KINEMATICAL SYMMETRIES IN MOLECULAR QUANTUM MECHANICS

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1. Historical background

At the very beginning of quantum mechanics, in 1927 Hermann Weyl [1] stressed the fact that the kinematical structure of a physical system is described by a group of automorphisms. In particular, he showed that the kinematical group of elementary quantum mechanics is given by an irreducible Abelian group of ray representations on the state space. The kinematics of the spinning electron is described by the irreducible 2-dimensional group of unitary rotations, while Heisenberg's kinematics of a system with F degrees of freedom is expressed by the irreducible ray representation of a 2F-parameter continuous Abelian group [1,2].

Weyl's proposal to exponentiate the Lie algebra of Heisenberg's canonical commutation relation $QP - PQ \subset i$ and to introduce the two-parameter group $\{U(p),V(q) : p,q \in \mathbb{R}\}$ of unitary operators $U(p) = \exp(ipQ)$ and $V(q) = \exp(-iqP)$ fulfilling the commutation relations

$$U(p)\,V(q) = e^{ipq}\,V(q)\,U(p) \quad , \qquad (1)$$

has become generally accepted but his conceptually more important idea to consider quantum kinematics as a group did not generate much interest. Nowadays it is popular to relate the canonical commutation relations of nonrelativistic quantum mechanics to the projective unitary representations of the Galilei group (compare [3] and [4]). Nevertheless, it should not be ignored that Weyl's remark that the kinematics of a physical system is determined by a group of automorphisms is more general and conceptually deeper. It is not at all superseded by the

relation between the Weyl group over the Euclidean space and Galilean invariance (apparently unnoticed by Weyl).

In order to avoid a possible misunderstanding about the significance of the kinematical group in quantum mechanics, we quote a footnote from Weyl's paper: "Diese Verknüpfung mit der Gruppentheorie liegt in ganz anderer Richtung als die Untersuchungen von Herrn Wigner, die erkennen lassen, dass die Struktur der Spektren nach ihrer qualitativen Seite hin durch die bestehende Symmetriegruppe bestimmt ist" [1,p.2]. While Wigner discussed the consequences of the symmetries of the Hamiltonian, Weyl adressed himself to the problem of observables: "Wie komme ich zu der Matrix, der Hermiteschen Form, welche eine gegebene Grösse in einem seiner Konstitution nach bekannten physikalischen System repräsentiert?" [1,p.1]. The kinematical group determines the pattern of feasible abstract motions apart from considerations of mass and force, and is therefore conceptually independent from the dynamical laws and the symmetries of the Hamiltonian. Surprisingly, this viewpoint is still in its development phase so that there are only few applications to actual physical and chemical problems. The purpose of this lecture is to give a general definition of kinematical symmetries for arbitrary molecular systems, to discuss some of the properties of kinematical groups, and to sketch an approach to the difficult problem of determining the appropriate kinematical group for a given scientific inquiry.

2. Logical symmetries

A logical symmetry of a theory is an automorphism of its propositional system which preserves the logical structure of the theory. Modern nonrelativistic quantum theory assumes that its logical structure is given by a complete orthomodular lattice $\mathcal{L}$ of propositions, where the partial order of $\mathcal{L}$ is interpreted as the logical implication and the orthocomplementation of $\mathcal{L}$ is interpreted as the logical negation. A logical symmetry of a quantum theory is an automorphism of the orthomodular lattice $\mathcal{L}$. i.e. a bijection of $\mathcal{L}$ which preserves the partial order and the orthocomplementation. The set of logical symmetries form a group, the logical group $\mathrm{Aut}(\mathcal{L})$.

In the Hilbert-space model of generalized quantum mechanics, the lattice $\mathcal{L}$ is represented as the lattice of all projections of a certain Neumann algebra $\mathfrak{N}$ of operators acting on a separable complex Hilbert

space $\mathfrak{H}$. A generalization of Wigner's theorem due to Uhlhorn [5], Emch and Piron [6], and Kruszyński [7] asserts that each automorphism of $\mathfrak{L}$ is represented as a Jordan *-automorphism in $\mathfrak{N}$, provided that $\mathfrak{N}$ does not contain type I_2-factors as direct summands. In the special case where $\mathfrak{N}$ equals the algebra $\mathfrak{B}(\mathfrak{H})$ of all bounded operators acting on a Hilbert space of dimension not less than three, a logical symmetry is represented by a *-automorphism or by a *-anti-automorphism on $\mathfrak{B}(\mathfrak{H})$ and can be implemented by a unitary or antiunitary operator which is unique up to a factor of modulus one. Here we are not interested in anti-automorphisms (which can be related to the time-inversion symmetry) so that for $\mathfrak{N} = \mathfrak{B}(\mathfrak{H})$ the group $\mathrm{Aut}(\mathfrak{L})$ of logical symmetries can be associated with the group $\mathfrak{U}(\mathfrak{H})$ of all unitary operators acting on $\mathfrak{H}$.

3. Dynamical symmetries

In a closed quantal system the time evolution is a logical symmetry. In the Hilbert-space model, the time evolution is represented by a weakly measureable Abelian one-parameter group $\mathfrak{T}$ of unitary operators T_t acting on the state space $\mathfrak{H}$,

$$\mathfrak{T} = \{T_t : T_t \in \mathfrak{U}(\mathfrak{H}) \quad , \quad t \in \mathbb{R}\} \; . \tag{2}$$

For the present purpose, the notion of a state is a suitable primitive notion. Conceptually, we define a state of a system at time t as the set of all temporal propositions of the universe of discourse that are true at time t (for details compare [8]). In the Hilbert-space model, an atomic state is represented by a projection $S \in \mathfrak{B}(\mathfrak{H})$ of rank one, or equivalently, by a ray (i.e. a one-dimensional subspace of $\mathfrak{H}$). A unit vector $\Psi \in \mathfrak{H}$ with $\Psi = S\Psi$ is called a state vector. The time evolution $\Psi \to \Psi_t$ of a state vector is given by the dynamical group $\mathfrak{T}$,

$$\Psi_t = T_t\Psi \quad , \quad t \in \mathbb{R} \quad , \quad T_t \in \mathfrak{T} \; . \tag{3}$$

Note that we are working <u>always</u> in the Schrödinger picture and that we do <u>not</u> assume that the Schrödinger picture is equivalent to the Heisenberg picture. Accordingly, we do not require that the dynamical group $\mathfrak{T}$ induces an automorphism of the algebra of observables (to be defined in the next section).

4. Kinematical symmetries

The pair $(\mathfrak{H},\mathfrak{T})$ gives a complete and intrinsic characterization of a given closed system. Accordingly we call $(\mathfrak{H},\mathfrak{T})$ the universal theory for the given universe of discourse [9]. From the viewpoint of the universal theory, there exists no objective physical property by which one could distinguish one atomic proposition in $\mathfrak{L}$ from another, or one state vector from another. We say that in the universal theory all states are kinematically equivalent. The group corresponding to this equivalence is the group $\mathfrak{U}(\mathfrak{H})$ of all unitary operators on $\mathfrak{H}$. That is, the universal theory possesses the maximal kinematical symmetry allowed. Therefore, all its atomic predicates have the same importance so that it is impossible to define classes of similar objects without extralogical arguments. This fact has the consequence that the universal theory $(\mathfrak{H},\mathfrak{T})$ is observationally empty. There is a striking correspondence between the emptiness of universal theories and the impossibility of inductive inference [10] and classifications [11,chapt.8] by pure logical handling of empirical data. The fact that we do classify and predict, that even classification and prediction are basic objectives of science, shows that equivalence classes of similar predicates are not intrinsic properties of systems. Accordingly it is impossible to detect similarity between phenomena without forming classes by abstracting so-called irrelevant features. Emphasis and abstraction presuppose some aim, the question whether one abstraction is "better" than another cannot be answered without asking "better for what purpose". This corresponds to the view that the central problem of cognition and recognition is that of weighting the importance of predicates [11.p.382] and that the description of a system depends on the question we ask.

In order to adapt the theory $(\mathfrak{H},\mathfrak{T})$ to the equivalence classes generated by the abstractions associated with a particular cognition and classification method we introduce a subtheory of the universal theory $(\mathfrak{H},\mathfrak{T})$ in which not all atomic states are equivalent. The automorphism group which induces the corresponding equivalence relation on the set of all states of the universal theory is called the group of kinematical symmetries of the subtheory in question. In the Hilbert-space model, the corresponding subgroup of $\mathfrak{U}(\mathfrak{H})$ is called the kinematical group $\mathfrak{K}$

$$\mathfrak{K} \subset \mathfrak{U}(\mathfrak{H}) \tag{4}$$

Technically it is convenient to associate to the kinematical group $\mathfrak{K}$ a weakly closed algebra $\mathfrak{N}$, defined by

$$\mathfrak{N} \stackrel{\text{def}}{=} \{\mathfrak{K}\}'' \quad , \tag{5}$$

where" denotes the double commutant with respect to $\mathfrak{B}(\mathfrak{H})$. Traditionally the Neumann algebra $\mathfrak{N}$ has the rather misleading name "algebra of observables". What really is "observable" has to come from detailed analysis of measurements and is by no means already evident from the fundamental axioms of the theory. Without a serious discussion of actual measurements, the relevance of a statement that a quantity is considered as observable remains obscure. Nevertheless, we adopt the time-honored name observable for the self-adjoint elements of $\mathfrak{N}$ without, however, accepting the frivolous claim that these observables are related in a clear-cut way to measurable quantities. The algebra $\mathfrak{N}$ of observables delineate the universe of discourse of a particular subtheory. Accordingly, we characterize a subtheory of the universal theory $(\mathfrak{H},\mathfrak{T})$ by a triple $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ where $\mathfrak{N}$ is the weakly closed group algebra of the kinematical group $\mathfrak{K}$. The study of kinematical groups in quantum mechanics is the same as the study of the nature of the algebra of observables of quantal systems. Conceptual problems are discussed preferrably in the group theoretical language while analytical-mathematical questions are often easier in the algebraic embedding.

5. Kinematical supersymmetries and primary states

In order to classify states in correspondence to the transformation properties of the kinematical group $\mathfrak{K}$ we introduce its center $\mathfrak{Z}(\mathfrak{K})$ defined as the set of those elements of $\mathfrak{K}$ that commute with every element of $\mathfrak{K}$,

$$\mathfrak{Z}(\mathfrak{K}) \stackrel{\text{def}}{=} \{U : U \in \mathfrak{K} \ , \ UK = UK \text{ for every } K \in \mathfrak{K}\} \quad . \tag{6}$$

The elements of the Abelian subgroup $\mathfrak{Z}(\mathfrak{K})$ are called the kinematical supersymmetries [12]. A state which is invariant under all kinematical supersymmetries is called a primary state of the quantal system $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$. If a state is represented by a state vector $\Psi \in \mathfrak{H}$, it is primary if and only if it is an eigenvector of every element of the center $\mathfrak{Z}(\mathfrak{K})$, i.e.

$$\Psi \text{ is primary} \quad \text{iff} \quad U\Psi = u\Psi \quad \text{for every } U \in \mathfrak{Z}(\mathfrak{K}) \quad , \tag{7}$$

where u is a complex number of unit modulus. In general, the symmetries also have continuous spectra so that the set of all primary state vectors do not span the state space $\mathfrak{H}$. For that reason we have to discuss the general central decomposition of the kinematical group.

Since all elements of the center $\mathfrak{z}(\mathfrak{K})$ are mutually commuting unitary operators, there exists a metrizable compact spectrum space Λ and a spectral measure $E : \Sigma \to \mathfrak{B}(\mathfrak{H})$, where Σ is the σ-field of Borel subsets of Λ, such that for every $U \in \mathfrak{z}(\mathfrak{K})$ there exists a complex-valued measurable function $u : \Lambda \to \mathbb{C}$ with $|u| = 1$ such that

$$U = \int_{\Lambda} u(\lambda)\, E(d\lambda) \quad . \tag{8}$$

Since every Abelian Neumann algebra on a separable Hilbert space has a separating vector, there exists a unit vector $\Omega \in \mathfrak{H}$ with $E(\mathcal{B})\Omega \neq o$ for all $\mathcal{B} \in \Sigma$. We define a probability measure $\mu : \Sigma \to \mathbb{R}^+$ by $\mu(\mathcal{B}) = \langle \Omega | E(\mathcal{B})\Omega \rangle$, $\mathcal{B} \in \Sigma$, and the associated direct integral decomposition of the state space $\mathfrak{H}$ by

$$\mathfrak{H} = \int_{\Lambda}^{\oplus} \mathfrak{H}(\lambda)\, \mu(d\lambda) \quad . \tag{9}$$

Accordingly, every vector $\Psi \in \mathfrak{H}$ can be decomposed into components $\Psi(\lambda) \in \mathfrak{H}(\lambda)$, and we write

$$\Psi = \int_{\Lambda}^{\oplus} \Psi(\lambda)\, \mu(d\lambda) \quad . \tag{10}$$

In this central decomposition, every unitary operator $K \in \mathfrak{K}$ is reduced by the direct integral decomposition

$$K\Psi = \int_{\Lambda}^{\oplus} K(\lambda)\, \Psi(\lambda)\, \mu(d\lambda) \quad , \quad \Psi \in \mathfrak{H} \tag{11}$$

where the component $K(\lambda)$ is a unitary operator on the Hilbert space $\mathfrak{H}(\lambda)$. This central decomposition gives all we need but it is somewhat inconvenient since $\mathfrak{H}(\lambda)$ is a subspace of $\mathfrak{H}$ if and only if $\mu(\{\lambda\}) > o$.

For our comfort we introduce the nuclear spectral theorem [13,14]. For the spectral measure $E : \Sigma \to \mathfrak{B}(\mathfrak{H})$ there exists a nuclear space $\mathfrak{H}_+ \subset \mathfrak{H}$, dense in $\mathfrak{H}$, and a topological dual $\mathfrak{H}_-$, such that $\mathfrak{H}_+ \subset \mathfrak{H} \subset \mathfrak{H}_-$ is a rigged Hilbert space and such that μ-almost all Hilbert spaces $\mathfrak{H}(\lambda)$ are subspaces of $\mathfrak{H}_-$,

$$\mathfrak{H}(\lambda) \subset \mathfrak{H}_{-} \quad \text{for} \quad \mu\text{-almost all } \lambda \in \Lambda \ . \tag{12}$$

If $\mu(\{\lambda\}) > 0$, then $\mathfrak{H}(\lambda)$ is even a subspace of $\mathfrak{H}$ and the elements of $\mathfrak{H}(\lambda)$ are eigenvectors of every $U \in \mathfrak{G}(\mathfrak{K})$ with the eigenvalue $u(\lambda)$. If $\mu(\{\lambda\}) = 0$, then the Hilbert space $\mathfrak{H}(\lambda)$ is not a subspace of $\mathfrak{H}$ but in virtue of eq.(12) it is called a generalized subspace. The elements of $\mathfrak{H}(\lambda)$ are called generalized eigenvectors of the group $\mathfrak{G}(\mathfrak{K})$, they form a complete set.

A Hilbert space $\mathfrak{H}(\lambda)$, $\lambda \in \Lambda$, arising from the central decomposition (9) induced by the kinematical group $\mathfrak{K}$, is called a sector of the quantal system $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$. An element in a sector is called a generalized primary state vector. The set of all generalized primary state vectors spans the set of all invariants of the kinematical supersymmetries. A generalized primary state vector $\Psi(\lambda) \in \mathfrak{H}(\lambda)$ induces on the algebra $\mathfrak{N}$ of observables a primary positive linear functional (a "factor state" in the terminology of algebraic quantum mechanics); if $\Psi(\lambda) \in \mathfrak{H}$, then this positive linear functional is normal.

6. Physically pure states and classical mixtures

By definition, a sector corresponds to the equivalence class of quasiequivalent primary states, so that in every sector the superposition principle holds unrestrictedly. However, different sectors are kinematically inequivalent and we say that they are disconnected by superselection rules. The impossibility of coherent superpositions between primary state vectors from different sectors means that systems in disjoint primary states can be distinguished classically. In a primary state the elements of the center $\mathfrak{G}(\mathfrak{N}) = \mathfrak{N} \cap \mathfrak{N}'$ of the algebra $\mathfrak{N}$ of observables have dispersionfree values [15]. Therefore we call the self-adjoint elements of $\mathfrak{G}(\mathfrak{N})$ classical observables, they can be observed with arbitrarily small disturbances of the state of the system. On that account, a system in a nonprimary state can be considered as a classical mixture of systems in primary states. Any further decomposition of a primary state would infringe the superposition principle, hence the central decomposition (10) of a state vector into (generalized) primary state vector is the physically finest possible. That is, a (generalized) primary state represents a physically pure state. This concept replaces the notion of a pure state in elementary quantum mechanics with an irreducible algebra of observables. Note that in general a primary state is

not extremal (i.e. not a pure state in the mathematical sense).

A convex linear combination of disjoint primary states is called a classical mixture. In terms of state vectors, the operation of mixing can be described as follows. Let Ψ_1 and Ψ_2 be the state vectors of two arbitrary states of a quantal system $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$. A state with the state vector Ψ_3 is called a classical mixture (with respect to the group $\mathfrak{G}(\mathfrak{K})$ of kinematical supersymmetries) of Ψ_1 and Ψ_2 if there exists a real number c , $0 < c < 1$, such that for every $\lambda \in \Lambda$ we have

$$f_3(\lambda) = c\, f_1(\lambda) + (1-c) f_2(\lambda) \quad , \tag{13}$$

where

$$f_j(\lambda) \stackrel{\text{def}}{=} \|\Psi_j(\lambda)\|^2_{\mathfrak{H}(\lambda)} \quad , \quad j = 1,2,3, \quad , \quad \lambda \in \Lambda \tag{14}$$

and $\Psi_j(\lambda)$ is the part of Ψ_j in the sector $\mathfrak{H}(\lambda)$.

This operation of mixing induces a partial order on the set of all state vectors. The function

$$f : \Lambda \to \mathbb{R}^+ \quad . \tag{15}$$

with

$$f(\lambda) \stackrel{\text{def}}{=} \|\Psi(\lambda)\|^2_{\mathfrak{H}(\lambda)} \tag{16}$$

is Borel measurable and μ-integrable, hence

$$f \in \mathcal{L}_1(\Lambda,\Sigma,\mu) \quad . \tag{17}$$

For a state vector Ψ, the corresponding distribution function f is normalized,

$$\int_\Lambda f(\lambda)\, \mu(d\lambda) = 1 \quad . \tag{18}$$

The mixing operations of normalized distribution functions can be represented by doubly stochastic operators [16-19]. A linear operator $\mathcal{S} : \mathcal{L}_1(\Lambda,\Sigma,\mu) \to \mathcal{L}_1(\Lambda,\Sigma,\mu)$ is called doubly stochastic if it satisfies for all $f \in \mathcal{L}_1(\Lambda,\Sigma,\mu)$ the following conditions

$$\text{(i)} \qquad f \geq o \ \text{ implies } \ \mathscr{A}\{f\} \geq o \quad , \tag{19a}$$

$$\text{(ii)} \qquad \int_{\Lambda} \mathscr{A}\{f\}(\lambda)\, \mu(d\lambda) = \int_{\Lambda} f(\lambda)\, \mu(d\lambda) \quad , \tag{19b}$$

$$\text{(iii)} \qquad \mathscr{A}\{1\} = 1 \quad , \tag{19c}$$

where 1 denotes the function whose constant value equals one. Let f_1, f_2 be two normalized distribution functions; if there exists a doubly stochastic operator $\mathscr{A}$ such that $f_2 = \mathscr{A}\{f_1\}$, then we write $f_2 \succ f_1$ and say that f_2 is <u>more mixed</u> than f_1. This partial order corresponds to the strong spectral order [20], i.e.

$$f_2 \succ f_1 \quad \text{iff} \quad \int_{\Lambda} \{f_2(\lambda)-t\}^+ \mu(d\lambda) \leq \int_{\Lambda} \{f_1(\lambda)-t\}^+ \mu(d\lambda) \tag{20}$$

for all $t \in \mathbb{R}$, where f^+ denotes the positive part of the function f.

Let $\varphi : \mathbb{R}^+ \to \mathbb{R}$ be an arbitrary convex function, then we define a generalized information-theoretical entropy $S_\varphi[f]$ of a probability distribution function $f \in \mathscr{L}_1(\Lambda,\Sigma,\mu)$ by

$$S_\varphi[f] \stackrel{\text{def}}{=} -\int_{\Lambda} \varphi\{f(\lambda)\}\, \mu(d\lambda) \quad . \tag{21}$$

A generalization of an important theorem by Hardy, Littlewood and Pólya [21, theorem 108] due to Chong [22] provides the following characterization of the partial ordering $\succ$ in terms of information-theoretical entropies: Let f_1 and f_2 be two probability distribution functions in $\mathscr{L}_1(\Lambda,\Sigma,\mu)$, then

$$f_2 \succ f_1 \quad \text{iff} \quad \begin{cases} S_\varphi[f_2] \geq S_\varphi[f_1] \\ \\ \text{for } \underline{\text{every}} \text{ entropy } S_\varphi \end{cases} . \tag{22}$$

Traditionally, the mixedness of distribution functions has been measured by the Boltzmann-Shannon entropy S,

$$S[f] = -\int_{\Lambda} f(\lambda)\, \ln\{f(\lambda)\}\, \mu(d\lambda) \quad . \tag{23}$$

It has been stressed by Ruch [23] that the mixing character of a probability distribution cannot be characterized by a single numerical quantity such as the Boltzmann-Shannon entropy but that the mixing character

is a qualitative concept defined by a partial ordering on the set of all probability distributions. Each entropy S_φ is a concave and homomorphic mapping of this partial ordering. The result (22) implies that this partial ordering can be characterized by the set of all concave entropies.

Consider now a quantal system $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$. We say that a state with the state vector Ψ_2 is more mixed than another state with the state vector Ψ_1 if the associated distribution functions (14) fulfill the relation $f_2 \succ f_1$. The entropy difference $S_\varphi[f_2]-S_\varphi[f_1]$ corresponds to the classical mixing entropy. The conceptual meaning of these entropies follows from the interpretation of primary states as physically pure states: the entropy $S_\varphi[f]$ of a nonprimary state with the associated distribution function f is a measure for the lack of knowledge of the observer. Since classical observables can be measured with arbitrarily small perturbations, it is always possible to acquire a more detailed knowledge by decomposing the mixture into less mixed states. This concept of information-theoretical entropies associated to nonprimary states should be distinguished clearly from the intrinsic entropies associated with type III primary states which represent undecomposable physical systems (compare section 7). The classical mixing is governed solely by the group $\mathfrak{g}(\mathfrak{K})$ of kinematical supersymmetries.

If the time evolution group $\mathfrak{T}$ of a quantal system $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ does not induce an automorphism of the center $\mathfrak{z}(\mathfrak{N}) = \mathfrak{N}\cap\mathfrak{N}'$, then the mixing character of the states of this system is not invariant in time. It is possible to give examples of quantal systems where the mixing character increases monotonically with time (i.e. fulfilling Ruch's [23] "principle of increasing mixing character") as well as examples of quantal systems where the mixing character decreases monotonically with time [8].

7. The meaning of reducibility: entropy of primary states

Traditionally, group theoretical investigations of symmetry properties of physical systems have been closely connected with the study of irreducible representations of the corresponding symmetry groups. Often it is presupposed that there is a one-to-one correspondence of physical concepts and the classification into irreducible representations. This idea makes sense for finite groups, and can easily be generalized to compact groups. Every unitary representation of a compact

group can be written uniquely as a direct sum of irreducible subrepresentations. Noncompact groups are much more complicated. Already a locally compact Abelian group need not be discretely decomposable but the replacement of the direct sum by a direct integral of irreducible representation is a complication of technical rather than conceptual importance. A conceptually new situation arises only with non-compact non-Abelian groups: there exist groups with reducible primary representations that contain no irreducible subrepresentations.

Recall that two unitary representations U,V of the same group are called disjoint if no subrepresentation of U is unitarily equivalent to any subrepresentation of V. Two unitary representations U,V are called quasiequivalent if no subrepresentation of U is disjoint from V, and no subrepresentation of V is disjoint from U. A representation is called a primary representation if all its subrepresentations are pairwise quasiequivalent. A representation is called reducible if there exists a nontrivial invariant subspace of the representation space, otherwise it is called irreducible. Via the central decomposition (discussed in section 5), every unitary representation can be decomposed uniquely into primary representations, so that we can restrict our discussion to primary representations. Following Mackey [24,25], a primary representation is said to be of type I if it contains an irreducible subrepresentation. A primary representation is said to be of type III if every representation quasiequivalent to it is unitarily equivalent to it. A primary representation is said to be of type II if it is neither of type I nor of type III. A group is called of type I if all its unitary representations are of type I. The compact groups, the locally compact Abelian groups, the Galilei group and the Lorentz group are examples for type I groups.

Every primary representation of a type I group is a multiple of an irreducible representation so that every unitary representation of a type I group is uniquely (up to equivalence) decomposable into a direct integral of irreducible representations. Even for type II and type III unitary representations of a locally compact group with a countable basis there always exist direct-integral decompositions into irreducible representations but these decompositions are pathologically nonunique. For example, there exist decompositions such that no irreducible component occuring in the one decomposition occurs in the other. The fact that no canonical decomposition into irreducible components can be given for type II and type III representations is often described

as unsatisfactory or even as pathological. For example, Kirillov [26] calls type I groups tame and non-type I groups wild. Ten years ago, A.J. Colemann [27] still posed the question "whether such type II and type III monsters need actually be taken into account in a reasonable physical theory". The answer is a clear yes.

The question of the conceptual relevance of irreducible representations in quantum theory cannot be settled by armchair philosophizing. The relevant decomposition of the representation of the kinematical group is uniquely given by the formalism and the interpretation of the theory. For the interpretation we have adopted it turns out that the all-important decomposition is the decomposition into primary representations. The decomposition into irreducible parts has no fundamental physical relevance. With this, any objections against II and type III representations (which cannot have irreducible subrepresentations) fade away. A well known example of great relevance for molecular theory are the thermodynamic systems whose algebras of observables are of type III [28].

For the tame type I kinematical groups reducibility has a simple meaning. The central decomposition (9) of the kinematical group $\mathfrak{K}$ reduces the algebra (5) of observables,

$$\mathfrak{A} = \int_{\Lambda}^{\oplus} \mathfrak{A}(\lambda)\, \mu(d\lambda) \quad , \tag{24}$$

where $\mathfrak{A}(\lambda)$ is a factor on $\mathfrak{H}(\lambda)$,

$$\mathfrak{A}(\lambda) \cap \mathfrak{A}(\lambda)' = \mathbf{1}.\mathbf{C} \quad . \tag{25}$$

For a type I representation, the Neumann algebra $\mathfrak{A}(\lambda)$ is a factor of type I so that there is a (up to unitary equivalence) unique decomposition of the Hilbert space $\mathfrak{H}(\lambda)$ into a tensor product

$$\mathfrak{H}(\lambda) = \mathfrak{H}_1(\lambda) \otimes \mathfrak{H}_2(\lambda) \quad , \tag{26}$$

such that

$$\mathfrak{A}(\lambda) = \mathfrak{B}\{\mathfrak{H}_1(\lambda)\} \otimes \mathbf{1}\cdot\mathbf{C} \quad , \tag{27}$$

$$\mathfrak{A}(\lambda)' = \mathbf{1}\cdot\mathbf{C} \otimes \mathfrak{B}\{\mathfrak{H}_2(\lambda)\} \quad . \tag{28}$$

A primary state vector $\Psi(\lambda) \in \mathfrak{H}(\lambda)$ has a unique canonical Schmidt decomposition

$$\Psi(\lambda) = \|\Psi(\lambda)\|_{\mathfrak{H}(\lambda)} \cdot \sum_n c_n \varphi_n(\lambda) \otimes \chi_n(\lambda)$$

where $\{\varphi_n(\lambda)\}$ and $\{\chi_n(\lambda)\}$ form a orthonormal set in $\mathfrak{H}_1(\lambda)$ and $\mathfrak{H}_2(\lambda)$, respectively. Since the operators acting on $\mathfrak{H}_2(\lambda)$ are "nonobservable", all expectations can be expressed by the reduced density operator $D(\lambda)$ acting on $\mathfrak{H}_1(\lambda)$,

$$D(\lambda) \stackrel{\text{def}}{=} \sum_n |c_n|^2 \, |\varphi_n(\lambda)\rangle\langle\varphi_n(\lambda)| \quad . \tag{29}$$

To this density operator we can associate a Shannon type entropy $S(\lambda)$ by

$$S(\lambda) \stackrel{\text{def}}{=} -\mathrm{tr}_{\mathfrak{H}(\lambda)}\{D(\lambda) \ln D(\lambda)\} = -\sum_n |c_n|^2 \ln |c_n|^2 \, . \tag{30}$$

We call $S(\lambda)$ the Shannon entropy of the primary state vector $\Psi(\lambda)$. The algebra (27) of observables gives only a partial description since the degrees of freedom in $\mathfrak{H}_2(\lambda)$ are not accounted for. The entropy $S(\lambda)$ is a measure for this loss of information; $S(\lambda)$ vanishes if and only if $\mathfrak{H}_2(\lambda)$ is one-dimensional, i.e. if the primary representation is irreducible.

If all factors $\mathfrak{N}(\lambda)$, $\lambda \in \Lambda$, are of type I , we call $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ a type I theory. If Dirac's [29] requirement of the existence of a complete set of commuting observables is fulfilled, then $\mathfrak{N}$ contains at least one maximal Abelian algebra [30] so that $\mathfrak{N} = \mathfrak{G}'$, i.e. of type I. Such a type I theory $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ with $\mathfrak{N} = \mathfrak{G}'$ will be called a Dirac system. The relation $\mathfrak{N}' = \mathfrak{G}$ implies that all primary representations of the kinematical group of a Dirac system are irreducible. Accordingly, the entropy of every primary state of a Dirac system is zero. If a type I theory $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ is not a Dirac system, it can always be completed by the addition of new observables to a dominating Dirac system $(\mathfrak{H},\mathfrak{T},\mathfrak{G}')$ where $\mathfrak{G}' = (\mathfrak{N} \cup \mathfrak{N}')''$. With this, the reducibility in type I theories is rather uninteresting: the associated incompleteness in principle can always be eliminated.

The situation in non-type I theories is entirely different. In a type II or III theory no primary state vector induces an extremal linear functional on the algebra of observables, and no extremal linear

functional can be expressed by a state vector. The reducibility of type II and type III factors enforces an inherent fuzziness of primary states which is inaccessible and cannot be eliminated. To every primary state on a factor $\mathfrak{N}(\lambda)$ one can associate a Shannon entropy $S(\lambda)$ relative to a faithful normal positive linear functional ρ by

$$S(\lambda) \stackrel{\text{def}}{=} -\rho\{D(\lambda)\ \ln D(\lambda)\} \quad , \tag{31}$$

where $D(\lambda)$ is the Radon-Nikodym derivative of the primary state with respect to ρ [31]. In contrast to the entropy (30) of a primary state of a type I theory, the entropy (31) of a primary state of a type II or type III theory is not due to an incomplete description but represents an objective and inherent property of the state of the system.

For example, one can consider classical thermodynamics (in contradistinction to statistical mechanics) of a single and finite system as a subtheory $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$, where $\mathfrak{N}$ is a type III algebra and the dynamical group $\mathfrak{T}$ is related to the modular automorphism group of $\mathfrak{N}$. A primary state of this subtheory characterizes a single thermodynamic phase with a dispersion-free value of temperature. A primary state has to be considered as indecomposable, any finer decomposition would go beyond the limits of a thermodynamic description with the effect that the concept of temperature would get lost. The entropy (31) of a primary state represents an objective property of the state of the thermodynamic system, it is related to the traditional thermodynamic entropy.

8. Generalized kinematics and the pattern group

Every group $\mathfrak{K} \subset \mathfrak{U}(\mathfrak{H})$ of unitary operators defines a particular subtheory $(\mathfrak{H},\mathfrak{T},\mathfrak{N})$ of the universal theory $(\mathfrak{H},\mathfrak{T})$. The question of how one has to choose the correct kinematical group is adequately answered by the Cheshire Cat in Lewis Caroll's "Alice in Wonderland": "Would you tell me, please, which way I ought to go from here?" "That depends a good deal on where you want to get to," said the Cat. "I don't much care where - " said Alice. "Then it doesn't matter which way you go," said the Cat. " - so long as I get somewhere", Alice added as an explanation. "Oh, you're sure to do that," said the Cat, "if you only walk long enough."

While the Galilei group is the kinematical group associated with Euclidean geometry, one may think of generalized kinematical groups as being related to generalized geometries in the sense of Weyl's [32] generalization of Klein's [33] Erlanger program. Every kinematical group

represents a particular perspective. The crucial point is that there are no observable facts without abstractions so that every point of view is a caricature portraying reality in a distorted manner. Good caricatures show relevant features by suppressing irrelevant details. Well-chosen abstractions can reveal regularities and give better insight than more elaborate theories. We do not suppose that the views presently fashionable are intrinsically distinguished, so that we propose that every subgroup $\mathfrak{K} \subset \mathfrak{U}(\mathfrak{H})$ whatsoever may serve as a kinematical group.

Whenever the space-time background of the phenomena we are interested in is essential, the appropriate kinematical group will be related to the Galilei (or Lorentz) group. Most formulations of molecular quantum mechanics take the postulates of particle mechanics and Galilean relativity as starting point. With this, the kinematical group is given by a Weyl system over an appropriate phase space. For a molecular system with F degrees of freedom, the phase space equals the locally compact Abelian group $\mathbb{R}^F$ so that the algebra of observables is of type I and irreducible. As we know today, this choice is not always an appropriate model. For many molecules it turns out that such a model without radiation field is structurally unstable against the inclusion of the interactions with the infinitely many soft photons of extrem low frequency (the so-called infrared part of the radiation field). The correct discussion of this problem is elaborate and difficult but the final result is simple: if the model without radiation field results in an almost degenerate ground state (like with molecules which phenomenologically are known to be chiral), then this model is structurally unstable and the inclusion of the radiation field generates inequivalent sectors. This result can be incorporated into a new structurally stable molecular model by replacing the irreducible system by a Dirac system with appropriate kinematical supersymmetries. In this case, the appropriate kinematical supersymmetries can be understood dynamically: the kinematical supersymmetry of the modified model accounts in a qualitatively exact manner for the interactions of the system with its surroundings. Such dynamically generated supersymmetries are very common in chemical systems and account for the partially classical behavior of such systems. Indeed one can even characterize chemical and biological systems as quantal systems that involve at the same time both quantal and classical properties in an essential way. As a paradigmatic example one may take a biomolecule with its molecular stability, its photochemical properties, its primary, secondary and tertiary structure.

Philosophers of science often fail to pay sufficient attention to the fact that chemistry is not the science of molecules but the science of substances and of the transformations they undergo. All-important concepts of chemistry like the notions of halogens, alkali metals, acids, oxidation , catalysis, temperature do not refer to single molecules but to classes and require for their description variables of logically higher type. That is, the patterns of genuine chemistry and biology generate new abstractions with an associated type hierarchy in the spirit of Russel's [34] theory of types. Contemporary theoretical chemistry is confused by many category mistakes. Such category mistakes [35] occur when categories of different logical type (e.g. individual objects, classes of individual objects, classes of classes) are treated as being on par. This confusion can be illustrated by that of taking a substance as being on equal footing with molecules, of taking chemical kinetics as being on equal footing with a theory of collisions, of taking the π-electrons of the organic chemist as being on equal footing with particular Hartree-Fock orbitals.

Insofar chemistry deals with individual molecules, it is well mirrored by Dirac systems which are type I theories. Classes of molecules are not themselves molecules but that does not a priori exclude the possibility of treating classes as objects of a particular subtheory. Of course, for entities belonging to categories of a higher logical type, the Galilei group is irrelevant so that we cannot expect that classes are described by Dirac systems. Moreover, the idea of "elementary objects" is out of place for a theory of classes so that the nonatomic type II and type III algebras seem to be appropriate.

The introduction of type II and type III kinematics leads to a significant evolution in our theoretical outlook. The referents of non-type I theories are no longer elementary building blocks (like electrons, molecules, phonons, excitons, bogoliubons) but entities of higher logical type. If we isolate a phenomenon and assign an individuality to it, we create a entity which we call <u>pattern</u>. Pattern cognition is understood here quite generally as a logically consistent method to discover structures from empirical data. Theoretically it is governed by a group of transformations whose equivalence classes are generated by the chosen abstractions. The role that the Galilei group plays for the type I theories is taken over by a <u>pattern group</u> which characterizes patterns by their invariant properties [36]. In order to find or to guess the gen-

eralized kinematical group we have to learn what criteria the experimentalist uses to recognize patterns. Concept formation and pattern recognition are characterized by the pattern group which in turn determines the kinematical group of the corresponding subtheory. In spite of much research efforts, the theory of pattern cognition and recognition still is in its infancy: unfortunately no comprehensive theory of pattern recognition is available at present.

9. Asymptotology

The detailed description of a complex chemical or biological system in terms of its elementary constituents is a painful and not very illuminating exercise. We are never interested in all the minute details the Weyl kinematical group or a Dirac system can provide for a molecular system having very many degrees of freedom. Even if we could deal analytically or numerically with this problem, the number of results would be larger than we could possibly survey. What we need are exact but less detailed alternative descriptions that provide an impressionistic painting.

At present, the only practicable approach to type II and type III kinematical groups seems to be asymptotics. From many examples we know that it is the limiting behavior that often presents regularities, and on the basis of experience in statistical mechanics we may expect that the relevant information for type II or type III kinematical groups should be available as limiting cases of type I theories. Examples for useful limits are the long-time behavior and the so-called thermodynamic limit. However, as the classical thermodynamic theory of capillarity exemplifies, thermodynamics is not a theory of infinite systems but an asymptotic theory. Even for a simple one-component system the Gibbs free enthalpy G is not only a function of the temperature T and the pressure P but depends also on the number n of moles in the sample, for examples as

$$G = f(P,T)\, n + g(P,T)\, n^{2/3} + \cdots \quad , \tag{32}$$

where the term proportional to $n^{2/3}$ is a surface energy. The beauty and power of the principles of phenomenological thermodynamics lies just in this generality which is destroyed in the thermodynamic limit. In spite of the fact that modern algebraic quantum statistics [28] is

tailored to infinite systems, it provides us with the relevant kinematical structure for a theory of the first term in the asymptotic expansion (32) : it is a type III Neumann algebra. The usual interpretation of algebraic statistical mechanics as a theory whose referent is an ensemble of molecules is not very convincing because a type III theory has no atoms so that it cannot describe molecules. A more natural view is that this type III theory is the first asymptotic term of a subtheory dealing with a single finite system. The referent of the theory is then macroscopic matter in a thermodynamic state what is not the same as a Gibbs ensemble of molecules. Molecules can be described only by type I theories, and thermodynamic systems in which temperature is a kinematical supersymmetry can be described only by type III theories [37]. This result is very natural and accounts for the well-known complementarity between molecular and thermodynamic descriptions [38]. Molecules and thermodynamic matter are entities of different logical type; the thermodynamic limit is nothing but a clever mathematical trick to get the first asymptotic term of a theory of higher type.

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