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THE GESTALT PROBLEM IN QUANTUM THEORY: GENERATION OF MOLECULAR SHAPE BY THE ENVIRONMENT

ABSTRACT. Quantum systems have a holistic structure, which implies that they cannot be divided into parts. In order to *create* (sub)objects like individual substances, molecules, nuclei, etc., in a universal whole, the Einstein–Podolsky–Rosen correlations between all the subentities, e.g. all the molecules in a substance, must be suppressed by perceptual and mental processes.

Here the particular problems of *Gestalt* (≡ *shape*) *perception* are compared with the attempts to *attribute a shape to a quantum mechanical system* like a molecule. Gestalt perception and quantum mechanics turn out (on an informal level) to show similar features and problems: holistic aspects, creation of objects, dressing procedures, influence of the 'observer', classical quantities and structures. The attribute 'classical' of a property or structure means that *holistic* correlations to any other quantity do not exist or that these correlations are considered as irrelevant and therefore eliminated (either deliberately and by declaration or in a mental process that is not under rational control). An example of an *imposed* classical structure is the nuclear frame of a molecule. Candidates for classical properties that are *not* imposed by the observer could be the charge of a particle or the handedness of a molecule. It is argued here that at least part of a molecule's shape can be *generated 'automatically' by the environment*. A molecular shape of this sort arises in addition to Lamb shift-type energy corrections.

1. THE GESTALT CONCEPT

> What we call reality consists of a few iron posts of observation between which we fill in by an elaborate papier-mâché construction of imagination and theory.
> John Archibald Wheeler (1980, p. 149)

There has been much controversy between psychologists so far as the concept of an object's shape is concerned. From a 'structuralist' (reductionist) point of view, perception of objects (patterns, textures, etc.) is explained in terms of perceptual 'atoms', that is to say, in terms of *local* entities and structures (Julesz, 1991). Gestalt psychologists on the other hand claim that the 'Gestalt' (≡ shape, configuration) of an object can only be perceived in a global, nonlocal manner (Köhler, 1971). From their point of view, the Gestalt of an object is a *holistic* concept,

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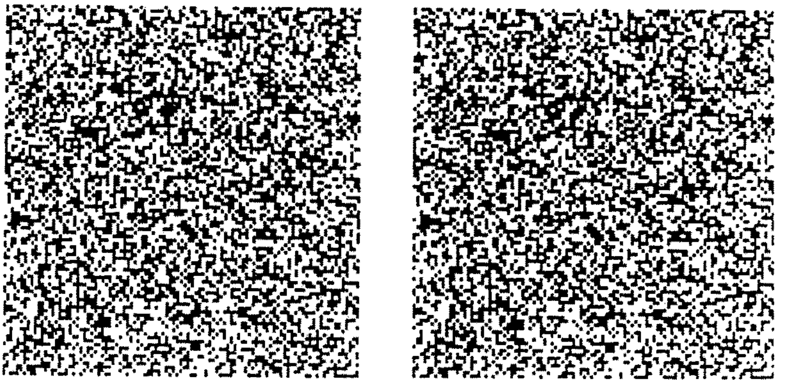

Fig. 1. Random-dot stereogram to be fused binocularly with the help of a stereoscope. The isolated left or right pattern, respectively, is built up from randomly chosen squares. Binocular fusion rests on certain correlations between the left and the right pattern. (Reprinted from Julesz (1971) with permission given by B. Julesz and the University of Chicago Press, © 1971 by Bell Telephone Laboratories.)

and this view is summarized in the slogan "*The whole is different from the sum of its parts*".

This slogan has constantly irritated and annoyed the critics of the Gestalt concept. Karl Popper (1980, p. 75), for example, remarks:

> Köhler, and other Gestalt theoreticians, asserted that the opposite of a *Gestalt* is a heap – '*ein Haufen*'. To this I have replied that a heap is also a Gestalt, and that therefore it has not been shown that the Gestalt idea – of a whole as being more than the sum of its elements – is really very important, because everything which consists of elements is more than the sum of its elements. The thing which the Gestalt theoreticians in those days were opposed to was the idea of a structure built of atoms; of things that were regarded as if they were built out of bricks. But the point is, of course, that atomic structures are not built of bricks; and bricks are not like heaps. Rather, bricks are also Gestalten. Everything in that sense is ultimately a Gestalt. In other words, I do not say that the Gestalt concept is empty, but that it is almost all-embracing.

Surely, Popper is right to state that a brick also has a Gestalt. But that accepted, one observes that an object may emerge out of a heap of bricks and that the Gestalt of an object made out of bricks and the Gestalt of the underlying bricks composing this object are on *different levels of perception*. This point of view is nicely illustrated by *random-dot stereograms* (Julesz, 1971, 1991) as that given in Figure 1. There the bricks used are little squares. As long as the respective pattern is viewed monocularly, one sees nothing more than an aggregate

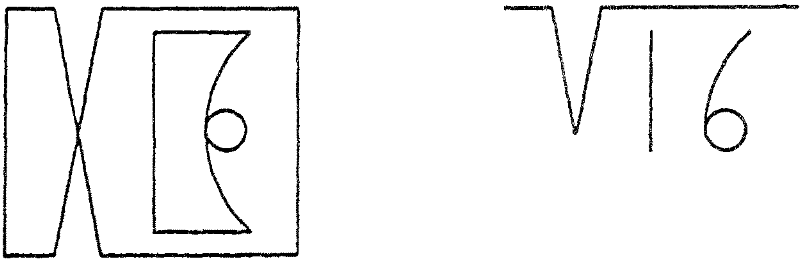

Fig. 2. Demonstration of holistic effects in Gestalt organization: The square root of 16 disappears if it is imbedded into some larger object (Köhler, 1971).

of little squares. As soon as the two pictures are fused binocularly (with the help of a stereoscope), a diamond-shaped object is perceived hovering over the random background.

Hence *a heap of bricks* (*to keep Popper's nomenclature*) *can unexpectedly acquire a Gestalt.* The process may take some time (say, from seconds to minutes) if the observer is not acquainted with the underlying pictures to be fused. During this organizational process, a flickering, unsteady image is observed (in particular, if one uses the anaglyph version of the stereogram, fused binocularly by use of 3-dimensional 'red-green' glasses (Julesz, 1971)). Since the organizational procedure is usually completed in too short a time, we do not even realize that *the images we observe are constructed in an 'internal', subconscious process* and are not simply 'there'. *Random-dot stereograms are used here to make this organizational process apparent.*

In the following, the *holistic aspect of Gestalt perception* is illustrated by various examples. The square root of 16 (in Fig. 2) is easily perceived in isolation, but disappears as soon as it is viewed as part of the larger object on the right-hand side (Köhler, 1971). Only careful inspection reveals that $\sqrt{16}$ is contained in it. Hence $\sqrt{16}$ has *lost its identity* as 'part' of the larger object, it no longer exists in a certain sense. Or consider Figure 3, which can be seen either as a collection of patches or as a 'contemplating man'. Perception of depth arises only if the respective pattern is seen in the latter way. Thereby the whole image is completely reorganized and the patches constituting it 'disappear', i.e., lose their identity just as in the example illustrated in Figure 2. If Figure 3 is seen as a collection of patches, there may and do already exist certain holistic 'correlations', i.e., these patches are not completely

Fig. 3. This picture can be seen either as a collection of patches or as a 'contemplating man' (Rock, 1984, p. 131). It illustrates the reorganization of holistic correlations in Gestalt perception. (Efforts made to contact the copyright holder, Craig M. Money, were unsuccessful, consequently this figure is reproduced without his consent. We hope this will cause no offense.)

uncorrelated. The critical point is really the *reorganization* of these correlations that turns it into the face of a man.

> 'Holistic' is *not* to mean here that 'the whole is different from the sum of its parts'. This slogan may be misleading. '*Holistic' is to say:* if one sees the *whole*, then the parts lose their identity, i.e., no longer exist in a certain (perhaps not precisely defined) sense. If one fixes on certain *parts*, on the other hand, then it seems strange that these parts can ever be re-collected as a whole.

As an example of the latter claim, one might concentrate on the short 'lines' of Figure 3, situated in the region that refers to cheeks and

Fig. 4. Dalmatian dog (Rock, 1984, p. 130). This picture is used to illustrate that giving structure to a bulk of visual information means to eliminate *and* to create holistic correlations. (Efforts made to contact the copyright holder, Ronald James, were unsuccessful, and consequently this figure is reproduced without his consent. We hope this will cause no offense.)

mouth of the man depicted. Fixing these 'lines' makes it difficult to integrate all the patches of the picture into a Gestalt (a head or a face in the present situation). Artists knew of course to use such holistic effects. Fascinating examples can be found among the paintings of Giuseppe Arcimboldo (Andreose et al., 1987).

Incidentally, shaping processes are not restricted to visual sensory material, but may also be observed with structuring of sense-impressions, auditory perception, communication (Watzlawick et al., 1967, Sec. 2.4), or with the structuring of ideas (e.g., in a mathematical proof).

In Gestalt formation of any kind, one should always be aware that two processes with opposite tendencies take place. On the one hand subentities lose their existence when being incorporated into some Gestalt. On the other hand the created Gestalt gains its existence by separation from the rest of the little universe considered. In Figure 4 one may see a dog and a tree, both of which are holistically organized just as in the examples above, and both have to be 'separated' from each other and from the rest of additional patches: this implies, in particular, that holistic correlations between the collection of patches making up the 'dog', on the one hand, with the surrounding patches, on the other, must be eliminated! Giving structure to a bulk of visual information means creating (within a Gestalt to be) *and* eliminating (between distinguished objects) holistic correlations. Effectively, *the creation of a Gestalt then involves two processes (artificially separated here for the sake of the argument)*:

- An object is established by elimination of holistic correlations with the 'environment'.
- This object obtains a form.

The creation of a contour, for example, would be attributed to the 'second' step. Interestingly, a contour may arise even if detailed inspection shows that it is not justified by the underlying visual material: inspection by scrutiny reveals that the Dalmatian in Figure 4 has no fourth leg (in the direction of the observer). Nevertheless, a respective contour arises if the dog is seen as a whole (cf. also Kanizsa, 1976).

Everyone is familiar with 'patterns' that allow (apart from just seeing a collection of patches) more than one interpretation, e.g., showing a young *or* an old lady. Particularly beautiful examples have been prepared by the Dutch artist M. C. Escher (Locher, 1984), one of them is reprinted in Figure 5: contemplating the whole picture (and not just some few objects in it), one sees either the black devils *or* the white angels.

Gestalt perception has a *stability property* (related to what is called *Dingkonstanz* in German). 'Stable' is not to say 'stationary', of course! It is to say that once a given pattern is attributed a certain shape, this shape is 'conserved': let that be in dynamical processes (a random-dot cinematogram, for example) or let that be in the situation where a Gestalt (such as the diamond-shaped object in the random-dot stereogram or the two different interpretations of a picture, as discussed in the previous paragraph) is immediately recognized even after a long intermission. 'Stable' is also to say that a Gestalt remains unperturbed by 'side-effects': by a flickering stochastic background or by perturbations arising in the attempt of eye and brain to create additional visual structure in the underlying pattern. Summarizing, 'stable' is to say that a Gestalt does *not* admit holistic correlations with the rest of the visual information, such as the flickering background just mentioned.

Perception of random-dot stereograms and visual perception in gen-

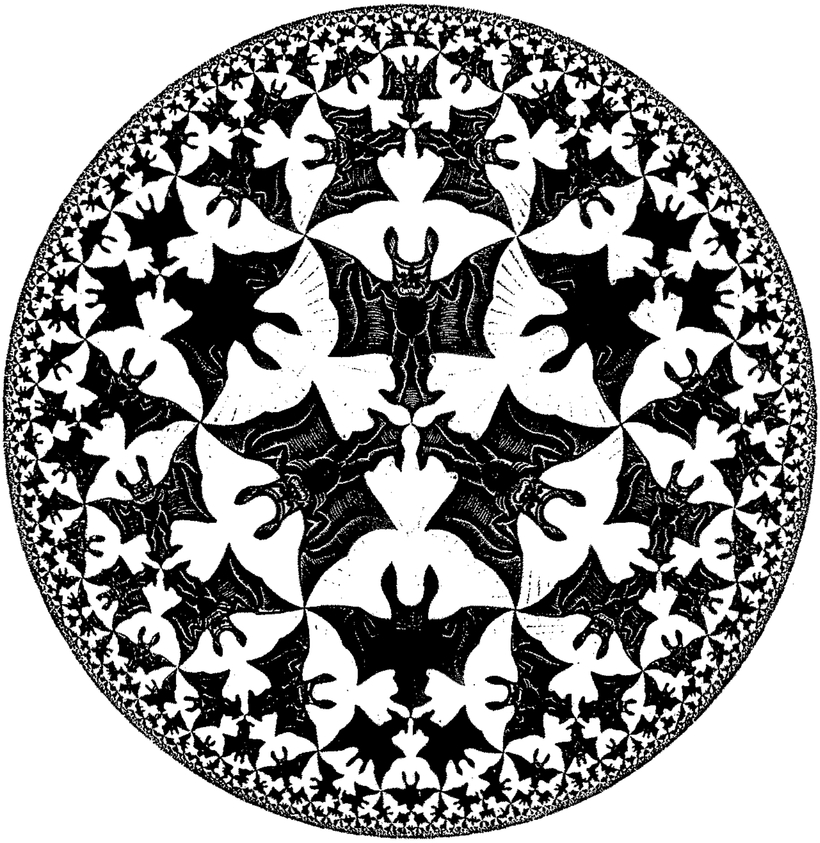

Fig. 5. One of the famous paintings created by M. C. Escher (Locher, 1984). It can be interpreted in (at least) two different ways, seeing devils *or* angels. (Reproduced with permission: © 1963 M. C. Escher/Cordon Art – Baarn – Holland.)

eral is a feedback process: the brain tries hard to make sense of incoming information. *As soon as the brain has 'created' some shape, it tries to keep and to stabilize it.* The particular way in which the two parts of our random-dot stereogram are fused is chosen such that the diamond-shaped object arises.

It seems therefore that the Gestalt of an object, and even the object itself, is *not* codified in the information we receive from our senses, hence is *not* part of the external physical reality (Gombrich, 1979; Maturana, 1982; Maturana and Varela, 1987; Resnikoff, 1989; Rock, 1984). This is not to say that an object's shape exists *only* in our mind; nor is it to say that *only* shapes already 'preexisting' in our mind can be perceived, though such preexisting shapes (such as Plato's or as C. G. Jung's archetypes) may play a role.

Leaving ontological questions aside, our interest focuses on *quantum mechanics*, where the problems mentioned with Gestalt theory arise again, but in sharper relief. Quantum mechanics does *not* explain Gestalt perception, of course, but in quantum mechanics and Gestalt psychology there exist almost isomorphic conceptions and problems:

> Similarly as with the Gestalt concept, the shape of a quantum object does *not* a priori exist but it depends on the interaction of this quantum object with the environment (for example: an observer or a measurement apparatus).
> Quantum mechanics and Gestalt perception are organized in a holistic way. Subentities do *not* necessarily exist in a distinct, individual sense.
> In quantum mechanics and Gestalt perception *objects have to be created* by elimination of holistic correlations with the 'rest of the world'.

The modern formalisms of quantum mechanics (Primas, 1983) offer the opportunity to give a stable (classical) shape to quantum objects. Just as in the context of Gestalt theory, 'stable' is to say that this shape does *not* admit holistic correlations with other physical quantities in the system under discussion (see Sec. 4). The dynamic 'measurement-type' process in which such a stable shape is formed corresponds (in a parabolic, loose sense) to the perceptual processes shaping reality in order to make the latter accessible to the human mind.

Quantum mechanics does not explain Gestalt perception, but *Gestalt perception is necessary to create 'objects' in a quantum world*: Einstein–Podolsky–Rosen correlations (see the next section) exist between *arbitrary* micro- or macroscopic entities if the latter admit at least *some* quantum properties. These Einstein–Podolsky–Rosen correlations must be suppressed in order to put into existence individual objects, which otherwise would be drowned in an all-devouring whole. 'Elimination' of Einstein–Podolsky–Rosen correlations is done precisely by the perceptual apparatus. Gestalt perception, in particular, creates objects out of the flickering unsteady background of a quantum system, just as with the random-dot stereograms above.

2. THE HOLISTIC STRUCTURE OF QUANTUM MECHANICS

> In the end it is practically impossible to say where the whole ends and the parts begin, so intimate is their interaction and so profound their mutual influence. In fact so intense is the union that the differentiation into parts and whole becomes in practice impossible, and the whole seems to be in each part, just as the parts are in the whole.
> Jan Christian Smuts (1987, p. 126)

It is one of the major merits of quantum mechanics that the dialectics of the whole and its parts can be studied on the level of a fully developed *formalism*. But merit seldom receives its true reward: most textbooks of quantum mechanics present a mutilated version, restricting themselves to the Schrödinger equation and, finally, to the production of *numerical* results. Notable exceptions are a book by Jauch (1968) and the elementary course offered by Primas and Müller-Herold (Primas and Müller-Herold, 1984). A proper introduction to quantum mechanics for the layman is still missing.

In quantum mechanics, the existence of *isolated* (*sub*)*objects* is no longer guaranteed. Einstein, Podolsky, and Rosen showed that quantum mechanical systems admit *holistic correlations that cannot be traced back to any interactions* (Einstein et al., 1935). Similarly, as in the example illustrated by Figure 2, subsystems lose their identity. But, whereas before only qualitative considerations were accessible, now things can be expressed in the quantum mechanical *formalism* (Schrödinger, 1935a, 1935b, 1936).

Illustration of holistic effects is best given by the famous experiments of Aspect and his coworkers (Aspect et al., 1982a, 1982b; Clauser and Shimony, 1978), which are presented here in a sketchy way: a ^{40}Ca-atom is excited to a state with total angular momentum $J = 0$. This state decays via a cascade

$$J = 0 \rightarrow J = 1 \rightarrow J = 0$$

into the original ground state, emitting two photons at wave lengths $\lambda_1 = 551.3$ nm and $\lambda_2 = 422.7$ nm. Conservation of momentum implies that these photons fly in opposite directions. With two polarizers oriented the same way (x- or y-direction, each about 6 meters distant from the source), the two photons are forced into *linearly* polarized states.

> The important fact then is: either *both* photons pass the respective polarizers or *both* fail to pass and are absorbed (due to conservation of angular momentum).
> The behavior of the photon system at *one* of the polarizers cannot be predicted. But if one knows that a photon has been absorbed at one of the polarizers, then it *follows* that 'the other' photon has been absorbed, too.

This result is independent of the actual direction of the polarizers. To prevent signal transmission, the direction of the polarizers can be changed with a frequency corresponding to 10 ns (the photons' flying time from the source to the polarizer being about 20 ns). The conclusions inferred from such experiments with time-varying polarizers is the same as before:

> The polarizers in the Aspect experiment can be installed at an arbitrarily large distance (between Paris and Tokyo, for example, or between different galaxies).
> Einstein–Podolsky–Rosen correlations (in short: EPR correlations) exist independently of interactions.
> *Quantum systems are not separable.* It is already careless to number photons. Aspect's experiment uses *one* 2-photon system. One-photon subsystems do *not* exist as individual entities.
> Note that EPR effects arise with arbitrary quantum systems, not just with photons. Subsystems (e.g., one of the photons in Aspect's experiment) of a quantum system are influenced by interventions far apart and therefore are *not* in a specified state. *Subsystems of a quantum system do not exist as an individual entity* (Primas, 1983).

In fact, the 'nonexistence of subsystems' is the characteristic property of any holistic system. Hence, in a strict interpretation, the slogan "The whole is different from the sum of its parts" (see Sec. 1) is *not* applicable to a holistic system, since its parts are *not* individual objects. Often this point is not worked out clearly enough. Most authors do not distinguish between holistic systems and merely complicated networks. 'Parts' of the latter exist perfectly well and the whole system can be described in terms of its parts and their interactions. The point with holistic correlations (such as EPR correlations) is precisely that one cannot explain them in terms of interactions.

The general idea of Aspect's experiment goes back to the article of Einstein, Podolsky, and Rosen (1935). It is principally to Einstein that the credit is due for bringing to light the nonseparability of quantum mechanics, though his intention was to show that quantum mechanics is either incomplete or unsensible, neither of which has turned out to be convincingly true. This lesson teaches us that *realism should not* be combined with specific physical ideas like atomism, localizability, separability, or determinism (Primas, 1993). Aspect's experiments – which confirm Einstein's 'absurd' quantum mechanical predictions perfectly well – do not exclude a realistic intepretation of the world. Often a more judicious formulation of 'reality' helps to escape contradictions: the holistic structure of quantum mechanics advises, for example, *not* to say that matter is *made* of elementary particles (like electrons) but that material reality can be described – under appropriate circumstances – in terms of elementary systems (ibid.). In Gestalt perception, one might be equally cautious and say that a given pattern (image) behaves as if being shaped in a particular way.

The holistic structure of quantum mechanics can also be viewed as a straightforward consequence of the quantum mechanical formalism (Primas, 1983; Raggio, 1981; Schrödinger, 1935a, 1935b, 1936): if a joint system, consisting of various subsystems, is in a pure state, then the same need *not* be true for the subsystems composing it. Only in the exceptional case that a subsystem is in a *pure* state can it be called an *individual (sub)object* or (sub)entity. As an example, consider an atom possessing more than one electron: the whole atom is described by a wave vector (≡ state vector ≡ wave function, corresponding to a pure state), whereas the composing electrons admit only a description by mixed states (density operators). If all the composing electrons were described by wave vectors, then the global wave vector would be a product vector (this corresponds to a Hartree ansatz without directly taking into account the Pauli principle), and conversely. The description of a subsystem (e.g., a composing electron) by a mixed state reflects the fact that the subsystem admits no description as individual object. A mixed state of a quantum system cannot be *uniquely* decomposed into pure states, hence not even the proportion of a given pure state in the mixed one is clearly determined. In classical systems (such as ordinary classical mechanics), no similar phenomenon arises: in the description of the planetary system, for example, every planet (every subsystem) is in a well-defined pure state and the global state of the planetary system is a product state composed of the states of the involved planets. The latter situation may also arise in Gestalt perception: two shapes can trivially be composed of a single one, 'trivially' meaning without holistic correlations between the two.

A quantum mechanical state associates a complex number $\phi(A)$, the 'expectation value', to every physical quantity A of the system in question. In case A is specified by an operator and Ψ is a state vector ($\equiv$ wave vector), the expectation value is given by $\langle\Psi|A\Psi\rangle$, where $\langle|\rangle$ is the scalar product of the underlying Hilbert space. In the present paper, the concepts 'state' and 'state vector' are not consequently distinguished. The technical terms 'pure state' (corresponding to an individual description) and 'mixed state' (corresponding to a statistical interpretation) are used to make the situation more transparent for the experts. The reader is kindly asked to tolerate residues of quantum mechanical slang in this paper.

The holistic structure of a Gestalt (see Sec. 1, e.g., Fig. 2) *illustrates* quantum holism, but of course only on the level of a parable. Nevertheless, the parallelity (isomorphism) between quantum and Gestalt holism goes far enough that one could even think of devising Aspect-type experiments in Gestalt perception. On the level of neurons (with some formalization work done), EPR correlations should not be excluded too quickly. One might also recall the 'Hilbert-space formalism' of Watanabe in pattern recognition processes (Watanabe, 1969).

It is interesting to note that holistic views were revived in different fields during the first decades of this century: philosophers and physiologists (Meyer-Abich, 1989), Gestalt psychologists (Köhler, 1971), and physicists (Heisenberg, 1986) independently used similar concepts. The actual term *holism* was coined by Jan Smuts in 1926 (Boeyens, 1986; Meyer-Abich, 1989; Smuts, 1987) (from the Greek word *ολος* meaning *whole*). Holistic concepts are extremely difficult to work with when no proper formalism (such as quantum mechanics) is at hand. This makes it easy to refute holistic concepts altogether. From Smuts's book (1987), for example, not much can be defended, apart from the holistic concept itself.

Holistic problems played an important role in ancient philosophy, mythology, and religion. Notably, the famous exponents of Neoplatonism (for example, Plotinos and Proklos in the third and fifth centuries, respectively) invented an extensive ϑεολογια dealing with holistic problems. These considerations were taken up by renaissance thinkers such as Ficino and Pico della Mirandola. A tradition of holistic thinking persisted with Leibniz, Schelling, Hegel, Goethe and with the romantic writers of the early nineteenth century. The mechanistic, antiholistic movement in science was headed by Ernst Haeckel during the second half of the nineteenth century (Meyer-Abich, 1989).

3. MUST A MOLECULE HAVE A SHAPE?

> If, however, there were no preconceptions about what a molecule ought to look like, there is nothing in the solutions of the space-fixed problem that would force or even guide one towards looking at them in the traditional molecular way. The most likely analysis of the results would be much more akin to the traditional methods for atoms.
> Brian T. Sutcliffe (1992, p. 43)

Chemists do not doubt that molecules should be described by quantum mechanics. Once this point of view is accepted, the holistic quantum mechanical structure comes into play. Not only are EPR correlations with neighbor or former neighbor molecules important, but also the coupling to the radiation or gravitation field. The latter two fields can never be decoupled and can only be very partially screened (but see the remarks on dressing processes, Section 5). Starting with a molecule coupled to the vacuum state of the electromagnetic field, the dynamics of the joint system leads immediately to EPR correlations between the molecule and the field. Hence single molecules do not necessarily exist as individual entities.

Even if a *single isolated* molecule is considered, the concept of a molecular shape is highly dubious (Claverie and Diner, 1980; Claverie and Jona-Lasinio, 1986; Sutcliffe, 1990, 1991; Weininger, 1984; Wilson, 1979; Woolley, 1978, 1986, 1988, 1991). This is mainly due to the *Pauli principle* and the *superposition principle*, which belong to the most important characteristics of quantum mechanics. Hence, just to cite an example, the overall wave function of a molecule describing nuclei *and* electrons should be antisymmetric with respect to permutation of two

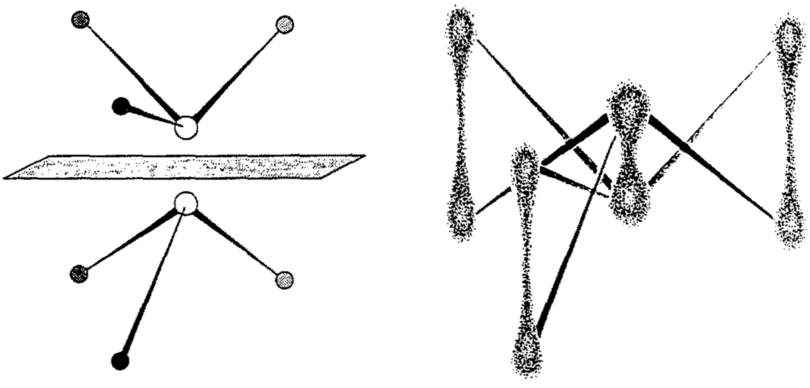

Fig. 6. A sketch of various structures of an ammonia-type molecule. The molecules on the left-hand side (mirror-images of each other) possess a nuclear frame. In their superposition, on the right-hand side, the nuclear frame has disappeared.

arbitrarily chosen hydrogen atoms (Thomas, 1969). Consequently, the latter automatically lose their individual identity and the nuclear frame of the underlying molecule ceases to exist. Or consider (approximate) ground states of a molecular Hamiltonian, e.g., left- and right-handed states of a potentially chiral molecule (Barron, 1991; Pfeifer, 1980; Quack, 1989; Amann, 1988, 1991a, 1991d) or the 'pyramidal' states of ammonia (Kukolich et al., 1973; Thomas, 1969). Then, in traditional quantum mechanics, there is no reason at all not to consider a superposition of these states! But superposition of molecular states with different nuclear structure gives rise to a state no longer admitting a nuclear frame: the position of the nuclei is described by a probability distribution, and this probability distribution changes if the particular superposition (e.g., the underlying scalar coefficients attributed to the states one started with) is changed. Hence even for a completely isolated molecule there is no guarantee of something like a shape! Any 'shape' would be EPR-correlated with (suitably chosen) molecular properties and hence 'destroyed' by a measurement of the latter! Incidentally, superpositions of ammonia's pyramidal states resulting in the proper ground and first excited states (and conversely) can be prepared without difficulty (Kukolich et al., 1973). For chiral molecules, the respective situation is not so clear (Quack, 1989; Amann, 1991a, 1991d). Figure 6 is an attempt to sketch the effect of a superposition: on the left-hand side the pyramidal states of an ammonia-type molecule (but with distinguished ligands, such as NHDT instead of NH_3) are drawn. They admit a nuclear frame. On the right-hand side *one particular* superposition of these states is sketched: there the nuclear frame has vanished.

If one *wants* to have individual molecules, individual nuclei and a molecular shape, or even individual electrons (as it may happen), then one may *impose* these additional wishes on the quantum mechanical formalism. In traditional quantum mechanics, such individual entities do *not* exist, but it may of course be sensible to proclaim their existence, be it that this corresponds well to traditional prejudices or be it that this guarantees success in the scientific community. Here *prejudice* is surely *not* meant in a pejorative sense: one tries to introduce as much structure as possible to a given situation without affecting too much certain (e.g., energetic) theoretical predictions. That corresponds again to perceptual processes where the brain tries to create shapes (Gestalt) so long as this shaping is more or less compatible with the incoming visual (retinal) or auditory material and other 'experience'.

The problems to solve then are: What approximations have been implicitly made in order to arrive at a particular concept? When do these approximations eventually break down? Are there alternative ways to go? What is the relation to more fundamental theories such as quantum mechanics?

In this paper I want to sketch *one* conceivable approach in that direction. Other approaches may work equally well or better.

4. CLASSICAL STRUCTURES AND GESTALT: AN INTERLUDE

> We can never neatly separate what we see from what we know. . . what we call seeing is invariably coloured and shaped by our knowledge (or belief) of what we see.
>
> Ernst H. Gombrich (1960, p. 394)

Holistic correlations between two systems can be 'eliminated' by declaring that only product states are admitted. Hence, if the combined system is in a pure (product) state, every subsystem is (effectively, by declaration) in a pure state and can be considered an object. Any intervention (measurement) concerning one of the two subsystems does not disturb the other one.

Holistic correlations can also be viewed from the perspective of two physical quantities in *one* given quantum system, which is not considered as being divided or being divisible into two or more components. One may ask if a measurement of one of those quantities, say the quantity A, changes the situation with another, say B. *If* the measurement of A does *not* preclude anything about the results of measurements of B *in any (pure) state* of the system, then we call them EPR-***un***correlated. Position and momentum operators of an electron, for example, are *not EPR-**uncorrelated**:* measuring the position of an electron, i.e. preparing the electron in a state with more or less well-defined position, changes the measured values of the electron's momentum.

Again, holistic correlations between physical quantities can be excluded, either by declaration or by giving more fundamental reasons (see Sec. 5). *Henceforth, a quantity **not** admitting holistic correlations with **any** other quantity of the system under discussion will be called **classical**.* This nomenclature acknowledges that holistic correlations do not arise in 'classical' physical theories such as classical mechanics.

In the formalism of *generalized quantum mechanics* (Primas, 1983), classical quantities are represented by operators that commute with all other operators of the system. Heisenberg's commutation relations for position and momentum assert that position and momentum are *not* classical quantities in quantum mechanics. 'Generalized quantum mechanics' stands for one of the various different formalisms incorporating classical observables *and* admitting the description of systems with infinitely many degrees of freedom: algebraic quantum mechanics (Bratteli and Robinson, 1981, 1987), quantum logics (Jauch, 1968; Piron, 1976), the convex state approach (Davies and Lewis, 1970; Ludwig, 1986). They are more less equivalent but use a slightly different language. In all these formalisms, traditional quantum mechanics *and* traditional classical (Hamiltonian) mechanics can be incorporated (Primas, 1983). Furthermore, 'generalized quantum mechanics' can be used to discuss thermodynamical systems and phase transitions (Sewell, 1986; Strocchi, 1983): recall that traditional quantum mechanics admits only *one* phase at a given temperature (since there is at most *one* canonical state, described by the density operator $\exp\{-\beta H\}/\text{trace}[\exp\{-\beta H\}]$, for a given inverse temperature β). This deficiency does not fit together well with the phenomenological situation and is cured in the generalized formalism.

Deriving classical observables and their dynamics in genuine quantum systems is a nontrivial matter (Bóna, 1988, 1989; Duffner and Rieckers, 1988; Fleig, 1983; Hepp and Lieb, 1973; Morchio and Strocchi, 1985, 1987; Unnerstall, 1990), often related to 'broken' symmetries. Discussion of the latter is already very difficult in the context of classical statistical mechanics (Ellis, 1985). The derivation of a relatively simple classical observable is sketched in Section 5 below.

Classical quantities have an unambiguous value at any time, which is unaffected by observations of any other quantity of the system under discussion (in particular, unaffected by observation of the classical quantity itself). That's precisely the property that was attributed to a Gestalt in Section 1.

> *Therefore, it is proposed here to extend and to make more precise the 'dictionary' translating between Gestalt psychology and quantum mechanics: the (visual, auditory, mental . . .) Gestalt of an object corresponds to the (unambiguous) value of some classical quantity in quantum mechanics.*

A molecule, for example, has a shape if its nuclei sit at unambiguously defined places. This shape is encoded by the parameters (distances, angles, etc.) determining the molecule's nuclear frame. The respective classical quantity that can take continuously varying values. As another example, consider a pattern that can be seen in two ways (cf. Sec. 1): then these two ways of attributing a Gestalt to the pattern correspond to a classical quantity with only two possible outcomes. *Chirality* could be a chemical example with similar background: a chiral molecule is either left- or right-handed, with no intermediate possibility (which would be the superposition of left- and right-handed states) remaining.

The two-valued classical quantity in these situations (i.e., Gestalt recognition or chiral molecules) describes only a very partial and almost trivial classical structure. The angels/devils painting of Escher has much more classical structure than just that two-valued one. Or a chiral molecule *with only a two-valued classical structure* would *not* possess a nuclear frame!

With Gestalt perception, the nature of a classical shape can be understood in more detail. Consider again the situation of a pattern that admits two interpretations: there the two-valued classical quantity comparison is only sensible as long as one cannot see behind the process that creates these two interpretations! As soon as this process is revealed (as in the example with random-dot stereograms), or *as soon as the 'bare' pattern appears without any interpretation at all (consisting* *only of black and of white points without any Gestalt appearing*), *the classical shape is no longer classical* (*or not yet classical*). In the particular example of Figure 5, the devil or the angel interpretation of the whole pattern can be built up by looking specifically at *one* devil or *one* angel, respectively. During these 'creational' processes, more than just two interpretations are available, and such that the two-valued classical quantity may perhaps not be extended to a three-valued one (incorporating the two interpretations and some other pattern): one then *no* longer has (overall) Gestalt, *no* longer an (overall) classical quantity. In the language of quantum mechanics, one might compare the bare pattern to a superposition of states. Quite similarly one might expect that the two-valued classical quantity describing chirality can disappear by preparation of a 'bare', 'undressed', potentially chiral molecule (see Sec. 5).

5. CAN THE ENVIRONMENT SHAPE MOLECULES?

> Zweiteilung und Symmetrieverminderung, das ist des Pudels Kern.
> Wolfgang Pauli (in Heisenberg, 1959, p. 663)

Twentieth-century chemists, as a rule, cannot see molecules without their having a shape, without their having a nuclear frame. Preconceptions of this sort are useful for sociological reasons, but they may change. It would therefore be interesting to single out certain cases where there may exist some deeper reason for molecules to acquire a kind of shape.

It has already been mentioned that molecules are coupled to the radiation and to the gravitation fields and that the influence of these fields cannot easily be screened. The interesting point with fields is that they have *infinitely many degrees of freedom* (corresponding to the modes of the field). The same is true for the joint quantum system {molecule and field} to be investigated.

Trying to eliminate EPR correlations between the molecule and the field (≡ the environment) leads to the concept of a *quasimolecule* or *dressed molecule*. The joint system remains unchanged but is split up in a new way:

$$\{\text{molecule and field}\} \equiv \{\text{quasimolecule and quasifield}\}.$$

The quasimolecule incorporates field properties and the quasifield (≡ dressed field) incorporates molecular properties. The new splitting is done in a way to guarantee that the *EPR correlations between the quasimolecule and the quasifield are minimized*, demanding, for example, that distinguished states of the joint system are product states with respect to the new splitting.

This dressing concept can be understood by comparison to a free ion that is transferred into an aqueous solution, thereby acquiring several water layers. The resulting solvated ion corresponds to the above quasimolecule. It's properties differ substantially from the properties of a free ion. Due to solvation, the Coulomb field of the free ion is screened by the solvent molecules, so that the solvated ion interacts only weakly with the remaining aqueous solution (the latter corresponding to the quasifield above). Moving in an external electric field, the solvated ion behaves like an individual entity.

The concept of a system dressed by environmental influence has been used in various situations with a system-environment structure (Primas, 1990d). In the solvation example (which has nothing to do with quantum mechanics and EPR correlations), the hope is to minimize the interaction between the dressed ion and the environment. In our quantum mechanical example above, the goal is first of all to minimize the EPR correlations between the dressed molecule and the dressed environment. *The dressing process break the holistic symmetry and creates a quasisystem as soon as the (minimized) EPR correlations are eliminated by declaration.* Incidentally, the dressed systems are mainly of interest to experimenters, such as the solvated ion in aqueous solution (compared to the bare one), or a chiral molecule (compared to the nonchiral undressed molecule of traditional quantum mechanics) (Amann, 1991a, 1991c, 1991d; Pfeifer, 1980), or boson-like electron pairs dressed by a cloud of phonons in superconductivity (McKenna and Blatt, 1962).

Dressing processes are useful to 'create' quasisystems that are (almost) decoupled from their environment. Note that some correlations between the dressed system and its dressed environment persist even after the dressing process has been performed. The spontaneous decay of excited molecular states, for example, is due to such correlations. Complete screening/decoupling of molecular properties from the dressed environment can only be reached if these properties are classical (see discussion below).

Important problems of molecular quantum mechanics therefore are:

(1) Which part of the joint system {bare molecule and field} should be considered as the quasimolecule used in chemistry?

(2) Does the quasimolecule chosen possess classical properties (≡ molecular shape)? Can these classical properties be derived?

As far as (1) is concerned, a *first step* is achieved by the choice of the Coulomb gauge in the molecule-field interaction: consider the bare molecule *without* Coulomb interaction between the involved nuclei and electrons (Heitler, 1954). When this bare molecule is coupled to the electromagnetic field, then one *may* (and does in chemistry) use the Coulomb gauge and view the vector potential of the field as composed of a transverse and a longitudinal part, where the latter incorporates the Coulomb interaction between the particles involved (ibid.). These Coulomb interactions – which were mediated by the *field* before – are then *ascribed* to the molecule. Hence *part of the field now is incorporated into the original bare molecule, resulting in a quasimolecule*. There is no a priori reason to stop the dressing procedure at that point.

As for (2), let me give another illustration: for a thalidomide consumer it makes a big difference if she/he takes the left- or the right-handed form! That fact couldn't be understood if only the bare molecule were involved (where the superposition principle holds unrestrictedly). *How does that classical structure left/right come in?!* It is surely not just an artifact, coming along by choice of an appropriate point of view! For this and other classical structures and observables (charge of a particle, position of a billiard ball (Born, 1969), temperature (Takesaki, 1970), and chemical potential (Müller-Herold, 1980, 1982, 1984) of substances, etc.), one should find a reasonable explanation.

Hence: accepting quantum mechanics results in the fading away of reality! Studying seriously environmental influences should lead us back to the reality chemists believe in!

A molecule isolated completely from its environment is expected to show quantum behavior only. A quasimolecule, which already incorporates environmental influences, is expected to show partial classical behavior, just as the molecules in chemistry do.

Even chemical bonds (Coulson, 1955) and chemical systematics (which refers to substances and thus lives on a different level) should be derivable from a proper discussion of quantum mechanics (including systems with infinitely many degrees of freedom and environmental influences). Such ambitious goals will, of course, be very difficult to achieve! But *the task of theoretical chemistry is to sharpen and to explain chemical concepts, not to reject a whole area of inquiry* (Primas, 1983).

In the following, I shall try to *sketch the emergence* of a simple two-valued classical property. This classical property will turn out to admit two distinguished values. The respective states will be called L- and R-states. One *might* (but need not) think here of chirality.

'The' environment of a molecule, i.e. the rest of the universe, is of course inaccessible to any precise theoretical reasoning and must be replaced by some model environment. Here *the environment is simply chosen to consist of infinitely many harmonic oscillators*, coupled to the molecule in a *dipole-type manner*. The simplest model of this then is the ubiquitous *spin-boson model* (Emery and Luther, 1974; Fannes and Nachtergaele, 1988; Fannes et al., 1987, 1988a, 1988b; Leggett et al., 1987; Nachtergaele, 1987; Pfeifer, 1980; Silbey, 1991; Harris and Silbey, 1985; Silbey and Harris, 1984, 1989; Spohn, 1989; Spohn et al., 1990; Zwerger, 1983; Amann, 1991a, 1991b, 1991c, 1992a, 1992b), which describes the molecule in the caricature of a *two-level system* coupled to a boson field. The two levels (≡ a spin) represent two carefully chosen stationary states of the isolated molecule. Every field mode corresponds to a position operator, Q_n, and a momentum operator, P_n (with n numbering the modes), fulfilling the Heisenberg commutation rules. Position and momentum operators referring to *different* modes commute. Hence the spin-boson Hamiltonian has the form

$$H = \tfrac{1}{2}\epsilon\sigma_1 + \sum_{n=1}^{\infty} \tfrac{1}{2}\{P_n^2 + \omega_n^2 Q_n^2\} + \sigma_3 \sum_{n=1}^{\infty} g_n Q_n,$$

with σ_1 and σ_3 being Pauli matrices, with ϵ being the level splitting of the isolated molecule, and with g_n being the coupling constant between the molecule (the spin) and the nth mode of the field. Physical constants such as $\hbar$ have been eliminated. *For the present purpose it is not important to know many details.* The results below are based on calculations with this spin-boson Hamiltonian (Amann, 1992a; Silbey, 1991; Silbey and Harris, 1984, 1989; Zwerger, 1983), but similar results could be expected with other models.

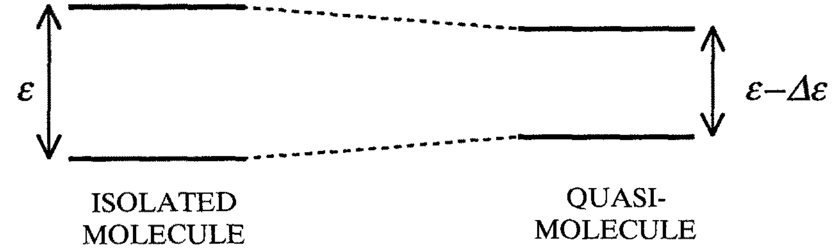

Fig. 7. The coupling of a two-level system with *large* level splitting ϵ to its environment results in a small 'Lamb-shift type' change of ϵ. The structure of two-level system remains unchanged.

The spin-boson model is a paradigmatic example (but also an extreme caricature) of the coupling between a 'small' quantum system and a quantum environment. The coupling between a molecule and the radiation or the phonon fields gives rise to the spin-boson model, but only after some uncontrolled idealizations have been introduced. Hence any result concerning this model has to be treated with care. A slightly more general model would consist of a double-minimum potential coupled to harmonic oscillators by means of 'springs'.

Qualitatively, one arrives at one of the following two scenarios (Amann, 1992a; Silbey and Harris, 1989; Zwerger, 1983), depending on the particular level splitting and coupling constants chosen:

- For a (relatively) large level splitting ϵ of the isolated molecule, the coupling to the field results in a small energy shift of the two molecular levels considered (see Fig. 7). Hence the quasimolecule is identical with the isolated molecule, apart from the fact that its level splitting is slightly changed. This is a Lamb-shift type effect.
- For a 'small' level splitting of the isolated molecule, an additional effect may arise (depending on the particular coupling constants (Amann, 1992a)), leading to a *two-valued-classical quantity:* each pure state of the quasimolecule is an eigenstate of this classical quantity and therefore labeled by one of the two possible eigenvalues. Here a nomenclature is chosen that calls these states L- or R-states, respectively. In particular, *two ground states* can be shown to arise: an L-ground state and an R-ground state (Spohn, 1989; Amann, 1991b). The two-level systems

arising in each of these ‘sectors’ show an identical modified level splitting (see Fig. 8).

A well-known candidate for a classical two-valued quantity is the molecular *handedness* (*chirality*). A (single) chiral molecule seems to be *either* left- *or* right-handed, with no intermediate superposition-type states (yet) known (Barron, 1986; Pfeifer, 1980; Quack, 1986, 1989; Amann, 1991a, 1991c, 1991d). The nomenclature above can be derived from this particular example or simply be thought to refer to the ‘left’ and ‘right’ sector in Figure 8.

Superpositions of (pure) L- and R-states are ‘forbidden’, in the sense that these superpositions lead to *mixed* states, corresponding, for example, to a racemate in the example of chirality and *not* describing a *single molecule* (Amann, 1992b; Müller-Herold, 1985; Pfeifer, 1980). Hence a single dressed molecule is *either* in an L- *or* in an R-state.

The set of L-states (or the set of R-states) is called a *sector*. Only state vectors (≡ wave vectors) in a given sector (but not superposition of state vectors in different sectors) give rise to pure states. The dressed molecule therefore has *acquired a two-valued shape*. This shape is *not* imposed and shows *no holistic EPR correlations* to any other physical quantities of the joint system {molecule and environment}, hence it is classical.

‘Derivation’ of this classical structure means that once the coupling constants between spin (≡ molecule) and field are given, one may decide without any further physical considerations, just by mathematical reasoning, if a classical shape arises or not. The critical point in this derivation consists in showing that L- and R-states exist such that their superposition is a mixed state. This then implies the existence of an explicitly constructable (Amann, 1992b) classical observable, i.e., an operator (just like a position and a momentum operator) that commutes

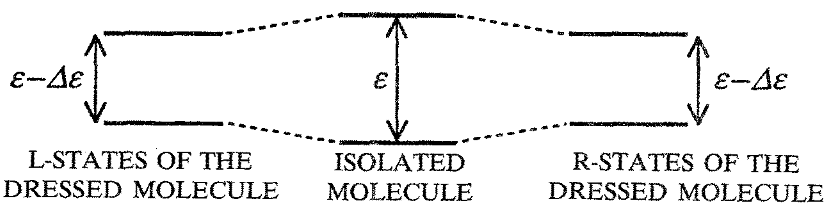

Fig. 8. The coupling of a two-level system with very *small* level splitting ϵ to its environment may give rise to a two-valued classical structure.

with all other observables of the system in question. In case of the spin-boson system, these other observables are the spin-operators σ_1, σ_2, σ_3 and the field operators Q_n and P_n for all modes n of the field.

Einstein–Podolsky–Rosen correlations between this derived classical shape and the rest of the environment are *strictly nonexistent*. And let me say that again: the L- and the R-structures arising stand for a general two-valued situation. We are far from discussing a realistic model, we are far from discussing chirality: this would be much more difficult. In a realistic model, it could, for example, not be accepted that the molecule is replaced by a two-level system. Nevertheless, the two-valued classical observable is not a consequence of the use of a *two*-level system for the molecule (Spohn et al., 1990)!

Note furthermore that the L- and the R-structures do not give rise to a nuclear frame! The latter would admit continuously many choices (corresponding to all bond lengths and angles), whereas in the present case only *two* choices (L and R) are offered. It might well be that *additional classical structure* arises by some other mechanism. Anyway, deriving classical structure is a difficult but not impossible goal.

To explain the two-valued classical quantity of above in heuristic terms, it is formulated in a slightly different (but equivalent) way: superpositions of two pure state vectors, Φ_L and Φ_R, are 'forbidden', i.e., do *not* lead to a pure state again, if and only if *all* transition probabilities between them vanish (Amann, 1992b; Müller-Herold, 1985; Pfeifer, 1980),

$$|\langle \Phi_L | T\Phi_R \rangle|^2 = 0,$$

with 'all' meaning that the 'mediating' operator T can be chosen to be an *arbitrary* observable of the system in question (dipole or quadrupole moment operator, etc., and with $\langle | \rangle$ being the scalar product of the underlying Hilbert space). The states Φ_L and Φ_R are then said to be *separated by a superselection rule*.

> Two states Φ_L and Φ_R are separated by a superselection rule if and only if there exists a *classical* observable X, such that the (dispersion-free) expectation values of X with respect to Φ_L and Φ_R are different. Hence there is a one-to-one correspondence between classical observables and superselection rules.

The heuristic explanation for the superselection rule (classical observable) arising in the spin-boson model then reads as follows: the more modes of the field are taken into account, the smaller the transition probabilities become between states in the respective two sectors (to be) of the spin-boson model. The L- and R-states incorporate a 'cloud of modes' (cloud of phonons, cloud of photons, etc.); in a transition it would be necessary to transform this 'cloud' into its counterpart as well, which may turn out to be impossible (Pfeifer, 1980). It is more impossible, the more modes of the field are considered. For a large (but finite) number of modes, an approximate superselection rule arises that turns into a strict superselection rule (classical observable) if all the infinitely many modes of the field are considered.

It should be stressed here that a classical quantity always refers to a particular context. When the *dynamical generation* of a classical quantity is investigated, then one must go *beyond* it, just as for the dynamical generation of a Gestalt. Hence in that situation the classical structure or Gestalt under discussion has to be 'broken up'. With random-dot stereograms this can be (partially) done in the case of Gestalt perception. In this respect, one might also think of the process that *mediates* between two different interpretations of a picture (such as between the interpretations of Figure 5). If processes of this type are considered, the Gestalt or its corresponding classical structure are lost. Similarly, the classical chiral structure of a molecule can in principle be removed. For an experimental investigation of this dynamical process, it would be necessary to prepare the bare molecule (of traditional quantum mechanics), i.e., to screen the molecule from its environment completely. From a theoretical point of view, this measurement-type process is notoriously difficult to describe (Primas, 1990a, 1990b, 1990c, 1991; Zaoral, 1991).

6. QUANTUM MECHANICS AND THE GESTALT PROBLEM: FINAL REMARKS

> The rabbi spoke three times. The first talk was brilliant – clear and simple. I understood every word. The second was even better – deep and subtle. I didn't understand much, but the rabbi understood all of it. The third was by far the finest – a great and unforgettable experience, I understood nothing, and the rabbi himself didn't understand much either.

(A favorite story of Niels Bohr, as cited in French and Kennedy, 1985, p. 299)

Speaking of an 'isomorphism' between quantum mechanics and Gestalt perception does *not* mean that Gestalt perception can be explained in terms of quantum mechanics. The 'isomorphism' mentioned refers to structural similarities between these two subjects and has the status of a parable. It rests on the fact that quantum mechanics in its modern formalisms (Primas, 1983) deals with general concepts such as complementarity, holism, broken symmetries, and others that have their counterparts in various fields and cannot be restricted to physics alone.

Here, primarily, the concepts of an *object* and of an object's *shape* have been considered. The problem arising with holistic theories is that objects do not necessarily exist as part of an all-embracing whole. Objects have to be *created* by elimination of holistic symmetries between the object-to-be and the environment-to-be (one might think here of the pattern in Figure 4 and think of dressing procedures discussed in Section 5). This creational process can at least in principle be done in various different ways and there is no clear recipe telling us how this separation into object and environment (*or* into object and subject *or* into observed and observer *or* into system and measurement apparatus *or* into Dalmatian and grounds) has to be done.

Holistic correlations between quantum systems can only rarely be shown to vanish completely; the alternative one has is to minimize these correlations with respect to certain states and with respect to a certain separation into parts. This was done in the dressing process described in Section 5. The next step – 'elimination' of the remaining minimized holistic correlations – can only be attained by *ignorance* or *declaration of nonexistence* in the perceptual apparatus. Nevertheless, holistic correlations are still there with any two quantum systems and may have considerable effect (for example, resulting in the spontaneous decay of excited molecular states).

Once an object is established, it may acquire shape, a contour, for example. It has been argued in this article that *Gestalt is a classical concept*, hence it is unambiguously defined at any time and does not admit *holistic* correlations with other quantities in the system under discussion. The identification

$$\text{Gestalt} \leftrightarrow \text{value of a classical quantity}$$

in the dictionary translation from Gestalt perception to quantum mechanics was based on these properties.

Classical quantities in quantum mechanics do not necessarily belong and refer to an object in 3-dimensional space: the charge of a particle, the temperature (Takesaki, 1970), and the chemical potential (Müller-Herold, 1980, 1982, 1984) of a substance are classical quantities of this type. Similarly a Gestalt need not have any direct interplay with 3-dimensional space (think of a chord). *The concept of a Gestalt therefore has been used here in a very broad sense.* Let me hasten to admit that the concept of a Gestalt has also been used in an informal manner and that it has not been clearly defined. It might well be that the Gestalt concept is connected with the *symmetry group* of some classical quantity and not so much with the classical quantity itself. These more delicate questions were not attacked here.

The structural similarities between Gestalt perception and quantum mechanics are on the level of a parable, but even parables can teach us something, for example, that quantum mechanics is more than just production of numerical results or that the Gestalt concept is more than just a silly idea, incompatible with atomistic conceptions. Ideas of holism, complementarity, generation of classical structures, broken symmetries, and other concepts have been used in disguised forms in mythology, religion, alchemy, philosophy, psychology and various 'scientific' fields before quantum mechanics was invented. Revealing their relationship with quantum mechanics might help to see these old ideas in new light and to give them back the credit they deserve.

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