformations are those that preserve the Hermitian character of a matrix and leave the trace of a matrix unchanged. This leads us into a topic in irreversiblity in quantum systems and a quantum Boltzmann equation, often referred to as the "Lindblad form", or "Lindblead master equation".

Matrices As Vectors

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Introduction Continued

- One key element I emphasize is that of Spectral Decomposition. One can justly claim this to be the master of all theorems for finite dimensional vector spaces. It is uncanny how it keeps surfacing up in any discussion.
- As an application, I show how the general structure boils down to Bloch's Relaxation Equations for two level systems, when secular terms can be ignored.
- The topic of a Quantum Boltzmann equation is currently (2020) a big topic and often presented in complicated mathematical language. These notes attempt to dial this back. This is, in part, a question of style but also that of the relationship between mathematics, especially modern mathematics, and physics. Other's have commented on this situation e.g. S. Weinbergs lament of mathematical expositions of differential forms (Gravitation & Cosmology)
- The popular method of constructing "super operators" via Lexigraphical ordering and Kronecker products is covered. While useful, there are cases where a simpler result is obtained by judicious choices for an outright operator expansion. This is particularly true for the Lindbladian operator, especially from an analytical perspective.
- The topic of course is well worn. A classic exposition in magnetic resonance is J. Jeener's in volume 10 of "Advances in Magnetic Resonance" (1982). However, I never thought this was a good introduction. Another more recent exposition is Gyamfi's EJP 41 (2020) which I found more useful. I mention "Halmo's book repeatedly "Finite Dimensional Vector Spaces", now out as a Dover edition.

Matices as Vectors

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- Due to the rules of matrix addition and scaling (element by element) it is clear that matrices of the same dimension (rows and columns) form a vector space. This then engenders one to form a column or row vector by some systematic reordering scheme.
- We can use Lexigraphical ordering on columns or rows

Eg. for 2×2 matrices

$$\underset{\sim}{A}_c \equiv \text{cvector}(A) = \begin{pmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{pmatrix} \qquad \underset{\sim}{A}_r \equiv \text{rvector}(A) = \begin{pmatrix} a_{11} \\ a_{21} \\ a_{12} \\ a_{22} \end{pmatrix}$$

where $$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad A^+ = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} \quad \text{"Adjoint"}$$

- These are related through the matrix operation of transposition, often denoted by $\tilde{A}$. $A^+ = \tilde{A}^*$
- Once extracted, one can form a dual vector, and an inner product. Following the example above

$$(a_{11}^* \; a_{12}^* \; a_{21}^* \; a_{22}^*) \begin{pmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{pmatrix} = |a_{11}|^2 + |a_{12}|^2 + |a_{21}|^2 + |a_{22}|^2$$

- It is easy to show that this inner product is identical to the matrix operation $\text{Trace}(AA^+)$

But the dual of $\text{cvector}(A)$ is not $\text{cvector}(A^+)$ but rather $[\text{rvector}(\tilde{A})]^+ = [\text{cvector}(A)]^+$

This follows the usual convention that the dual of a column vector $(N \times 1)$ is a $(1 \times N)$ row vector with complex conjugate elements.

- The preceding demonstrates that there are nuances to "vectorizing a matrix". Why not just keep the matrix form? After all, the elements are all readily available. And Lexicographical ordering has cumbersome aspects.

- The major reason was to see, briefly, how things go <u>without</u> matrix multiplication. Since matrices posses a decent definition of multiplication, we have entered the realm of <u>Vector Algebra</u> [Halmos, of course]. This is a horse of a different color, because vectors can now be multiplied. We can take $Tr(AA^+)$ as an inner product and A^+ is "dual" to A.

- Though unremarkably trival (almost) for mathematicians (Halmos, again), the topic is important for physics and other practical problems. For example, one could be confronted with a <u>matrix</u> differential equation such as $\dot{\rho} = A \rho A^+$. This must be dealt with element by element, and vectorized in some way.

- Before proceeding, lets take one more example with two matricies A and B from which we construct "c vectors"

$$\underset{\sim}{a} = \begin{pmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{pmatrix} \quad \text{and} \quad \underset{\sim}{b} = \begin{pmatrix} b_{11} \\ b_{12} \\ b_{21} \\ b_{22} \end{pmatrix}$$

with duals $a^+ = (a_{11}^* \; a_{12}^* \; a_{21}^* \; a_{22}^*)$ and likewise for b^+.

then $b^+ a = a_{11} b_{11}^* + a_{12} b_{12}^* + a_{21} b_{21}^* + a_{22} b_{22}^* = (a^+ b)^*$

This corresponds to $Tr(AB^+)$ so the "apparent" order is given by the adjoint. Inner products, are after all, <u>ordered</u>, due to their "conjugate bilinearity" (Halmos). Since $Tr\, C^+ = (Tr\, C)^*$ everything fits nicely, <u>viz</u> $Tr(AB^+) = Tr\, B^+ A$ $\star$

Matrices as Vectors

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- The vectorization procedure can be expressed clearly by the use of the "fundamendal" matrix basis $X^{\alpha\beta}$ with matrix elements $X^{\alpha\beta}_{ij} = \delta_{\alpha i}\delta_{\beta j}$ for the i^{th} row and j^{th} column as usual. We list some properties ($\tilde{X}$ is matrix transpose)

$$\tilde{X}^{\alpha\beta} = X^{\beta\alpha} \qquad Tr\, X^{\alpha\beta} = \delta_{\alpha\beta} \qquad Tr\left(X^{\alpha\beta}\tilde{X}^{\alpha'\beta'}\right) = \delta_{\alpha\alpha'}\delta_{\beta\beta'}$$

$$X^{\alpha\beta}X^{\alpha'\beta'} = \delta_{\alpha'\beta}X^{\alpha\beta'} \qquad \sum_{\alpha} X^{\alpha\alpha} = \underline{1}$$

$$X^{\alpha\beta}\tilde{X}^{\alpha\beta} = X^{\alpha\beta}X^{\beta\alpha} = X^{\alpha\alpha} \quad \text{Factoring of } X^{\alpha\alpha}$$

$$\sum_{\alpha} X^{\alpha\beta}\tilde{X}^{\alpha\beta} = \sum_{\alpha} X^{\alpha\alpha} = \underline{1} \quad \text{Closure identity}$$

$$X^{\alpha\alpha}X^{\alpha\alpha} = X^{\alpha\alpha} \quad \text{Projectors} \quad X^{\alpha\alpha}X^{\beta\beta} = \delta_{\alpha\beta}$$

- Clearly we can expand a matrix V as

$$V = \sum_{\alpha}\sum_{\beta} V_{\alpha\beta}X^{\alpha\beta} \qquad V_{\alpha\beta} = Tr\left(V X^{\beta\alpha}\right)$$

- Because of the projection and closure of $X^{\alpha\alpha}$ we can also write $V = \sum_{\alpha}\sum_{\beta} X^{\alpha\alpha} V X^{\beta\beta} = \sum_{\alpha\beta} E_{\alpha} V E_{\beta}$

  Each Expansion has certain advantages. The later dovtails nicely with spectral decomposition.

- Since $X^{\alpha\beta}$ are matrices, one should perhaps specify their dimension, say $X^{\alpha\beta}(n)$ for an $n \times n$ matrix, of course, there are n^2 such matracies.

- By ordering Lexigraphically, eg $X^{11}, X^{12}, X^{21}, X^{22}$ we have a set of basis "vectors".
- Construction of $X^{\alpha\beta}$, though seemingly trivial, has many uses.

- With the use of $X^{\alpha\beta}$ as a basis, one could proceed to vectorize every matrix under consideration. Doing so, one obtains a vector algebra via matrix algebra. However, in many applications, only one matrix is of interest dynamically. Say the matrix ρ (density matrix) is such a matrix and evolves dynamically as $\dot{\rho} = A\rho + \rho B + A\rho B$

and in this type of situation we only need to vectorize ρ.

Consider $\dot{\rho} = A\rho$ so $\dot{\rho}_{ij} = \sum_k A_{ik}\rho_{kj}$

Let's use $\rho_{kj} = \sum_l \delta_{lj}\rho_{kl}$ and create the double sum

$$\dot{\rho}_{ij} = \sum_k \sum_l A_{ik}\delta_{lj}\rho_{kl}$$

Now that k and l are free indicies, we are free to interpret $A_{ik}\delta_{lj}$ as a Kronecker product of A with the identity, and with lexigraphical ordering by columns to contruct the vector $\underset{\sim}{\rho}_c$ then

$\dot{\underset{\sim}{\rho}}_c = (A \otimes \underline{\underline{1}})\underset{\sim}{\rho}_c$. It is allways usefull to illustrate with a simple example.

$$\begin{pmatrix} \dot{\rho}_{11} \\ \dot{\rho}_{12} \\ \dot{\rho}_{21} \\ \dot{\rho}_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & 0 & A_{12} & 0 \\ 0 & A_{11} & 0 & A_{12} \\ A_{21} & 0 & A_{22} & 0 \\ 0 & A_{21} & 0 & A_{22} \end{pmatrix} \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ \rho_{22} \end{pmatrix}$$

$$\begin{pmatrix} A_{11}\underline{\underline{1}} & A_{12}\underline{\underline{1}} \\ A_{21}\underline{\underline{1}} & A_{22}\underline{\underline{1}} \end{pmatrix} = A \otimes \underline{\underline{1}}$$

- It is then easy to see that $\dot{\rho} = \rho A$ translates into $(\underline{1} \otimes \tilde{A})\rho_c$. Since matrix multiplication is associative then $\dot{\rho} = A\rho B = A(\rho B)_c$
$= (A \otimes \underline{1})(\underline{1} \otimes \tilde{B})\rho_c = (A \otimes \tilde{B})\rho_c$.

- Similar expressions result for the choice of <u>row vectorization</u> eg $\dot{\underset{\sim}{\rho}}_r = (\underline{1} \otimes A)\underset{\sim}{\rho}_r$ for $\dot{\rho} = A\rho$

and $\dot{\underset{\sim}{\rho}}_r = (\tilde{A} \otimes \underline{1})\underset{\sim}{\rho}_r$ for $\dot{\rho} = \rho A$.

$$\dot{\underset{\sim}{\rho}}_r = (\tilde{B} \otimes A)\dot{\underset{\sim}{\rho}}_r \quad \text{for } \dot{\rho} = A\rho B$$

But column vectorization seems more natural since certain orderings are preserved.

- With the matrix ρ extracted as a column vector, our difficult matrix dynamics is now straight forward.

$$\dot{\underset{\sim}{\rho}}_c = [A \otimes \underline{1} + 1 \otimes \tilde{B} + A \otimes \tilde{B}]\underset{\sim}{\rho}_c$$

$$= L\underset{\sim}{\rho}_c \quad \text{where } L \text{ is now } n^2 \times n^2$$

L is a "super operator"!

- This approach may not produce the simplest matrix (see later sections)
- with such a large dimensional problem, it is important to take advantage of <u>any</u> symmetry that may exist. For example, ρ may be Hermitian, $\rho^+ = \rho$. Fortunately, these can be prescribed at the matrix formulation, and demand for example that

$$\dot{\rho} = A\rho + \rho A^+ + B\rho B^+$$

$$\dot{\rho}^+ = \dot{\rho} \quad \text{if } \rho = \rho^+$$

- Let us take an important specific example namely quantum evolution for a finite number of states where Schrodinger's equation is

$$\dot{c}_i = -i \sum_k \mathcal{H}_{ik} c_k \quad \text{for } \psi = \sum_i c_i \, \underset{\sim}{b}_i \equiv \underset{\sim}{c}$$

with basis vectors $\underset{\sim}{b}_i$. VIZ $\dot{\underset{\sim}{c}} = -i \mathcal{H} \underset{\sim}{c}$

- The density matrix $\rho_{ij} = \langle c_i c_j^* \rangle$ evolves as a commutator with $\mathcal{H}$ $\dot{\rho} = -i[\mathcal{H}, \rho]$ and we can render ρ as a column vector ρ_c, so that

$$\dot{\underset{\sim}{\rho}}_c = -i(\mathcal{H} \otimes \underline{1} - \underline{1} \otimes \tilde{\mathcal{H}})\, \rho_c$$

Since $\mathcal{H}^+ = \mathcal{H}$ $\tilde{\mathcal{H}} = \mathcal{H}^*$ and $(A \otimes B)^+ = A^+ \otimes B^+$

we have $\mathcal{L} \equiv (\mathcal{H} \otimes \underline{1} - \underline{1} \otimes \mathcal{H}^*) = \mathcal{L}^+$

$\therefore$ $\dot{\underset{\sim}{\rho}}_c = -i \mathcal{L} \rho_c$ similar to $\dot{\underset{\sim}{c}} = -i \mathcal{H} \underset{\sim}{c}$

In many places in the literature, one see's the notation "$\mathcal{H}^\times$" for $\mathcal{L}$ without much exposition. The super operator $\mathcal{L}$ is often referred to as the Louivillian

- One can find eigenvalues and eigenvectors for $\mathcal{L}$ and if $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ with $\mathcal{L}_0$ diagonal and $\mathcal{L}_1$ a perturbation, the usual techniques of perturbation theory can be utilized. This approach is basically finding "eigen matrices" VIZ $[\mathcal{H}, Q] = \lambda Q$, a problem that is related to spectral decomposition which is explored later.

- Of course there are other ways of vectrizing a matrix such as an expansion in a complete set of Hermitian matrices which is given after the spectral theorem.

The Spectral Theorem

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Magnetic Resonance

- a Hermitian matrix $\mathcal{H}$ is decomposed into a sum over eigenvalues ω_k and projectors E_k

$$\mathcal{H} = \sum_k \omega_k E_k \qquad E_k E_l = E_k \delta_{kl}$$

- Let $\mathcal{H}$ be diagonalized by the similarity transformation

$$\Lambda = U^+ \mathcal{H} U \qquad \Lambda_{ij} = \omega_j \delta_{ij}$$

$$\mathcal{H} = U \Lambda U^+$$

$$U^+ \mathcal{H} U = \sum_k \omega_k U^+ E_k U = \sum_k \omega_k X^{kk}$$

where the set of matrices $X^{\alpha\beta}$ with components $X^{\alpha\beta}_{ij} = \delta_{\alpha i}\delta_{\beta j}$ are introduced. We can now write E_k in the original basis as $E_k = U X^{kk} U^+$

$$E_k = E_k^+ \qquad \mathrm{Tr}\, E_k = 1 \qquad \det E_k = 0 \qquad \sum_k E_k = \underline{1}$$

Also note that $X^{\alpha\beta} X^{\alpha'\beta'} = \delta_{\alpha'\beta} X^{\alpha\beta'}$ $\qquad \mathrm{Tr}\, E_k E_\gamma = \delta_{k\gamma}$

Since $[\mathcal{H}, \mathcal{H}] = \sum_{ij} \lambda_k \lambda_j [E_k, E_j] = 0$

$[E_k, E_j] = 0$ $\qquad$ NB $[X^{\alpha\beta}, X^{\alpha'\beta'}] = \delta_{\alpha'\beta} X^{\alpha\beta'} - \delta_{\alpha\beta'} X^{\alpha'\beta}$

$$[X^{kk}, X^{k'k'}] = \delta_{k'k} X^{kk'} - \delta_{kk'} X^{k'k}$$

The spectral theorem gives an operator expansion of $\mathcal{H}$, but $\sum_k E_k = \underline{1}$
(none of the E_k are orthogonal to the identity matrix)

The Spectral Theorem

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Magnetic Resonance

- By using the properties of the E_k we see that for a given matrix V

$$[\mathcal{H}, E_k V E_{k'}] = (\omega_k - \omega_{k'}) E_k V E_{k'}$$

and

$$e^{i\mathcal{H}t} E_k V E_{k'} e^{-i\mathcal{H}t} = e^{i(\omega_k - \omega_{k'})t} E_k V E_{k'}$$

$$\sum_k \sum_{k'} E_k V E_{k'} = V$$

- The projectors generate eigen operators for the quantum mechanical equations of motion for the density matrix $\dot{\rho} = -i[\mathcal{H}, \rho]$. $E_k V E_k$ are invariants and correspond to eigen values of zero. $E_k V E_{k'}$ and $E_{k'} V E_k$ to eigenvalues of opposite sign. This is reflected in the real, orthogonal character of the "superoperator" of the equation of motion.
- This is, of course, an artsy way of looking at the problem. If V is also expressed in the eigenbasis of $\mathcal{H}$, then the projectors are trivial, even unneeded.

$$(e^{i\mathcal{H}t} V e^{-i\mathcal{H}t})_{ij} = V_{ij} e^{i(\omega_i - \omega_j)t}$$

- In the eigenbasis of $\mathcal{H}$, then the $X^{\alpha\beta}$ basis matrices are eigen matrices

$$e^{i\mathcal{H}t} X^{\alpha\beta} e^{-i\mathcal{H}t} = e^{i(\omega_\alpha - \omega_\beta)t} X^{\alpha\beta}$$

- Let's take another look at

$$\mathcal{H} = \sum_k \omega_k E_k = \sum_k \omega_k U X^{kk} U^+$$

Since $X^{kk} X^{kk} = X^{kk}$

$$U X^{kk} U^+ = U X^{kk} X^{kk} U^+ = V_k V_k^+$$

with $V_k = U X^{kk} \quad V_k^+ = X^{kk} U^+$

$$\mathcal{H} = \sum_k \omega_k V_k V_k^+ \qquad \text{and} \quad V_k^+ V_k = X^{kk}$$

So the V_k are not normal in this factoring scheme

- If the ω_k are positive, complete factoring is possible. $N_k = \sqrt{\omega_k}\, V_k$ and $\mathcal{H} = \sum_k N_k N_k^+$

- The importance of positivity is very dependent on the role played by $\mathcal{H}$. In quantum evolution this is related to the "zero of energy". For finite dimensional problems, shifting all levels by a constant amount $\alpha \underline{\underline{1}}$ is a common phase factor $e^{i\alpha t}$ for pure states. The density matrix $\rho_{ij} = c_i c_j^*$ is independant of this common phase which is reflected in $\dot{\rho} = -i[\mathcal{H}, \rho] = -i[\mathcal{H} + \alpha \underline{\underline{1}}, \rho]$.

- Other dynamical equations will not have this property.

- Shifting the zero of energy so that $\mathcal{H}$ can be expressed as $\sum_k N_k N_k^+$ is often used in Laser Physics [Loudon Quantum theory of Light]

Matracies As Vectors

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- General matrix basis

  any matrix B can be decomposed as a sum

  $B = H + iJ$ where H and J are Hermitian.

  $$B = \tfrac{1}{2}(B + B^+) + \tfrac{1}{2}(B - B^+) = H + iJ$$

  If O_k is a complete set of Hermitian matrices such that $Tr\, O_k O_l = \delta_{kl}$ then $\quad O_k^+ = O_k$

  $$B = \sum_k (h_k + i j_k) O_k = \sum_k b_k O_k$$

  Define $N_k = (1+i)/\sqrt{2}\; O_k = e^{i\pi/4} O_k$

  $$Tr(N_k N_l^+) = Tr(O_k O_l) = \delta_{kl}$$

  So $Tr\, N_k^+ B = h_k + i j_k = b_k$

  and the set N_k is a general basis for <u>any</u> complex matrix. Note that the N_k are <u>normal</u> $[N_k, N_k^+] = 0$

- The normality is trivial and this is due to the fact that a Hermitian basis is all that is required.

- For 2x2, the classic basis set elements are the normalized Pauli matrices

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\sigma_x \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\sigma_y \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\sigma_z$$

and the normalized identity $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

- For 3x3 we can take the spin 1 operators $I_x\ I_y\ I_z$ and their products eg $I_xI_y + I_yI_x$, $I_zI_x + I_xI_z$, $I_x^2 - I_y^2$ etc, all of which have normalizations of $1/\sqrt{2}$, except $3I_z^2 - 2\underline{1}$.

General Matrix Expansion

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- Let's return to the example of $\dot{\rho} = -i[\mathcal{H}, \rho]$
Given that ρ and $\mathcal{H}$ are Hermitian, we only need the Hermitian set $\{O_i\}$ so $\rho = \sum_i \rho_i O_i$ and $\mathcal{H} = \sum_i h_i O_i$ with $h_i = Tr(\mathcal{H} O_i)$ $\rho_i = Tr(\rho O_i)$.
Substituting these into $\dot{\rho} = -i[\mathcal{H}, \rho]$ gives

$$\sum_k \dot{\rho}_k O_k = -i\left\{\sum_\ell h_\ell O_\ell \sum_m \rho_m O_m - \sum_m \rho_m O_m \sum_\ell h_\ell O_\ell\right\}$$

$$= -i \sum_\ell \sum_m h_\ell [O_\ell, O_m] \rho_m$$

$$\dot{\rho}_k = -i \sum_\ell \sum_m h_\ell \rho_m Tr\{[O_\ell, O_m] O_k\}$$

$$= -i \sum_m M_{km} \rho_m$$

$$M_{km} = \sum_\ell h_\ell Tr\{[O_\ell, O_m] O_k\} = \sum_\ell h_\ell Tr\{[O_m, O_k] O_\ell\}$$

where the cyclic properties of Trace has been used.
Since $Tr A^\dagger = (Tr A)^*$ we have $M^*_{km} = -M_{km}$
so M_{km} is pure imaginary as well as antisymmetric

$$M_{kk} = 0 \qquad M_{km} = -M_{mk}$$

Let's redifine $-iM \rightarrow M$ so that now

$$\dot{\rho}_k = \sum_m M_{km} \rho_m \qquad \tilde{M} = -M \qquad M^* = M$$

The evolution of ρ now "vectorized" is $\dot{\underset{\sim}{\rho}} = M \underset{\sim}{\rho}$
where M now represents a <u>real</u> <u>orthogonal</u> <u>transformation</u>.
If we diagonalize M we have basically found the eigen operators for $[\mathcal{H}, Q] = \lambda Q$ which brings us back to spectral decomposition once again, namely if ω_α are the eigenvalues of $\mathcal{H}$, the eigenvalues for M will be $\pm i(\omega_\alpha - \omega_\beta)$ or zero. The "general" vectorization has merit over the one employing Kroenecker products.

① Kronecker Products of $x^{\alpha\beta}$ Tom Barbara

- Let's look at Kronecker products for our fundemental bases matrices for the case of 2×2. Here is a table, in a compact notation. Each entry is a 2×2 matrix embedded into the 4×4 matrices produced by Kronecker

$$\begin{array}{cc|cccc}
 & & \begin{pmatrix} x^{11} & 0 \\ 0 & x^{11} \end{pmatrix} & \begin{pmatrix} x^{12} & 0 \\ 0 & x^{12} \end{pmatrix} & \begin{pmatrix} x^{21} & 0 \\ 0 & x^{21} \end{pmatrix} & \begin{pmatrix} x^{22} & 0 \\ 0 & x^{22} \end{pmatrix} \leftarrow \underline{1} \otimes x^{\alpha\beta} \\
\hline
\underline{11} & \begin{pmatrix} \underline{1} & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} x^{11} & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} x^{12} & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} x^{21} & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} x^{22} & 0 \\ 0 & 0 \end{pmatrix} \\
\underline{12} & \begin{pmatrix} 0 & \underline{1} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & x^{11} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & x^{12} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & x^{21} \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & x^{22} \\ 0 & 0 \end{pmatrix} \\
\underline{21} & \begin{pmatrix} 0 & 0 \\ \underline{1} & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ x^{11} & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ x^{12} & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ x^{21} & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ x^{22} & 0 \end{pmatrix} \\
\underline{22} & \begin{pmatrix} 0 & 0 \\ 0 & \underline{1} \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & x^{11} \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & x^{12} \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & x^{21} \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & x^{22} \end{pmatrix}
\end{array}$$

1st row 2nd row

3rd row 4th row

$\uparrow$

$x^{\alpha\beta} \otimes \underline{1}$

$$x^{\alpha\beta} \otimes x^{\alpha'\beta'}$$

- These form a 4×4 basis. Notice that the rows of the 4×4 are grouped in quadrants in this table, as marked.

We take the example of the transpose operation

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ \rho_{22} \end{pmatrix} = \begin{pmatrix} \rho_{11} \\ \rho_{21} \\ \rho_{12} \\ \rho_{22} \end{pmatrix}$$

- The transpose of the vectorized matrix ρ can now be written as

$$O_T \underset{\sim}{\rho}_c = \left[X^{11} \otimes X^{11} + X^{12} \otimes X^{21} + X^{21} \otimes X^{12} + X^{22} \otimes X^{22} \right] \underset{\sim}{\rho}_c$$

$$= \left[X^{11} \otimes \tilde{X}^{11} + X^{12} \otimes \tilde{X}^{12} + X^{21} \otimes \tilde{X}^{21} + X^{22} \otimes \tilde{X}^{22} \right] \underset{\sim}{\rho}_c$$

- We can recognize this in matrix form as

$$\tilde{\rho} = \sum_{\alpha\beta} X^{\alpha\beta} \rho X^{\alpha\beta}$$

$$= X^{11} \rho X^{11} + X^{12} \rho X^{12} + X^{21} \rho X^{21} + X^{22} \rho X^{22}$$

- The transpose operation is one of the permutations of ρ_{ij} which is an easy case since the elements of the transformation are so simple (1 or 0).

- a general transformation will "mix-up" the coefficients according to quadrants as noted earlier, creating something of a "notational nightmare".

- anothere example is the identity transformation and this is given by

$$\rho = \sum_{\alpha\beta} X^{\alpha\alpha} \rho X^{\beta\beta}$$

and we are back to the spectral theorem

- a general transformation can be written as

$$\rho' = \sum_{\alpha\beta} \sum_{\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} \, X^{\alpha\beta} \rho X^{\alpha'\beta'} \qquad (1)$$

The index ordering chosen for $C_{\alpha\beta\alpha'\beta'}$ appears logical but there is a fly in the ointment. This is revealed when the above is converted to matrix elements ρ'_{ij}

$$(X^{\alpha\beta} \rho X^{\alpha'\beta'})_{ij} = \sum_k \sum_l X^{\alpha\beta}_{ik} \rho_{kl} X^{\alpha'\beta'}_{lj}$$

$$= \delta_{\alpha i} \, \rho_{\beta\alpha'} \, \delta_{\beta' j}$$

$$\rho'_{ij} = \sum_{\alpha\beta} \sum_{\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} \, \delta_{\alpha i} \, \rho_{\beta\alpha'} \, \delta_{\beta' j}$$

$$\rho'_{ij} = \sum_{\beta\alpha'} C_{i\beta\alpha' j} \, \rho_{\beta\alpha'}$$

One could argue that this ordering is not logical and therefore it gets switched around. For example, Redfield writes

$$(R\sigma)_{\alpha\alpha'} = \sum_{\beta\beta'} R_{\alpha\alpha'\beta\beta'} \, \sigma_{\beta\beta'}$$

(Advances in Magnetic Resonance, Volume 1 1965)

Whereas Weinberg writes

$$[\rho(t)]_{MN} = \sum_{M'N'} K_{MM',NN'} [\rho]_{M'N'}$$

(Lecture's on Quantum Mechanics 2nd Ed 2015)
which corresponds to the matrix equation with $X^{\alpha\beta} \rho \tilde{X}^{\alpha'\beta'}$

Notions Anent Notations

Tom Barbara

- It is of some interest to linger on aspects of the proceeding page regarding indexing. From an pure index perspective $\sum_{\beta\beta'} R_{\alpha\alpha'\beta\beta'} \rho_{\beta\beta'}$ appears logical

but this choice does not jibe well with (1) of the preceeding page. From (1) we can make various choices which we list, with the matrix index forms along side.

$$\sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} X^{\alpha\beta} \rho X^{\alpha'\beta'} \rightarrow \rho_{ij} = \sum_{\beta\alpha'} C_{i\beta\alpha' j} \rho_{\beta\alpha'}$$

$$\sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} X^{\alpha\beta} \rho \tilde{X}^{\alpha'\beta'} \rightarrow \rho_{ij} = \sum_{\beta\beta'} C_{i\beta j\beta'} \rho_{\beta\beta'}$$

$$\sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} \tilde{X}^{\alpha\beta} \rho X^{\alpha'\beta'} \rightarrow \rho_{ij} = \sum_{\alpha\alpha'} C_{\alpha i\alpha' j} \rho_{\alpha\alpha'}$$

$$\sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'} \tilde{X}^{\alpha\beta} \rho \tilde{X}^{\alpha'\beta'} \rightarrow \rho_{ij} = \sum_{\alpha\beta'} C_{\alpha i j\beta'} \rho_{\alpha\beta'}$$

- So $\sum_{\beta\beta'} R_{\alpha\alpha'\beta\beta'} \rho_{\beta\beta'}$ does not fit into (1)! But it gets used alot eg Redfield and Abragam.
- Weinberg's choice does fit, but the matrix form similar to (1) is never written down. Strange.....
- I mentioned earlier that the introduction of $X^{\alpha\beta}$ seems trivial but useful and now we can see why. It is a real advantage to move away from "pure matrix indexing".
- In much of the literature, these things are never carefully exposed. Instead people just talk about "Choi matricies" and one can follow down the "citation trail" and still not get to the nub.

(1) Hermiticity and Trace Conservation

Tom Barbara

- If our general transformation

$$\rho' = \sum_{\alpha\beta}\sum_{\alpha'\beta'} c_{\alpha\beta\alpha'\beta'}\, X^{\alpha\beta}\rho X^{\alpha'\beta'}$$

preserves the hermitian property of $\rho = \rho^{+}$ then $\rho'^{+} = \rho'$. Since $\tilde{X}^{\alpha\beta} = X^{\beta\alpha}$

$$(\rho')^{+} = \sum_{\alpha\beta}\sum_{\alpha'\beta'} c^{*}_{\alpha\beta\alpha'\beta'}\, X^{\beta'\alpha'}\rho X^{\beta\alpha}$$

$$= \sum_{\alpha\beta}\sum_{\alpha'\beta'} c^{*}_{\beta'\alpha'\beta\alpha}\, X^{\alpha\beta}\rho X^{\alpha'\beta'}$$

then $c^{*}_{\beta'\alpha'\beta\alpha} = c_{\alpha\beta\alpha'\beta'}$

- If $Tr\,\rho' = Tr\,\rho$ then

$$Tr\,\rho' = Tr\left\{\left[\sum_{\alpha\beta}\sum_{\alpha'\beta'} c_{\alpha\beta\alpha'\beta'}\, X^{\alpha'\beta'}X^{\alpha\beta}\right]\rho\right\}$$

which holds for arbitrary ρ if

$$\sum_{\alpha\beta}\sum_{\alpha'\beta'} c_{\alpha\beta\alpha'\beta'}\, X^{\alpha'\beta'}X^{\alpha\beta} = \underline{1}$$

Using the product rules for $X^{\alpha\beta}$ then gives

$$\sum_{\alpha'\beta}\left[\sum_{\alpha} c_{\alpha\beta\alpha'\alpha}\right] X^{\alpha'\beta} = \underline{1}$$

OR $$\sum_{\alpha} c_{\alpha j i \alpha} = \delta_{ij}$$

(2) Hermiticity and Trace Conservation and Kraus — Tom Barbara

- Lets express everything in a Hermitian basis by using the normal matricies intoduced earlier

$$N_k = e^{i\pi/4} O_k \qquad O_k^+ = O_k \quad \text{so that}$$

$$x^{\alpha\beta} = \sum_k \xi_k^{\alpha\beta} N_k \qquad k = 0, 1, \ldots N^2-1$$

$$O_0 \propto \underline{\underline{1}}$$

- This leads us to an expansion in the O_k

$$\rho' = \sum_k \sum_{k'} G_{kk'} O_k \rho O_{k'}$$

Now $G_{kk'} = G^*_{k'k}$ if $(\rho')^+ = \rho'$ and now that G is Hermitian in the k indicies we can factor $G_{kk'} = \sum_\ell U^*_{\ell k} \sqrt{\lambda_\ell} \sqrt{\lambda_\ell}\, U_{\ell k'}$

were λ_ℓ are the real eigenvalues of $G_{kk'}$ $\lambda_\ell^* = \lambda_\ell$

We now have NB $\sqrt{\lambda_\ell}$ may be imag unless $G_{kk'}$ is <u>positive</u>

$$\rho' = \sum_\ell \Big(\sum_k \sqrt{\lambda_\ell}\, U^*_{\ell k} O_k \Big) \rho \Big(\sum_{k'} \sqrt{\lambda_\ell}\, U_{\ell k'} O_{k'} \Big)$$

$$\rho' = \sum_\ell M_\ell \rho M_\ell^+ \qquad M_\ell = \sum_k \sqrt{\lambda_\ell}\, U^*_{\ell k} O_k$$

This is the famous "Kraus Form" for the transformation

Trace conservation is now $\sum_\ell M_\ell^+ M_\ell = \underline{\underline{1}}$

While very "artsy-fartsy", the direct connection on the $C_{\alpha\beta\alpha'\beta'}$ seems "easier", even with the muliple indicies. But the positivity requirement is clear when $G_{kk'}$ is factored.

The Lindblad Form Tom Barbara

Since $\rho' = \sum_{kk'} G_{kk'} O_k \rho O_{k'}$ (*)

with $G_{k'k} = G^*_{kk'}$; $\sum_{kk'} G_{kk'} O_{k'} O_k = \underline{1}$ (closure)

we can develope a difference equation for $\rho' - \rho$

Often this is approached withe the Kraus form as a starting point, but this is actually a "bridge to far". From Kraus, the $\{O_k\}$ basis must be introduced anyway so why not just start with (*)?

We can use the closure condition symmetrically

$$\rho' - \rho = \sum_{kk'} G_{kk'} O_k \rho O_{k'} - \frac{1}{2} (\rho \underline{1} + \underline{1} \rho)$$

- Since the identity is an element of $\{O_k\}$ let us treat that separately. Collecting terms for say, $k=0$ and/or $k'=0$ we get for their contribution the sum

$$\sum_k \frac{1}{2i} (G_{k0} - G^*_{k0}) \, i [O_k , \rho]$$

We are left with sums over $1, N^2-1$ $\{A,B\} = AB + BA$

$$\rho' - \rho = \sum_{kk'} G_{kk'} \left[O_k \rho O_{k'} - \frac{1}{2} \{ \rho , O_{k'} O_k \} \right]$$

Now that $O_0 \equiv \underline{1}$ has been eliminated $\mathrm{Tr}\, O_k = 0$, $k > 0$

The first part of the aboave is Hermitian evolution and the second part is the Lindblad Form. If one so desires, Kraus can then be invoked for $G_{kk'}$ positive resulting in a non-Hermitian operator expansion.

(2)

Lindblad Form Differential Equation

Tom Barbara

- $\sum_k \sum_{k'} G_{kk'} O_{k'} O_k = \underline{1}$ and $Tr\, O_\ell O_m = \delta_{\ell m}$

$$\Rightarrow \sum_k G_{kk} = N$$

Since $O_0 = \frac{1}{\sqrt{N}} \underline{1}$ drops out of the difference equation we need to go back to (A) to get a value for G_{00}

$$\rho' = 2 G_{00} \frac{1}{\sqrt{N}} \underline{1} \rho \frac{1}{\sqrt{N}} \underline{1} + \dots$$

$$\rho' = \frac{2 G_{00}}{N} \rho \qquad G_{00} = \frac{N}{2}$$

- If the transformation is viewed as a continuous one parameterized by the time, then

$$\lim_{t \to 0} \left\{ 2 G_{00} + \sum_{k \neq 0} G_{kk} \right\} = N$$

$$\lim_{t \to 0} \sum_{k \neq 0} G_{kk}(t) = 0$$

Therefore $G_{kk'}$ must be proportional to the size of the time step $\Delta\tau$ $\qquad G_{kk'} = \Delta\tau\, K_{kk'}$

$$\rho(t+\Delta\tau) - \rho(t) = \Delta\tau \sum_{kk'} K_{kk'} \left[O_k \rho O_{k'} - \tfrac{1}{2} \{ \rho O_{k'} O_k \right.$$

$$\dot{\rho} = \sum_{\substack{kk' \\ \neq 0}} K_{kk'} \left[O_k \rho O_{k'} - \tfrac{1}{2} \{ \rho, O_{k'} O_k \} \right]$$

$$K_{k'k} = K^*_{kk'}$$

Lindblad Form

Tom Barbara

- Notice that I have avoided the Kraus operators. This was pursued to see <u>exactly</u> the role that they played. Since $K_{k'k} = K^*_{kk'}$ we can express it in terms of eigenvalues

$$K_{kk'} = \sum_{l} \lambda_l V^*_{lk} V_{lk'}$$

which represents a partial factoring. A complete factoring would require that $\lambda_l = \mu_l \mu_l^*$ which implies $\lambda_l \geq 0$ as discussed earlier.

- If $K_{kk'} = \lambda_k \delta_{kk'}$ then the dynamics can be written as nested commutators

$$\dot{\rho} = \sum_{k} \tfrac{1}{2} \lambda_k [O_k, [O_k, \rho]]$$

- The general mathematical formalism is very complex. Since $K_{kk'}$ is $(N^2-1) \times (N^2-1)$ for a $N \times N$ matrix and even with $K_{kk'} = K^*_{k'k}$ the number of parameters is very large.

- We can proceed to find solutions by using the method of column vectorizing ρ as described earlier or we can also expand ρ in our basis set $\{O_m\}$. The second choice leads to a more compact matrix form as given next

Lindblad Master Equation Redux

Tom Barbara

$$\dot{\rho} = \sum_{kl} K_{kl} \left(O_k \rho O_l - \tfrac{1}{2}\left(\rho O_l O_k + O_l O_k \rho \right) \right)$$

$$= \sum_{kl} K_{kl} \tfrac{1}{2} \left\{ [O_k \rho, O_l] + [O_k, \rho O_l] \right\}$$

- These are very "compact" and we can glean more by being "verbose".

$$P^{kl} = \tfrac{1}{2} \left\{ [O_k \rho, O_l] + [O_k, \rho O_l] \right\}$$

$$\dot{\rho} = \sum_{kl} K_{kl} P^{kl}$$

$$= \sum_{kl} \tfrac{1}{2} K_{kl} P^{kl} + \tfrac{1}{2} K_{lk} P^{lk}$$

$$= \sum_{kl} \tfrac{1}{2} K_{kl} P^{kl} + \tfrac{1}{2} K^{*}_{kl} P^{lk}$$

$$= \sum_{kl} \tfrac{1}{2} (R_{kl} + i I_{kl}) P^{kl} + \tfrac{1}{2} (R_{kl} - i I_{kl}) P^{lk}$$

$$= \sum_{kl} \tfrac{1}{2} R_{kl} (P^{kl} + P^{lk}) + \tfrac{i}{2} I_{kl} (P^{kl} - P^{lk})$$

$$R_{kl} = R_{lk} \qquad I_{kl} = - I_{lk}$$

$$P^{kl} + P^{lk} = [O_k, [\rho, O_l]] + [O_l, [\rho, O_k]]$$

$$P^{lk} - P^{kl} = \{ O_l, [\rho, O_k] \} + \{ [O_l, \rho], O_k \} + 2 \{ [O_l, O_k], \rho \}$$

This shows the parts that have nested commutator evolution and that the "inhomogeneous part" comes from the imaginary part of K_{kl}. Viz for $\rho = \mathbb{1}$

$$\dot{\rho} = \sum_{kl} K_{kl} [O_k, O_l]$$

Operator Expansion

Tom Barbar

- Lets write out the operator expansion of the Lindbladian

$$\dot{\rho}_m = \sum_{n=0} \sum_{kl \neq 0} K_{kl} \rho_n \left[C_{lmkn} - \frac{1}{2}\left(C_{nmlk} + C_{mnlk} \right) \right]$$

where $C_{klmn} = Tr(O_k O_l O_m O_n) = \sum_p C_p^{kl} C_p^{mn}$

with $C_p^{kl} = Tr(O_k O_l O_p)$; $(C_p^{kl})^* = C_p^{lk} = C_k^{pl} = C_l^{kp}$

- Take care that the m, n and p indices include the identity while k l do not.

- The advantge here is the O_m are observables with expectation values $Tr(\rho O_m)$

- Symbolic Computation can be used to Calculate the C_{klmn}

For the 2x2 case we have the simplest example

$$O_0 = \frac{1}{\sqrt{2}} \mathbb{1} \quad O_1 = \frac{1}{\sqrt{2}} \sigma_x \quad O_2 = \frac{1}{\sqrt{2}} \sigma_y \quad O_3 = \frac{1}{\sqrt{2}} \sigma_z$$

$$\rho = \sum_n \rho_n O_n$$

Index shift! on K's

$$\begin{bmatrix} \dot{\rho}_0 \\ \dot{\rho}_1 \\ \dot{\rho}_2 \\ \dot{\rho}_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ i(K_{34} - K_{34}^*) & -(K_{44} + K_{33}) & \frac{1}{2}(K_{23} + K_{23}^*) & \frac{1}{2}(K_{24} + K_{24}^*) \\ i(K_{42} - K_{42}^*) & \frac{1}{2}(K_{23} + K_{23}^*) & -(K_{22} + K_{44}) & \frac{1}{2}(K_{34} + K_{34}^*) \\ i(K_{23} - K_{23}^*) & \frac{1}{2}(K_{24} + K_{24}^*) & \frac{1}{2}(K_{34} + K_{34}^*) & -(K_{33} + K_{22}) \end{bmatrix} \begin{bmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \rho_3 \end{bmatrix}$$

↳ K_{12} etc

- Since $\rho_0 = Tr(\rho O_0)$ $\dot{\rho}_0 = 0$ and this can be shown generally by evaluating C_{lmk0} explicitly.*

The matrix is <u>considerably</u> <u>simpler</u> than that obtained by vectorizing ρ and using Kroneker products.

* This means we will allways have at least one eigenvalue $= 0$.

Operator Expansion

Tom Barbara

- Since $\dot{\rho}_0 = 0$ we can take $\rho_0 = 1$ and then get an inhomogeneous equation

$$\begin{bmatrix} \dot{\rho}_1 \\ \dot{\rho}_2 \\ \dot{\rho}_3 \end{bmatrix} = \begin{bmatrix} -(k_4+k_3) & \mathrm{Re}\,K_{23} & \mathrm{Re}\,K_{24} \\ \mathrm{Re}\,K_{23} & -(k_2+k_4) & \mathrm{Re}\,K_{34} \\ \mathrm{Re}\,K_{24} & \mathrm{Re}\,K_{34} & -(k_3+k_2) \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{bmatrix}$$

$k_4 = K_{44}$
$k_3 = K_{33}$
etc

$$+ \begin{bmatrix} -2\,\mathrm{Im}\,K_{34} \\ -2\,\mathrm{Im}\,K_{42} \\ -2\,\mathrm{Im}\,K_{23} \end{bmatrix}$$

- The 2×2 case shows the "transport" matrix is real symmetric, but symmetric does not hold in general

- We can write $\dot{\rho}_m = \sum_n A_{mn}\rho_n$

with $$A_{mn} = \sum_{kl} K_{kl}\left\{ C_{lmkn} - \tfrac{1}{2}(C_{nmlk} + C_{mnlk})\right\}$$

but $C_{lmkn} = C_{nlmk} = C^*_{lnkm}$

$$A_{mn} = \sum_{kl} K_{kl}\left\{ \tfrac{1}{2}(C_{lmkn} + C^*_{lnkm}) - \tfrac{1}{2}(C_{nmlk} + C_{mnlk})\right\}$$

$$= \sum_{kl} K_{kl}\left(E^{lk}_{mn} - F^{lk}_{mn}\right)$$

$$E^{lk}_{mn} = E^{*lk}_{nm} \qquad F^{lk}_{mn} = F^{lk}_{nm}$$

So $A_{mn} \neq A_{nm}$ in general. This seems to go contrary to Onsager and his reciprocity theorem.... $A_{mn} = A_{nm}$ if K_{kl} is real symmetric $m,n \neq 0$ of course!

Bloch Equations via Lindblad

Tom Barbara

- The preceding dynamic matrix can be considerably simplified if symmetry prevails as with the case of magnetic resonance in liquids. We expect that no detectable change in behavior occurs upon rotation about the magnetic field axis. Taking the field along the z axis, the part independent of a rotation is

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -K_{44}-\frac{1}{2}(K_{22}+K_{33}) & 0 & 0 \\ 0 & 0 & -K_{44}-\frac{1}{2}(K_{22}+K_{33}) & 0 \\ -2I_{23} & 0 & 0 & -K_{33}-K_{22} \end{bmatrix}$$

$$I_{23} = \mathrm{Im}\,(K_{23})$$

- We can immediately identify this with

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -R_2 & 0 & 0 \\ 0 & 0 & -R_2 & 0 \\ -2I_{23} & 0 & 0 & -R_1 \end{bmatrix}$$

the solutions are easily found which then allows us to identify $-2I_{23}$ with $-R_1 M_0$ by comparing with $\dot{M}_z = -R_1(M_z - M_0)$, and therefore reproduce the Bloch relaxation matrix equations

$$\begin{bmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{bmatrix} = \begin{pmatrix} -R_2 & 0 & 0 \\ 0 & -R_2 & 0 \\ 0 & 0 & -R_1 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_1 M_0 \end{pmatrix}$$

- A less ad hoc connection to the physics requires a full treatment of Relaxation Theory developed by F. Bloch. Bloch's Theory incorporates all the features of Lindblad.