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Membranes and Meters

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We present a mathematical examination of the measurement and representation of membrane transport systems. Confronted with a coupled, multicomponent system, the experimentalist must choose meters which project out and make measurements upon subsystems in a rational manner. With a proper choice of projection operations, a representation of the composite system can be synthesized directly from the results of measurement. Starting from a set of basic axioms governing the measurement process, we apply the tenets of operator theory to the action of meters. We derive the projection operators associated with the representation of transport systems in terms of irreversible thermodynamics. The metric structure of this representation is explored from the viewpoint of measurement and the specification of identity. By means of concrete examples and a computational algorithm, the abstract, mathematical formalism is related to standard laboratory procedures.

1. Introduction

What does the biophysicist know about the transport of molecules across biological membranes? How is this knowledge obtained? How is this knowledge expressed, that is, represented symbolically? Ultimately, everything that the biophysicist knows about membrane transport processes is derived from the observation of meters in the laboratory. The data itself can be presented by tabulation or in graphical form. The data can also be used to determine some *ad hoc* mathematical function that "fits" the data. Thus, the set of meter readings is "reduced" to a smaller parameter set characteristic of the prescribed function. A third possibility is to reduce the data to a set of parameters pertaining to a mathematical model of permeation based upon underlying physical mechanisms. With a successful reduction to such a set of constitutive parameters, the biophysicist has some confidence that the associated transport equations represent the biological phenomena in an objective manner, independent of the measuring process. However, there is no *a priori* logical prohibition upon the possibility that the meter itself necessarily induces the form of the representation, thus making meter and representation inextricably linked.

This paper presents a mathematical examination of the measurement and representation of membrane transport systems. The first part is epistemological, with the development of a general, abstract theory. Though axiomatic, the theory is motivated by reflecting upon the task of the experimentalist, who, confronted with a complex, highly interacting biological system, must draw upon experience and intuition to

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devise a method to divide it into subsystems in a meaningful way. A commonplace representation resulting from such an isolation of and measurement upon component subsystems is the wall chart so often posted in biochemistry laboratories which depicts, in an integrated manner, the various subprocesses involved in the metabolism of glucose. The membrane biophysicist typically employs subsystems identified by the mobile molecular (possibly ionized) species: for example, sodium flux or water flux. These may not, however, be easy to measure in a direct manner, and the experimentalist may elect to work with subsystems identified by physical properties: for example, electric current or volume flux.

Certainly, any theory of measurement must address the problem of the reduction to (or, equivalently, the identification of) subsystems. In fact, we shall see that identification is central. In our theory, though it is concerned with the macroscopic, deterministic systems that one encounters in biology, the resolution into subsystems is analogous to the spectral decomposition of a quantum system into eigenstates. Just as quantum subsystems are identified by the specification of their associated eigenvalues (quantum numbers), the subsystems projected out of their biological context by the measurement process have identifying eigenvalues. A linear operator is ascribed to a given measurement process, and this operator determines the eigenvalues. The eigenstates comprise the set of appearances associated with the reduction to subsystems, and with them a representation of the composite system can be synthesized. It is, in fact, the best possible representation. At this point, the reader must be cautioned not to make too much of our appropriation of the mathematical forms and terminology of quantum mechanics. We use the forms but not the physics. We impose no quantum conditions, explicitly or implicitly.

The second part of this paper is practical. Our abstract theory of measurement has a concrete realization in the familiar transport equations of irreversible thermodynamics. However, the approach to these transport equations via an examination of the measurement process is unfamiliar. A membrane system in the context of a particular experimental situation can be represented by a single mathematical entity which we have called the response tensor. The response tensor varies as the external constraints on the membrane system are changed. The descriptions of all possible experiments on the system are thus contained in the space spanned by the response tensor. This space is a metric space, and the complete linear formalism of irreversible thermodynamics is provided by the geometric structure associated with the response tensor. The response tensor is composed of the eigenstates arising from actions of the operators used by the experimentalist to divide the system into the desired subsystems. As such, it is the optimal possible representation. We present a data reduction algorithm to calculate the constitutive parameters which characterize the membrane and determine the operators of the measurement process. Thus, the parameters of our unfamiliar theory can be determined from the familiar results of experiments by the membrane biophysicist.

The awesome success of 20th century physics has amply demonstrated what can be achieved by studying directly the mathematical structure underlying a phenomenon, rather than constructing in detail a mechanistic model. This paper is part of a continuing series devoted to a tensor algebra which has proved to be particularly

well suited for the study of complex systems. Although the paper is essentially self-contained, we shall draw upon notation and results from earlier papers, especially Richardson *et al.* (1982) and Richardson & Louie (1983).

2. The Measurement Process

Quantum mechanics, of all the sciences, possesses the most highly developed theory of measurement. Reduced to essentials, it posits that, by definition, *observables* are operators and that the result of a measurement is an eigenvalue of an observable. Furthermore, a representation of the state of the system can be given as a linear combination of the associated eigenvectors (eigenstates). Finally, a measurement repreated gives the same result as it did initially.

Operators, and hence observables, operate upon vectors, and in this case the vector describes the state of the system confronting the experimentalist. In principle and in practice the experimentalist cannot hope to obtain a "complete" description of the "whole" system that includes all possible modes of interaction with all other systems in its physical context. Experimentation proceeds by projecting out a series of subsystems, and any representation of the system is restricted to information gained by measurement on these subsystems. In Richardson & Louie (1983) we address the problem of how to synthesize a mathematical representation in an optimal manner directly from the results of measurements upon projected subsystems. We start with two basic postulates from that paper.

Postulate I

Nature is a Hilbert space N *over the real field, and it consists of invariants* $\mathbf{I}$, *which are not directly accessible.*

This is not as shocking as it might seem. At the very core of every scientific theory is the establishment of a direct correspondence between natural phenomena and mathematical objects. This remarkable abstraction is made even more audacious by the dictum that the correspondence is a full functor (in the terminology of category theory). Thus, any structure inherently associated with the mathematical objects must be manifested in the natural world. This, in fact, is the power and the test of any theory that purports to be more than mere curve-fitting. It is only reasonable to assume that the mathematical representation of natural phenomena as revealed to us by the mediation of *meters* must be done in a *metric* space. The distinction between real and complex fields corresponds to the distinction between the representation of deterministic, macroscopic phenomena, as addressed here, and the representation of probabilistic, quantum phenomena (see Richardson & Louie, 1986).

Postulate II

Real manifestations (*i.e. phenomena or appearances*) *are projections of* $\mathbf{I}$: *i.e.*

$$\mathbf{A}_\alpha = \hat{\mathfrak{P}}_\alpha \mathbf{I}, \tag{1}$$

where $\mathbf{A}_\alpha$ = *appearance* α *and* $\hat{\mathfrak{P}}_\alpha$ = *projector producing appearance* α.

In mathematical terms, a projector is a linear operator such that $\hat{\mathfrak{P}}_\alpha^2 = \hat{\mathfrak{P}}_\alpha$. In our earlier papers we made no distinction between the words *appearance* and *observable*,

although we did anticipate one and used the symbol $\mathbf{A}_a$ as a mnemonic notation. In the context of a theory of measurement, $\hat{\mathfrak{P}}_a$ is an *observable*. By its projector property, it operates on (1) to give

$$\hat{\mathfrak{P}}_a \mathbf{A}_a = \hat{\mathfrak{P}}_a^2 \mathbf{I} = \hat{\mathfrak{P}}_a \mathbf{I} = \mathbf{A}_a . \tag{2}$$

Therefore, the appearance $\mathbf{A}_a$ is an *eigenvector* (*eigenstate*) of the observable $\hat{\mathfrak{P}}_a$ associated with the *eigenvalue* (*quantum number*) $\lambda_a = 1$.

To get an intuitive notion of what this abstract formulation of a measurement means in the "real" world of experimentation, consider the use of flame-photometry to determine if, say, a sample of extracellular fluid contains sodium. The result of the measurement is binary: yes or no. Sodium, *per se*, is not measured. One uses an eyepiece or a photographic emulsion to determine whether or not there is a beam of light leaving the prism at a given angle ϑ (a rather old-fashioned spectrometer is assumed). The angle ϑ is determined by the wavelength of the sodium *D*-line and the index of refraction of the glass of the prism. The *observable* is the operation of projecting (via the prism) a beam of light to a detector at the angle ϑ. The light emanating from the sample in the flame is sent to the eigenstate $|\vartheta\rangle$. If the projected beam $|\vartheta\rangle$ is sent through a second spectrometer, the same result is found: namely a light band at ϑ. In the parlance of quantum mechanics this is called *wave-packet reduction*.

It was posited that the result of a measurement was the eigenvalue associated with the observable. If sodium is in the sample, the result of the experiment is *yes*, which corresponds to the eigenvalue $\lambda_\vartheta = 1$. Since there is a one-to-one correspondence between the eigenstate $|\vartheta\rangle$ and the eigenvalue $\lambda_\vartheta = 1$, the presence of sodium in the sample can be denoted $|\text{Na}\rangle \cong |\vartheta\rangle \cong |1\rangle$. The absence of sodium gives the null result $|\text{no Na}\rangle \cong |0\rangle$. Identity is thereby bestowed upon a system (i.e. a sample) by this particular observable. A system (or, to be more precise, the representation of its state) either "contains" the eigenstate or not. Its identity is either $|1\rangle$ or $|0\rangle$. Thus, its name is its eigenvalue (quantum number). If the experimentalist goes to the cabinet of reagents, takes a pinch of substance from a bottle labeled "sodium", and puts it into the flame, then he can make an empirical correlation between names: $|\text{sodium}\rangle \cong |\vartheta\rangle \cong |1\rangle$. However, as we shall see, science is deeper than mere convention.

3. Spectral Decomposition and Subsystems

The observable $\hat{\mathfrak{P}}_a$ projects out a subsystem. The subsystem is the eigenstate $\mathbf{A}_a$ (i.e. the appearance) and is identified by the related eigenvalue. If a set of observables $\{\hat{\mathfrak{P}}_i : i = 1, \ldots, m\}$ is carefully chosen so that they are orthogonal; that is,

$$\hat{\mathfrak{P}}_i \hat{\mathfrak{P}}_j = \hat{0} \quad \text{for } i \neq j \tag{3}$$

or, since $\hat{\mathfrak{P}}_i^2 = \hat{\mathfrak{P}}_i$,

$$\hat{\mathfrak{P}}_i \hat{\mathfrak{P}}_j = \delta_{ij} \hat{\mathfrak{P}}_i , \tag{4}$$

then this decomposition into subsystems provides a remarkably simple way to make a mathematical representation of the whole system using the eigenstates. The representation is

$$\mathbf{R} = \sum_i \mathbf{A}_i, \tag{5}$$

and not only is it simple, but it is also the best one possible in that $\|\mathbf{I} - \mathbf{R}\|$ is minimal [see Richardson & Louie (1983) Postulate III for details]. Rosen's (1984) "orthogonal projection experiment" uses this optimality principle in a powerful empirical procedure for parameter estimation in very large systems.

For this canonical set of observables, there is a set of eigenvalues associated with a given projector $\hat{\mathfrak{P}}_\alpha$; that is,

$$\hat{\mathfrak{P}}_\alpha \mathbf{A}_\alpha = \hat{\mathfrak{P}}_\alpha(\hat{\mathfrak{P}}_\alpha \mathbf{I}) = \hat{\mathfrak{P}}_\alpha^2 \mathbf{I} = \hat{\mathfrak{P}}_\alpha \mathbf{I} = \mathbf{A}_\alpha \tag{6}$$

gives an eigenvalue of 1, and

$$\hat{\mathfrak{P}}_\alpha \mathbf{A}_\beta = \hat{\mathfrak{P}}_\alpha \hat{\mathfrak{P}}_\beta \mathbf{I} = \hat{\mathfrak{O}} \mathbf{I} = 0 \mathbf{A}_\beta \tag{7}$$

gives an eigenvalue of 0 for all $\beta \neq \alpha$. This *spectrum* identifies the subsystem α, and thus the name of this subsystem is

$$|\alpha\rangle = |0, 0, \ldots, 1, \ldots, 0\rangle \tag{8}$$

with m entries and 1 at entry α.

To see what this means in concrete terms, return to the example of sodium. There are many ways to identify sodium besides naming it by its spectral band location $|\vartheta\rangle$. Much of the science of chemistry derives from naming atoms in terms of elementary constituents: electrons, protons, and neutrons. These comprise the three subsystems of all atoms and hence are associated with three observables: $\hat{\mathfrak{P}}_e$, $\hat{\mathfrak{P}}_p$, and $\hat{\mathfrak{P}}_n$. The spectra which identify the three subsystems are then

$$\begin{aligned} \mathbf{A}_1 &\cong |e\rangle \cong |\overset{e}{1}, \overset{p}{0}, \overset{n}{0}\rangle \\ \mathbf{A}_2 &\cong |p\rangle \cong |0, 1, 0\rangle \\ \mathbf{A}_3 &\cong |n\rangle \cong |0, 0, 1\rangle. \end{aligned} \tag{9}$$

Since sodium has 11 electrons, 11 protons, and 12 neutrons, its name in terms of the given subsystems is

$$\begin{aligned} |\mathrm{Na}\rangle &\cong 11|e\rangle + 11|p\rangle + 12|n\rangle \\ &\cong |11, 11, 12\rangle. \end{aligned} \tag{10}$$

Here sodium is identified by its hierarchical structure rather than by convention. As we indicated in Richardson & Louie (1983: section 7), such a *spectral decomposition* is general.

Consider an arbitrary linear operator $\hat{\mathfrak{R}}$, which is assumed to be self-adjoint. This condition has important physical significance because it ensures that the eigenvalues

are real: cf. Dirac (1958). Is $\hat{\mathfrak{R}}$ an observable? The question can be answered only operationally (in the empirical sense of the word), by considering what meters are available to measure the action upon the system by the physical process represented by $\hat{\mathfrak{R}}$ (in the mathematical realm, $\hat{\mathfrak{R}}$ acts upon the invariant $\mathbf{I}$, which is characteristic of the state of the system). The experimentalist has at hand a set of meters, compatible with the proposed observable, whose actions upon the system are determined mathematically by the basic projectors $\{\hat{\mathfrak{P}}_i: i=1, \ldots, m\}$ and whose unit readings correspond to the associated eigenvalues, 0 or 1. Therefore, the only empirically meaningful action of $\hat{\mathfrak{R}}$ is its restriction to the linear span of the basic projectors. All one can really "know" about $\hat{\mathfrak{R}}$ as an observable is given by the action of

$$\hat{\mathfrak{R}}|_D \equiv \hat{\mathfrak{P}} = \lambda_i \hat{\mathfrak{P}}_i, \tag{11}$$

where D denotes the space of possible descriptions of the system that can be obtained via the available meters. Here and in the following we use the Einstein summation convention over repeated Latin indices, but no summation over repeated Greek indices.

The expansion (11) is valid and unique, it being essentially a statement of the *Spectral Theorem*. The decomposition (11) is in fact called the *spectral resolution* of $\hat{\mathfrak{P}}$, giving a self-adjoint operator as a sum of projectors. The complete set of these projectors defines the class of *compatible* (but not necessarily *available*) meters. Thus, the self-adjoint assumption is seen to be crucial because it allows $\hat{\mathfrak{R}}$ to be decomposed according to subsystems defined by the actions of meters. Furthermore, as a sum of mutually orthogonal projectors, $\hat{\mathfrak{P}}$ is itself a projector and produces an appearance $\mathbf{A} = \hat{\mathfrak{P}}\mathbf{I}$. Obviously, $\mathbf{A}$ is an eigenstate of $\hat{\mathfrak{P}}$. The problem is to relate $\mathbf{A}$ to the various eigenstates, $\mathbf{A}_\alpha$, associated with the meters. Since

$$\begin{aligned}\hat{\mathfrak{P}}\mathbf{A}_\alpha &= (\lambda_i \hat{\mathfrak{P}}_i)\hat{\mathfrak{P}}_\alpha \mathbf{I} = (\lambda_i \hat{\mathfrak{P}}_i)\hat{\mathfrak{P}}_\alpha^2 \mathbf{I} \\ &= \lambda_i (\hat{\mathfrak{P}}_i \hat{\mathfrak{P}}_\alpha)\mathbf{A}_\alpha = \lambda_i \delta_{i\alpha} \mathbf{A}_\alpha \\ &= \lambda_\alpha \mathbf{A}_\alpha, \end{aligned} \tag{12}$$

it is seen that the λ_i in (11) are eigenvalues of $\hat{\mathfrak{P}}$. In addition,

$$\mathbf{A} = \hat{\mathfrak{P}}\mathbf{I} = \lambda_i \mathfrak{P}_i \mathbf{I} = \lambda_i \mathbf{A}_i. \tag{13}$$

Therefore, the composite appearance $\mathbf{A}$ is a linear combination of the basic appearances with coefficients provided by the eigenvalues of the operational (i.e. empirical) decomposition of the observable $\hat{\mathfrak{R}} \mapsto \hat{\mathfrak{P}}$. The name of the composite system in terms of subsystems is given by the spectrum of $\hat{\mathfrak{P}}$; thus

$$\begin{aligned}|\mathbf{A}\rangle &\cong \lambda_i |\mathbf{A}_i\rangle \\ &\cong |\lambda_1, \lambda_2, \ldots, \lambda_m\rangle, \end{aligned} \tag{14}$$

where this spectrum is simply an ordered set of meter readings. From this general argument, it is seen that the numbers in the name of sodium (10) are eigenvalues. Two levels of hierarchical description are related by the eigenvalues of the composite observable (projector) connecting the different levels. The proper task for theoretical

science is to discover the connections between different descriptions (representations). The representation $|\vartheta\rangle$ for sodium and that given by (10) are not hierarchically related, and their relationship is not as simple as the phenomenological connection (14). Given the atomic structure in (10), one can use quantum mechanics to calculate the emission frequencies. Given the frequency for the D-line and the index of refraction for the prism, one can then calculate the angle ϑ.

4. Constitutive Parameters and Projectors

In measurement by flame photometry, the name $|\vartheta\rangle$ is determined by a constitutive parameter of the meter: the index of refraction of the prism. In this section the relationship between observables (projectors) and constitutive parameters will be examined. The appearances $\mathbf{A}_\alpha$ are eigenvectors of the projectors. In the search for the mathematical connections between descriptions, it is obvious that the appearances must be assigned some mathematical structure. In Richardson *et al.* (1982) we postulate that the $\mathbf{A}_\alpha$ are elements of a subspace of the metric space $T^1_1(V)$ of dyadics over V, the vector space $\mathbb{R}^n$ [in Louie *et al.* (1982) this is generalized to $T^1_1(H)$ over Hilbert spaces, H]. This subspace is the space spanned by the *response tensor* (dyadic)

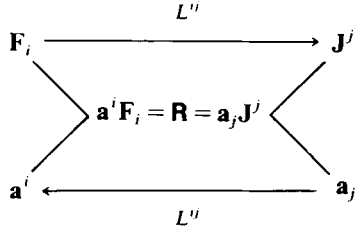
$$\mathbf{R} = \sum_i \mathbf{A}_i = \mathbf{a}^i \mathbf{F}_i, \tag{15}$$

where $\mathbf{F}_i \in V$ are generalized forces and $\mathbf{a}^i \in V^*$ are constitutive parameters. The tensor $\mathbf{R}$ is a mapping $V^* \mapsto V^*$ defined by

$$\begin{aligned} \mathbf{R}(\mathbf{a}^j, \cdot) &= \mathbf{a}^i \mathbf{F}_i(\mathbf{a}^j, \cdot) = (\mathbf{a}^i \cdot \mathbf{a}^j)\mathbf{F}_i \\ &= L^{ji}\mathbf{F}_i \\ &\equiv \mathbf{J}^j, \end{aligned} \tag{16}$$

where, by the symmetry of the dot product, $L^{ij} = L^{ji}$. By definition the $\mathbf{J}^i$ are generalized fluxes. At this point, the mathematical development is general, and we need not make any thermodynamic assumptions about the nature of the forces and fluxes.

The metric space spanned by $\mathbf{R}$ is called description space (D-space). In earlier work we have demonstrated that it provides a rich and powerful means for the representation of natural systems. We cannot present a full development of this phenomenological approach here, but shall indicate its most salient features in the following Duality-Invariance-Diagram (DID):



(17)

The mapping $\mathbf{a}^i = L^{ij}\mathbf{a}_j$ is a consequence of the invariance of $\mathbf{R}$ (indicated in the center of the DID) in the two representations.

A given D-space is determined by a fixed set of constitutive parameters $\{\mathbf{a}^i\}$. The index i refers to subsystem i as determined by the observable $\hat{\mathfrak{P}}_i$. This index ranges from $i=1$ to m, where m is independent of the dimension n of the underlying vector space V. Thus, $m = \dim D$ may be smaller, equal to, or larger than $n = \dim V$. The identity (name) of subsystem α is given by (8) as a spectrum.

A lucid and instructive example of the relationship between spectra, observables, and constitutive parameters is provided by an incorporation of Dirac's ket and bra notation into the metric geometry implied by (17). One should be alert to notice that the usage here is significantly different in mathematical content, if not in form, from that of Dirac (1958); see also Friedman (1956). Here $\mathbf{a}_i \in V$, and the associated ket belongs to the space of linear operators from N to V; that is, $|\mathbf{a}_i\rangle \in L(N, V)$. Likewise, $\mathbf{a}^i \in V^*$ and $\langle \mathbf{a}^i| \in L(N, V^*)$. The usual response tensor (which belongs to the product space $V \otimes V^*$) becomes the hybrid response tensor

$$\mathbf{R} = \mathbf{F}_i \langle \mathbf{a}^i| = |\mathbf{a}_j\rangle \mathbf{J}^j. \tag{18}$$

The exact interpretation of this "hybrid" is given in Appendix A. The actions of the kets and bras upon $\mathbf{R}$ are [cf. Richardson & Louie (1983: (46) and (47))]

$$\mathbf{R}|\mathbf{a}_\alpha\rangle = \mathbf{F}_\alpha \quad \text{and} \quad \langle \mathbf{a}^\beta|\mathbf{R} = \mathbf{J}^\beta, \tag{19}$$

where the Dirac notation necessitates the distinction between right-hand and left-hand operators.

What is the projector that sends $\mathbf{R} = \mathbf{I}$ to $\mathbf{A}_\alpha$ and thereby operationally establishes the identity of subsystem α? Consider the candidate projector

$$\hat{\mathfrak{P}}_\alpha = |\mathbf{a}_\alpha\rangle\langle \mathbf{a}^\alpha| \tag{20}$$

which operates (on the right-hand side) upon $\mathbf{R}$ as follows:

$$\hat{\mathfrak{P}}_\alpha(\mathbf{R}) = \mathbf{R}\hat{\mathfrak{P}}_\alpha = (\mathbf{R}|\mathbf{a}_\alpha\rangle)\langle \mathbf{a}^\alpha| = \mathbf{F}_\alpha \langle \mathbf{a}^\alpha| = \mathbf{A}_\alpha. \tag{21}$$

The dual projector [as regards D-space: cf. Richardson & Louie (1983: (15))] is

$$\hat{\mathfrak{Q}}^\beta = |\mathbf{a}_\beta\rangle\langle \mathbf{a}^\beta|, \tag{22}$$

which operates (on the left-hand side) upon $\mathbf{R}$ as follows:

$$\hat{\mathfrak{Q}}^\beta(\mathbf{R}) = \hat{\mathfrak{Q}}^\beta \mathbf{R} = |\mathbf{a}_\beta\rangle(\langle \mathbf{a}^\beta|\mathbf{R}) = |\mathbf{a}_\beta\rangle \mathbf{J}^\beta = \mathbf{A}^\beta. \tag{23}$$

An important relationship between the bra and ket operators is established by combining (18) and (19): namely,

$$\mathbf{R}|\mathbf{a}_\alpha\rangle = \mathbf{F}_i \langle \mathbf{a}^i|\mathbf{a}_\alpha\rangle = \mathbf{F}_\alpha \tag{24}$$

and

$$\langle \mathbf{a}^\beta|\mathbf{R} = \langle \mathbf{a}^\beta|\mathbf{a}_j\rangle \mathbf{J}^j = \mathbf{J}^\beta. \tag{25}$$

In effect, this states that

$$\langle \mathbf{a}^i | \mathbf{a}_j \rangle = L^{ik} \langle \mathbf{a}_k | \mathbf{a}_j \rangle = L^{ik} L_{kj} = \delta^i_j. \tag{26}$$

One should note that this "orthogonality" condition is on the linear operators and not upon the vectors $\mathbf{a}^i$ and $\mathbf{a}_j$. In D-space the action of the L^{ij} operator is that of a metric tensor, and thus the number of metrically related subsystems is not limited by $n = \dim V$ but rather is determined by $m = \dim D$. However, (26) does not imply that the matrix L^{ik} has a unique inverse (see Appendix B).

It is now possible to show that the candidate projector (20) does in fact satisfy the essential conditions (3) and (4); indeed,

$$\begin{aligned} \hat{\mathfrak{P}}_\alpha \hat{\mathfrak{P}}_\beta &= |\mathbf{a}_\alpha\rangle\langle \mathbf{a}^\alpha | |\mathbf{a}_\beta\rangle\langle \mathbf{a}^\beta| \\ &= |\mathbf{a}_\alpha\rangle \delta^\alpha_\beta \langle \mathbf{a}^\beta| \\ &= \delta^\alpha_\beta \hat{\mathfrak{P}}_\alpha . \end{aligned} \tag{27}$$

We are brought to a truly remarkable conclusion. The name of a subsystem, determined operationally by measurement, is the name of the measuring device. That is, the observable is determined completely by constitutive parameters via (20). To see that this is not so far-fetched, consider the following simple laboratory procedure. Cells are suspended in a solution, homogenized sonically, and then filtered through a millipore filter with pores of diameter d. The only name that can be given to the filtrate is "the stuff that goes through a millipore filter with pores of diameter d". This example can be extrapolated to a more sophisticated level by considering (17) to be the DID representing a transport system with $\mathbf{F}_i$ and $\mathbf{J}^i$ denoting the forces and fluxes of molecular (or ionic) species i. In this case the identity of species i is determined by the observable (20), which in turn is determined completely and solely by the constitutive parameter $\mathbf{a}_i$. Just as the diameter d determines the permeability properties of a millipore filter, the set $\{\mathbf{a}_i\}$ determines permeabilities via the phenomenological coefficients $L^{ij} \equiv \langle \mathbf{a}^i | \mathbf{a}^j \rangle$. As a final example, recall that pH is measured using an *ion-selective* glass electrode. In Appendix C we address a crucial question: namely, can the $\mathbf{a}^i$ be determined empirically? At first glance there appears to be a serious mathematical difficulty, which, however, is easily resolved.

The prototype of linear force–flux relationships is the phenomenological equation of Ohm: $E = RI$. A plot of E as a function of I for an incandescent lamp with a tungsten filament is essentially cubic. The behavior of this simple device does not mean that Ohm's law must be abandoned. Rather, the non-linearity is ascribed to the resistance. Ohm's law is then seen to be locally linear and globally non-linear, with the resistance operationally well defined by the ratio $R(I) = E(I)/I$. This observation can be generalized to the more complex systems described by the DID (17) by allowing the constitutive parameters $\mathbf{a}_j$ to be functions of one or more of the fluxes: that is, $\mathbf{a}_j = \mathbf{a}_j(\mathbf{J})$ or, in the dual space, $\mathbf{a}^i = \mathbf{a}^i(\mathbf{F})$. It remains to be seen what advantages a description of a complex biological system in terms of a non-linear geometry might have over a head-on modeling of detailed mechanisms and structures. Riemannian D-spaces have proved to be well suited for the analysis of dissipative systems that age (Richardson & Louie, 1986). Lastly, the fact that in every instance

the response tensor is bilinear has significant implications for the Principle of Superposition in highly-interacting systems, with, for example, practical consequences for the interpretation of tracer fluxes (Richardson, 1989).

5. Hierarchical Connections

A set of projectors $\{\hat{\mathfrak{P}}_i\}$ (chosen at the discretion of the experimentalist) "quantizes" the system by a division into discrete subsystems. Because of the basic physical composition of natural systems, it is not unexpected that subsystems often are physical particles (elementary or aggregated). In the case of transport across biological membranes, the division of fluxes and forces into subsystems is according to molecular and ionic species: for example, $i=1=\mathbf{J}^{\mathrm{Na}}$, $i=2=\mathbf{J}^{\mathrm{K}}$, $i=3=\mathbf{J}^{\mathrm{Cl}}$, etc. In this case the DID (17) provides a representation of the system at a *particulate* level in the hierarchy of descriptions. Nevertheless, the division of a system into subsystems need not result in "quanta" that are particles. In electrophysiology, for example, measurements are generally made of state variables such as electric current and pressure gradient which have no particulate character. Here the DID (17) provides a representation at the *systemic* level in the hierarchy of descriptions.

A hierarchical analysis of dissipative systems is given in Richardson (1985), and that formulation will be used here (with slight notational changes) in an investigation of the connection between observables and names belonging to representations at different hierarchical levels. The flux of particle k is denoted $\mathbf{J}^k$ and is related to the forces $\mathbf{F}_i$ $(i=1,\ldots,m)$ by the DID (17): $\mathbf{J}^k=L^{ki}\mathbf{F}_i$. Each particle carries with itself certain properties, such as mass and volume. The flux of such properties, $\mathbf{\Gamma}^i$, is obviously just

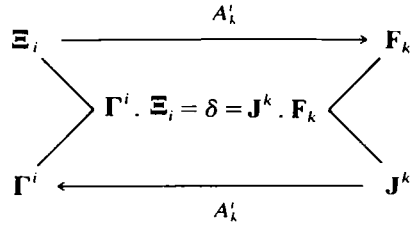
$$\mathbf{\Gamma}^i=A^i_k\mathbf{J}^k, \tag{28}$$

where the *scale factors* A^i_k are the partial molar quantities such as charge per mole of species k, $\bar{Z}_k$. The double index thus relates systemic properties such as charge to a given particle species. In this case $\mathbf{\Gamma}^i$ would be current, with (28) being $\mathbf{\Gamma}^i=\mathbf{I}=\bar{Z}_k\mathbf{J}^k$. Likewise, in the systemic description there are fields $\mathbf{\Xi}_i$ related to forces by

$$\mathbf{F}_k=\mathrm{A}^i_k\mathbf{\Xi}_i. \tag{29}$$

The fields commonly include $\nabla\psi$, ∇T, and ∇p, where $\psi=$electrostatic potential, $T=$temperature, and $p=$pressure [see Richardson (1985) for details, especially for the treatment of the concentration-dependent part of the Gibbs potential].

The hierarchical connections (28) and (29) between the particulate and systemic descriptions can be expressed by the following Adjoint-Invariance-Diagram (AID): see Louie & Richardson (1983) and Richardson & Louie (1983). The invariant connecting the two descriptions in (30) is the dissipation function δ (which is given a geometric representation as the norm on the response tensor by the metric $\|\mathbf{R}(p)\|^2=L^{ij}\mathbf{F}_i\,.\,\mathbf{F}_j=\mathbf{J}^i\,.\,\mathbf{F}_i\equiv\delta$). An explicit indication that the response tensor, $\mathbf{R}(p)$, refers to the particulate representation is required because the AID (30) does not itself establish $\mathbf{R}$ as an invariant of the hierarchical connection (it is, as will be seen). There is



(30)

a DID (17) for the systemic representation with constitutive parameters $\mathbf{b}^i$ and $\|\mathbf{R}(s)\|^2 = K^{ij}\Xi_j \cdot \Xi_i \equiv \delta$ with $K^{ij} = \mathbf{b}^i \cdot \mathbf{b}^j$.

The connections between the two descriptions are derived directly from the necessary congruences between the two DIDs and the AID. For example, from

$$\begin{aligned}\Gamma^i = A^i_k \mathbf{J}^k = A^i_k (L^{kj}\mathbf{F}_j) = A^i_k L^{kj}(A^h_j \Xi_h) \\ = A^i_k (\mathbf{a}^k \cdot \mathbf{a}^j) A^h_j \Xi_h\end{aligned} \tag{31}$$

one finds

$$\mathbf{b}^i = A^i_k \mathbf{a}^k \tag{32}$$

since

$$\Gamma^i = K^{ih}\Xi_h = (\mathbf{b}^i \cdot \mathbf{b}^h)\Xi_h. \tag{33}$$

The response tensor in the systemic representation is then

$$\mathbf{R}(s) = \mathbf{b}^i \Xi_i = A^i_k \mathbf{a}^k \Xi_i = \mathbf{a}^k \mathbf{F}_k = \mathbf{R}(p), \tag{34}$$

and so, indeed, the response tensor is an invariant. From the corresponding invariance of $\mathbf{R}$ as represented in the dual of D-space, it is easy to show that

$$\mathbf{a}_i = A^k_i \mathbf{b}_k. \tag{35}$$

The final question to be addressed is: can one hope to find a spectral resolution such as (11) and (13) that connects the observables and appearances at the two levels of description? Actually, the situation here is not so simple, but, nevertheless, is quite interesting.

The projectors are given as in (20) by

$$\hat{\mathfrak{P}}_\alpha(p) = |\mathbf{a}_\alpha\rangle\langle\mathbf{a}^\alpha| \tag{36}$$

and

$$\hat{\mathfrak{P}}_\alpha(s) = |\mathbf{b}_\alpha\rangle\langle\mathbf{b}^\alpha|. \tag{37}$$

Substituting (35) into (36) yields

$$\hat{\mathfrak{P}}_\alpha(p) = \mathrm{A}^k_\alpha |\mathbf{b}_k\rangle\langle\mathbf{a}^\alpha|; \tag{38}$$

while (32) into (37) yields

$$\hat{\mathfrak{P}}_\alpha(s) = |\mathbf{b}_\alpha\rangle\langle A_k^\alpha \mathbf{a}^k| = A_k^\alpha |\mathbf{b}_\alpha\rangle\langle \mathbf{a}^k|. \tag{39}$$

That is, the spectral resolutions, analogous to (11), are

$$\hat{\mathfrak{P}}_\alpha(p) = A_\alpha^k \hat{\mathfrak{E}}_k^\alpha \tag{40}$$

and

$$\hat{\mathfrak{P}}_\alpha(s) = A_k^\alpha \hat{\mathfrak{E}}_\alpha^k \tag{41}$$

where

$$\hat{\mathfrak{E}}_\alpha^\beta = |\mathbf{b}_\alpha\rangle\langle \mathbf{a}^\beta|, \tag{42}$$

which we shall call *relative operators*. Note that on the particulate level (40) the summation is over the upper index of the scale factors, while on the systemic level (41) the dual summation is over the lower index of the scale factors.

As for appearances, on the one hand

$$\hat{\mathfrak{P}}_\alpha(p)\mathbf{R} = \mathbf{A}_\alpha = \mathbf{F}_\alpha\langle \mathbf{a}^\alpha| = A_\alpha^k \Xi_k \langle \mathbf{a}^\alpha|, \tag{43}$$

and on the other hand

$$\hat{\mathfrak{P}}_\alpha(p)\mathbf{R} = A_\alpha^k \hat{\mathfrak{E}}_k^\alpha \mathbf{R}. \tag{44}$$

Thus, defining *relative appearances* as

$$\mathbf{e}_k^\alpha = \hat{\mathfrak{E}}_k^\alpha \mathbf{R} = \Xi_k \langle \mathbf{a}^\alpha|, \tag{45}$$

we have, analogous to (13),

$$\mathbf{A}_\alpha = A_\alpha^k \mathbf{e}_k^\alpha. \tag{46}$$

Dually, on the systemic level we have

$$\hat{\mathfrak{P}}_\alpha(s)\mathbf{R} = \mathbf{B}_\alpha = A_k^\alpha \mathbf{e}_\alpha^k. \tag{47}$$

6. The Transformation of Names

In (8) the name of subsystem α determined by the observable $\hat{\mathfrak{P}}_\alpha$ is given as an m-tuple of the m eigenvalues associated with $\hat{\mathfrak{P}}_\alpha$, with 1 at the αth entry and zeros elsewhere. There are m such spectra, or names. Mathematically (without regard to physical meaning) such a collection of m-tuples forms the standard basis of the vector space $\mathbb{R}^m$. The physical meaning of this vector space becomes apparent upon considering the name (14) of the spectral decomposition (12) and (13) of an arbitrary appearance $\mathbf{A}$ in the D-space determined by the given observables $\{\hat{\mathfrak{P}}_k\}$, $k = 1, \ldots, m$. For a better notation, let the name $|\mathbf{A}_k\rangle = |0, \ldots, 1, \ldots, 0\rangle$ (1 at the kth entry) be simply $|k\rangle$. Then (14) is

$$|\mathbf{A}\rangle = \lambda_k |k\rangle, \tag{48}$$

which shows immediately how any name $|\mathbf{A}\rangle$ can be expressed in terms of the set of m basis vectors $\{|k\rangle\}$. Therefore, this vector space will be called *name-space*.

There is no direct connection between the name-spaces of two different D-spaces which come about from dividing a given system into two different sets of subsystems. Consider the preceding division of a transport system into a particulate representation and into a systemic representation. If there are m species of particles, then there are m subsystems, and the dimension of this name-space is m. If, on the other hand, there are r fields, then the dimension of name-space in the systemic representation is r. Obviously, there is no one-to-one transformation between $\mathbb{R}^m$ and $\mathbb{R}^r$ for $m \neq r$. Nevertheless, there does exist a very interesting transformation of names connecting these two levels in the hierarchy of descriptions in a relative manner.

Let $|k(p)\rangle$ be the kth basis vector of the name-space in the particulate description. Consideration of the relative spectral decomposition (46) leads to the following transformation:

$$\overset{1 \ \ldots \ k \ \ldots \ m}{|0, \ldots, 1, \ldots, 0\rangle} \begin{pmatrix} A_1^1 & \cdots & A_1^i & \cdots & A_1^r \\ \vdots & & \vdots & & \vdots \\ A_k^1 & \cdots & A_k^i & \cdots & A_k^r \\ \vdots & & \vdots & & \vdots \\ A_m^1 & \cdots & A_m^i & \cdots & A_m^r \end{pmatrix} = |A_k^1, \ldots, A_k^i, \ldots, A_k^r\rangle. \quad (49)$$

The basis vector $|k(p)\rangle$, which is the name (spectrum) of subsystem k, is transformed to a vector of dimension r. This gives the name of $|k(p)\rangle$ relative to the systemic representation; hence the transformed vector will be denoted $|k(p;s)\rangle$. With this notation (49) is

$$|k(p)\rangle[A_k^i] = |k(p;s)\rangle, \quad (50)$$

where $[A_k^i]$ is the $r \times m$ matrix of the scale factors. Since the $|k(p)\rangle$ are basis vectors, any arbitrary name $|\mathbf{A}(p)\rangle = \lambda_k |k(p)\rangle$ as given by (48) transforms linearly by (50). Analogous to (49) and (50), the basis vectors of the name-space for the systemic representation transform via (47) as

$$[A_k^i]\langle i(s)| = \langle i(s;p)|. \quad (51)$$

The physical content of (49) is easy to see upon considering an example from transport theory, with subsystem $k(p)$ as sodium ($\mathbf{J}^k$ being the flux of sodium). Here $|k(p)\rangle = |\mathrm{Na}(p)\rangle$ is the name of sodium, which by (49) transforms to $|A_k^1, \ldots, A_k^i, \ldots, A_k^r\rangle = |\bar{M}_{\mathrm{Na}}, \bar{V}_{\mathrm{Na}}, \bar{Z}_{\mathrm{Na}}, \ldots\rangle$, where $\bar{M}$, $\bar{V}$, $\bar{Z}$ are, respectively, partial molar mass, volume, and charge (Richardson, 1985). This $|k(p;s)\rangle = |\mathrm{Na}(p;s)\rangle$ is obviously a name for sodium.

An important conclusion to be drawn from our discussion of measurements on complex systems is that there are no unique names. Names are bestowed operationally by the actions of the observables, $\hat{\mathfrak{B}}_i$. Any two objects having the same physical properties as regards the set of observables used by the experimentalist will receive the same name. Since the "restriction to subspace" operation $.|_D$ is not injective, it is possible to have two operators $\hat{\mathfrak{R}} \neq \hat{\mathfrak{M}}$ such that $\hat{\mathfrak{R}}|_D = \hat{\mathfrak{M}}|_D$. For example,

if the observable is an operator that determines ionic charge, then Na^+ and K^+ have the same name: |monovalent cation⟩. In the nomenclature of Rosen (1978), they belong to the same "equivalence class". This work should be consulted for a theory of measurement of natural systems which is mathematically and methodologically different from the one we have presented here. An analysis of measurement in terms of category theory is presented in Louie (1985). Though differing significantly in approach, these and the present theory are conceptually convergent—in spite of Rosen's (1978: 26) summary dismissal of the measurement theory of quantum mechanics as being "in a chaotic state". As an introduction to measurement theory and epistemology the Tarner lectures of Eddington (1939) remain unequaled.

IWR dedicates this paper to the memory of his teacher Aharon Katchalsky, a master of irreversible thermodynamics and a pioneer in its application to biophysics.

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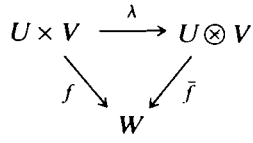
APPENDIX A

Adjoint Associativity

The ket and bra operators introduced in section 4, being linear operators from a tensor product space to a vector space, have very interesting properties. We shall start with a general concept. Let U, V, and W be vector spaces; then the theorem of adjoint associativity states that

$$L[U, L(V, W)] = L(U \otimes V, W) \tag{A.1}$$

[i.e. $-\otimes V$ is the left adjoint of the hom functor $L(V, -)$]. Another way of expressing this is that for every bilinear $f: U \times V \to W$ there exists a unique $\bar{f}: U \otimes V \to W$ such that the diagram



(A.2)

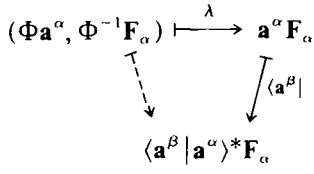
commutes [where λ is the "generator map" $(u, v) \mapsto u \otimes v$].

Now let $\mathbf{a}^\beta \in V^*$, and consider the bra operator $\langle \mathbf{a}^\beta | \in L(N, V^*) = L(V \otimes V^*, V^*)$. Recall that its action on $\mathbf{R} = \mathbf{a}^i \mathbf{F}_i$ is

$$\langle \mathbf{a}^\beta | \mathbf{R} = \mathbf{R}(\mathbf{a}^\beta, \cdot) = \mathbf{a}^i \mathbf{F}_i(\mathbf{a}^\beta, \cdot) = \langle \mathbf{a}^\beta | \mathbf{a}^i \rangle^* \mathbf{F}_i = L^{\beta i} \mathbf{F}_i = \mathbf{J}^\beta. \tag{A.3}$$

What is the bilinear map from $V \otimes V^*$ to V^* that corresponds to it?

Each term $\mathbf{a}^\alpha \mathbf{F}_\alpha$ of the dyadic $\mathbf{R}$ is in fact the generator $\Phi \mathbf{a}^\alpha \otimes \Phi^{-1} \mathbf{F}_\alpha$ (where $\Phi : V^* \to V$ is the isometric isomorphism; cf. Louie *et al.*, 1982). Thus, the following diagram commutes:



(A.4)

whence for $\mathbf{y} \in V$ and $\mathbf{b} \in V^*$, $[\mathbf{a}^\beta] : (\mathbf{y}, \mathbf{b}) \mapsto \langle \Phi \mathbf{a}^\beta | \mathbf{y} \rangle^* \Phi \mathbf{b}$ is the bilinear map that corresponds to $\langle \mathbf{a}^\beta |$.

In particular, the association with each $\mathbf{y} \in V$ of the map $[\mathbf{a}^\beta](\mathbf{y}, \cdot) = \langle \Phi \mathbf{a}^\beta | \mathbf{y} \rangle \cdot$ from V to V^* is the morphism (a scalar multiplication operator) in $L[V, L(V^*, V^*)]$ corresponding to $\langle \mathbf{a}^\beta | \in L(V \otimes V^*, V^*)$.

Thus, $\mathbf{a}^\beta \in V^*$ leads to two isomorphic operators, $\langle \mathbf{a}^\beta |$ and $[\mathbf{a}^\beta]$, the former mapping tensors to dual vectors, and the latter mapping vectors to scalar multiplications. It is in this latter sense that $\langle \mathbf{a}^\beta |$ can be considered itself a dual vector (i.e. a "co-ordinate" in the representation $\mathbf{a}^i \mathbf{F}_i$). Hence, $\mathbf{R} = \mathbf{F}_i \langle \mathbf{a}^i |$ can be interpreted as (isomorphic to) a tensor, thus justifying the term "hybrid response tensor".

Similarly, the ket vector $|\mathbf{a}_\alpha\rangle \in L(V^* \otimes V, V)$ is isomorphic to a morphism $[\mathbf{a}_\alpha] \in L[V^*, L(V, V)]$. Note that the bra and ket operators map responses to "components", and their isomorphic operators $[\mathbf{a}^\beta]$ and $[\mathbf{a}_\alpha]$ are equivalent to "co-ordinates". Co-ordinates belong to parameter space, and components belong to state space. Thus, this adjoint associativity states that parameters and states are in fact "adjoints". Another view on this universal duality is given in a different biological context by Rosen (1985), who considers a parameter space of genotypes and a state space of phenotypes.

APPENDIX B

Independent Subsystems

The number, m, of subsystems determined by the projectors (20) is not limited by the dimension, n, of the underlying vector space, V. If, as may well happen, $m > n$, then it is impossible for the $\mathbf{a}^i \in V^*$ $(i = 1, \ldots, m)$ to form a linear independent set. If k is the dimension of the subspace of V^* spanned by $\mathbf{a}^i$ $(k \leq m$ and $n)$, then the rank of the matrix (L^{ij}) is k. Thus, k is the number of *independent* subsystems determined by the projectors associated with a given set of constitutive parameters. To see that this is a natural definition for independence consider a co-ordinate transformation that uncouples the subsystems; that is, diagonalize the matrix (L^{ij}). All off-diagonal coupling coefficients become zero, and of the diagonal elements, only k of them will be non-zero. This means that for a transport system, where the forces and fluxes are in physical space $(V = \mathbb{R}^3)$, our metric theory of irreversible thermodynamics (as it stands) would allow for at most three independent mobile molecular species.

This apparent difficulty is solved by broadening our notion of tensor. Strictly speaking, a tensor is defined over a single vector space; hence the notation $T^1_1(V)$. However, with a little sacrifice of some elegant properties under co-ordinate transformations, one can define tensor products between distinct vector spaces (and their duals). Although transport processes take place in three-dimensional space, we shall make the argument general; let $\mathbf{F}_i \in V$ $(\mathbf{J}^i \in V^*)$ with dim $V = n$. Furthermore, let $\mathbf{a}^i \in U^*$ $(\mathbf{a}_i \in U)$ with dim $U = m$. For a fixed set of constitutive parameters $\{\mathbf{a}^i\}$, the response tensor is given by the $m \times n$ dyadic

$$\mathbf{R} = \mathbf{a}^i \mathbf{F}_i = \mathbf{a}_i \mathbf{J}^i, \tag{B.1}$$

with, as in (16),

$$\mathbf{J}^i = (\mathbf{a}^i \cdot \mathbf{a}^j)\mathbf{F}_j = L^{ij}\mathbf{F}_j. \tag{B.2}$$

The space spanned by $\mathbf{R}$ is a metric space with norm

$$\|\mathbf{R}\|^2 = (\mathbf{a}^i \cdot \mathbf{a}^j)(\mathbf{F}_i \cdot \mathbf{F}_j) = L^{ij}(\mathbf{F}_i \cdot \mathbf{F}_j) = \mathbf{F}_i \cdot \mathbf{J}^i \geq 0. \tag{B.3}$$

To prove this, one need only follow the proof that $\mathbf{R} \in T^1_1(V)$ is a metric space given in Richardson *et al.* (1982) or the alternate proof in Louie & Richardson (1986). Since dim $U = m$, it is obvious that a set $\{\mathbf{a}^i\}$ can always be found corresponding to m independent subsystems. With $\mathbf{F}_i \in V$ and $\mathbf{a}^i \in U^*$ it is seen more clearly that the response tensor, $\mathbf{R}$, is a tensor product between state space and parameter space. This is analogous to the procedure in quantum mechanics where tensor products are used to represent complex systems: for example, a tensor product between position space and spin space.

The opposite of independent subsystems is identical subsystems. Their proper specification and representation is of some practical importance because a naive superposition of identical subsystems results in a misinterpretation of tracer experiments and in the fallacious concept of unidirectional fluxes (Richardson, 1989).

APPENDIX C

Data Reduction Algorithm

For convenience, assume that dim $V = m =$ number of species (so $i = 1, 2, \ldots, m$). Thus, the set $\{\mathbf{a}^i\}$ which we wish to determine from the data contains m^2 components. The data consists of the coefficients L^{ij}, determined empirically from ratios of forces and fluxes. However, because of symmetry (Onsager's reciprocity) the set $\{L^{ij}\}$ contains only $m(m+1)/2$ independent values.

The apparent dilemma of having to obtain solutions to more unknowns than independent values is resolved by noting the form of the phenomenological connection between forces and fluxes: $L^{ij} = \langle \mathbf{a}^i | \mathbf{a}^j \rangle$. In the calculation of inner products, all information beyond lengths and angles is superfluous. That is, the constitutive parameters, $\mathbf{a}^i$, need be determined only up to an orthogonal transformation. This is analogous to the situation in quantum mechanics, where a wave function is unique up to a unitary transformation of its basis set.

The relation $L^{ij} = \langle \mathbf{a}^i | \mathbf{a}^j \rangle$ can be expressed as the matrix decomposition

$$L = AA^T \tag{C.1}$$

where

$$A = \begin{pmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^m \end{pmatrix} = \begin{pmatrix} a_1^1, a_2^1, \ldots, a_m^1 \\ a_1^2, a_2^2, \ldots, a_m^2 \\ \vdots \\ a_1^m, a_2^m, \ldots, a_m^m \end{pmatrix}. \tag{C.2}$$

Because of the Euclidean invariance observed above, we can set

$$\begin{aligned} \mathbf{a}^1 &= (a_1^1, 0, 0, \ldots, 0) \\ \mathbf{a}^2 &= (a_1^2, a_2^2, 0, 0, \ldots, 0) \\ \mathbf{a}^3 &= (a_1^3, a_2^3, a_3^3, 0, 0, \ldots, 0) \\ &\vdots \end{aligned} \tag{C.3}$$

That is, the $m \times m$ matrix A is lower triangular. The existence of such a lower triangular matrix A for a positive definite matrix L is a well-known theorem in linear algebra (cf. e.g. Stewart, 1973), and (C.1) for lower triangular A is the Cholesky decomposition of L.

The algorithm for Cholesky decomposition follows:

$$\begin{array}{l} \text{For } i=1, 2, \ldots, m \\ \qquad \left| \begin{array}{l} \text{For } j=1, 2, \ldots, i-1 \\ a_j^i = \left(L^{ij} - \sum_{k=1}^{j-1} a_k^i a_k^j \right) \Big/ a_i^i \end{array} \right. \\ a_i^i = \left[L^{ii} - \sum_{k=1}^{i-1} (a_k^i)^2 \right]^{1/2}. \end{array} \tag{C.4}$$

This algorithm requires about $m^3/6$ multiplications and can always be carried to completion for positive definite L.