Decoherence

The decoherence of the state functions of open quantum systems is known already since the twenties of last century. But only since the seventies it found appropriate attention in the debate about the interpretation of quantum theory. In this letter we derive and compare the basic concepts for the description of measurements of closed and open quantum systems. Thereby the density operator is introduced, and the notions PVM and POVM are explicated. Also the "measurement problem of quantum theory" and the "problem of the preferred basis" are discussed in this context. In the last section, the essential properties of projection operators and density operators will be evaluated.

For an amazing long time, the basic importance of decoherence of quantum systems, which are entangled with their environment, has been overlooked. Our central result (35) can be found already in §1, equation (4) of a publication by Landau [1] from the year 1927. Also in the following decades, these facts never have fallen into oblivion. As a typical example we mention the extensive discussion on the relationship between measurement and decoherence in the chapters 19 and 20 of the textbook on quantum mechanics by Gottfried [2]. Another example is a citation of Heisenberg from 1955, which we will quote on page 27. But only in the seventies and eighties, the phenomenon of decoherence of open quantum systems got the appropriate attention in the debate on the interpretation of quantum theory, starting with a publication by Zeh [3] in 1970.

1 Closed Quantum Systems

The state of a quantum system S is described by means of the state function $|\psi\rangle$. The state function is a vector in the Hilbert space $\mathcal{H}$. It is conveniently normalized to unity: $\langle\psi|\psi\rangle = 1$.

Measurable quantities (observables) are represented by hermitean operators. We consider the simple case of an observable Q, which has only discrete eigenvalues, and whose normalized eigenvectors $|q_j\rangle$ with eigenvalues q_j constitute an orthonormal basis, spanning the Hilbert space $\mathcal{H}$:

The $|q_j\rangle$ are eigenvectors of Q: $Q|q_j\rangle = q_j|q_j\rangle$ (1a)

The $|q_j\rangle$ are orthonormal: $\langle q_k|q_j\rangle = \delta_{kj}$ (1b)

The $|q_j\rangle$ are complete: $\sum_j |q_j\rangle\langle q_j| = 1$ (1c)

If the observed system is described by the state function $|\psi\rangle$, and if this state is normalized to unity, then the expectation value of the observable Q is

$$\begin{aligned}\langle Q\rangle_\psi = \langle\psi|Q|\psi\rangle = \sum_j \langle\psi|Q|q_j\rangle\langle q_j|\psi\rangle \ = \\ = \sum_j q_j \underbrace{\langle\psi|q_j\rangle}_{a_j^*}\underbrace{\langle q_j|\psi\rangle}_{a_j} = \sum_j q_j\,|a_j|^2 = \sum_j q_j\,w_j \ . \qquad (2)\end{aligned}$$

a_j is the probability amplitude, and w_j is the probability, for the value q_j to be observed in a particular measurement. The mean value $\langle Q\rangle_\psi$ is expected for measurements of a large ensemble of systems, which all were prepared in the state $|\psi\rangle$.

The measurement not only produces a measured value, but at the same time prepares a new state. The system, which was described by the state function $|\psi\rangle$ before the observable Q was measured, is described by the state function $|q_k\rangle$ after the measurement, if the eigenvalue q_k was observed:

$$\text{dynamic I:}\quad |\psi\rangle \xrightarrow{\text{measurement of } Q \text{ with result } q_k} |q_k\rangle \tag{3a}$$

With probability w_k the value q_k will be observed in a particular measurement of the observable Q, and the system will be prepared in the state $|q_k\rangle$, if it was described by the state $|\psi\rangle$ before the measurement. The measurement, which is described by dynamic I, is a discontinuous, irreversible process, which can not be explained deterministically. Only the probability w_k of the result q_k can be computed, but in general it is impossible to predict definitely, which result q_k will be observed in a particular single measurement.

The process of state preparation caused appreciable irritations since the discovery of quantum mechanics, because quantum systems are thus subject to two completely different types of dynamics. Dynamic I: A measurement changes the system's state discontinuously, irreversibly, indeterministically, in our example from $|\psi\rangle$ to $|q_k\rangle$. In contrast, the

$$\text{dynamic II:}\quad \frac{\partial|\psi\rangle}{\partial t} = -\frac{i}{\hbar}H|\psi\rangle \tag{3b}$$

is describing a continuous, unitary, reversible, deterministic evolution of the state according to the Schrödinger equation. The irritations are caused by the fact, that there exists no criterion, whether a cluster of atoms is to be considered a measurement device, which is inducing a discontinuous evolution according to dynamic I = (3a), or whether this cluster of atoms is to be considered a quantum system, whose interaction with the investigated object should be integrated into the Hamilton operator of the continuous dynamic II = (3b). What is qualifying a cluster of atoms, to be acknowledged as a measurement device, whose action can (and must) be described by dynamic I?

2 The invention of the “measurement problem”

It was John v. Neumann, who extensively stressed the strange appearance of the both completely different types of dynamics (3) to which the state functions of quantum systems are subjected, when he published by 1932 the first mathematically rigorous presentation [4] of the young quantum mechanics. He suggested to describe all types of objects — even macroscopic ones, including measurement devices — at least formally by the methods of quantum theory. If the measurement device is displaying the value q_k, then the quantum state $|m_k\rangle$ shall be ascribed to it according to v. Neumann’s theory of measurement.

v. Neumann considered two aspects of the measurement separately: One aspect is the combination of the investigated quantum system S, whose state is $|\psi\rangle = \sum_j a_j\,|q_j\rangle$, and the measurement device M, whose state is $|m_0\rangle$ before the measurement, such that they can interact and generate a common, merged quantum state:

$$\left.\begin{array}{r} |m_0\rangle \\ \sum_j a_j\,|q_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j\,|q_j\rangle\,|m_j\rangle \tag{4a}$$

This aspect of the measurement process creates a state, in which the state functions of the investigated system and of the measurement device are mutually entangled. Below we will explain the exact meaning of this notion. Note: (4a) does not state, that the state function $|\psi\rangle = \sum_j a_j\,|q_j\rangle$ of the measured system remains unchanged. Just the opposite. The state function $|\psi\rangle = \sum_j a_j\,|q_j\rangle$ has completely disappeared. Instead there is now a state function $\sum_j a_j\,|q_j\rangle\,|m_j\rangle$, which is representing the common state of object and measurement device.

The process of measurement is not yet completely described by (4a), because a measurement device never displays the superposition of different, macroscopically distinguishable values q_j. There still is a second aspect of measurement: The state function is reduced to the single state $|q_k\rangle\,|m_k\rangle$, and consequently the unique value q_k can be read off the measurement device:

$$\sum_j a_j\,|q_j\rangle\,|m_j\rangle \xrightarrow{\text{2. aspect}} |q_k\rangle\,|m_k\rangle \tag{4b}$$

This second aspect

$$a_j \xrightarrow{\text{2. aspect}} \begin{cases} 1 \text{ if } j=k \\ 0 \text{ if } j\neq k \end{cases}$$

of the measurement is called “reduction”, or “projection”, or “collapse” onto the state $|q_k\rangle\,|m_k\rangle$. The reduction is the not deterministically explainable, discontinuous, irreversible aspect of measurement, which above was named dynamic I.

But why is there a collapse in case of interaction with a measurement device, while there is no collapse in case of interaction with an other, arbitrarily complex aggregate of atoms? If the complex aggregate of atoms wasn’t a measurement device, the process would stop at (4a), and no collapse would happen. How does the investigated system recognize, that this is a measurement, and that therefore now a collapse is due? This question was dubbed “the measurement problem of quantum theory”.

With his presentation of the measurement process, v. Neumann deviated significantly from the “Copenhagen interpretation” [5] of quantum theory, which Bohr and Heisenberg had elaborated in 1927. According to the perception of the Copenhagen interpretation, set-up and sequence of an experimental observation of a quantum phenomenon, the applied measurement devices, and the achieved results, must all be described in the language and by the notions of classical physics. This is mandatory from the very beginning, not only after a “collapse”. As, according to the Copenhagen interpretation, measurement devices categorically must be described classically, there never can be the question, which of the dynamics (3) should be applied to their description: Neither the one nor the other, because measurement devices by definition never are to be considered as quantum systems. Thus the "measurement problem" is a home-made problem, which v. Neumann created by himself, when he — contrary to the instruction manual for quantum theory, as supplied from Copenhagen — extended the theory's application range to measurement devices.

v. Neumann was not the only one, who did not want to content himself with the postulates of the Copenhagen interpretation. It is beyond dispute, that measurement devices are systems, which are composed of atoms. The distinction between measurement devices, which categorically must be described classically, and other more or less complex aggregates of atoms and molecules, which can (and sometimes must) be described by the methods of quantum theory, is seeming arbitrary and dissatisfying to many scientists. But if one wants to consider and to describe arbitrary macroscopic objects in the first instance as — possibly quite complex — quantum systems, then one must find an explanation for the reduction (4b) of their state vectors, because it is also beyond dispute, that measurement devices and other macroscopic objects never are observed in superposition states of the type (4a).

The alternatives to the Copenhagen interpretation, which have been proposed in the following decades to explain the reduction of quantum states (4b), can essentially be grouped into four categories:

∗ There is initially no difference at all in-between measurement devices and other aggregates of atoms. Therefore there is initially no collapse. Instead the process stops at (4a). But if a human being is looking at the pointer of the measurement device, then he/she perceives a certain measured value displayed. Thus the appearance of the human being is the essential factor, which effects the collapse. But also the optical interaction between the measurement device and the human being's eyes, and also the transmission of the stimulus from the retina to the brain should be subject to the laws of quantum theory. Therefore ultimately the human being's consciousness remains as the only factor, which possibly can trigger the collapse. This was the point of view, which v. Neumann adopted in his book [4]. Thus a measurement result according to v. Neumann does not exist as an objective fact in the "outside world", but only within a human being's consciousness. He phrased it in these words: "Experience only makes statements of this type: an observer has made a certain (subjective) perception, but never of that type: a physical quantity has a certain value" [4].

∗ Modifications of quantum theory, by which the collapse is formally integrated into the theory: Additional factors have been inserted into quantum theory, which at random points of time trigger a collapse of the state function. These factors are constructed such, that the collapse is triggered the more frequently, the more complex and/or the heavier the quantum system is. This method was elaborated in detail by Ghirardi, Rimini, and Weber [6].

∗ Modifications of quantum theory, which don't need a collapse of state functions, because quantum systems never are in an superposition state of type (4a). Quantum objects still can interfere with other objects and/or with themselves in these modified theories due to additional, non-material guiding fields, or similar "hidden variables": The most prominent example is de Broglie's concept of the pilot wave [7], which was reconstructed and further developed by Bohm [8].

∗ The "many worlds"-interpretation of Everett [9] and deWitt [10]: While any measurement (and any other interaction) is creating superposition states of the type (4a), there is no collapse in this interpretation. Instead as the next step after (4a), the observer observes the measurement result. That might be called a “measurement of the measurement device”:

$$\left.\begin{array}{r} |b_0\rangle \\ \sum_j a_j\,|q_j\rangle\,|m_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j\,|q_j\rangle\,|m_j\rangle\,|b_j\rangle \tag{5}$$

The human observer as well is to be considered a quantum system, according to Everett’s interpretation. Before he reads the measurement device’s display, his state is $|b_0\rangle$. After he noted the measurement result, he is in the entangled state of the right-hand side of (5). With the j-component of his consciousness he is observing the result q_j, with the k-component of his consciousness he is observing the result q_k, and so on. The detailed evaluation is showing, that absolutely no communication is possible between the different components of the observer’s consciousness. With each component of his consciousness, the observer notes a unique result, and he does not know that with the infinitely many other components of his consciousness (“in infinitely many other worlds”) he is noting infinitely many other results. While this interpretation of course is bizarre (to say the least), it still seems to be compatible with all observable facts.

The second and third alternatives modify the theory’s formalism, while the first and the fourth alternatives merely give a different interpretation than the Copenhagen interpretation for the same formulas. Three of the four alternatives coincide in all experimentally verifiable predictions with the Copenhagen interpretation. Only the stochastically triggered collapse formulated by Ghirardi, Rimini, and Weber results in slight differences, which might become observable in future for mesoscopic systems due to improved experimental technology.

Heisenberg coined the notion “cut”, to emphasize the discontinuous character of the borderline in-between that part of the world, which must be described by quantum theory, and that part of the world, which must be described classically. According to the Copenhagen interpretation, the cut may be shifted within a wide range, but there are limits. Quantum systems like atoms or molecules in any case must be described by quantum theory. On the other hand, human observers (inclusive of their consciousness), and the measurement devices used for the detection of quantum phenomena, as far as they obviously (this notion is to be understood literally!) are behaving classically, must compulsory be described by classical theory. Usually several amplifiers are cascaded for the observation of quantum phenomena. Then according to Copenhagen understanding it doesn't matter, at which exact point the cut in-between quantum-theoretical description and classical description is placed.

v. Neumann shifted the cut beyond the obviously classical measurement devices (e.g. the observer's eyes) to the borderline(??) in-between(??) the human being's brain and consciousness, where it is likewise incomprehensible for both physical and philosophical analysis. Everett's and deWitt's point of view is significantly simpler than v. Neumann's, and even simpler than the Copenhagen point of view: It discards the cut and applies the same (quantum theoretical) type of description to each and everything within the universe. It even makes human consciousness an ordinary physical object, which is subject to quantum theory.

3 Projection Operators and Traces

To prepare for the definition and discussion of the decoherence of open quantum systems, first some formal clarifications are needed.

We resume equation (1):

The $|q_j\rangle$ are eigenvectors of Q: $$Q|q_j\rangle = q_j|q_j\rangle \tag{6a}$$
The $|q_j\rangle$ are orthonormal: $$\langle q_k|q_j\rangle = \delta_{kj} \tag{6b}$$
The $|q_j\rangle$ are complete: $$\textstyle\sum_j |q_j\rangle\langle q_j| = 1 \tag{6c}$$

On the left-hand side of (6c), there is the sum of projectors

$$P_j \equiv |q_j\rangle\langle q_j| \qquad\qquad \sum_j P_j = 1 \tag{7}$$

onto the states $|q_j\rangle$. As $\sum_j P_j$ is an operator, the 1 on the equation's right-hand side is an operator as well. It is the “identity operator”, which is leaving unchanged any state function onto which it is acting. Any arbitrary state function is an eigenfunction of the operator 1 with eigenvalue 1:

$$1|\phi\rangle = 1|\phi\rangle \tag{8}$$

Using the projector $P_j = |q_j\rangle\langle q_j|$ and an arbitrary system $|s\rangle$ of orthonormal state functions, which span the Hilbert space, the probability w_j, which was defined in (2), can be converted:

$$\begin{aligned} w_j &= \langle\psi|q_j\rangle\langle q_j|\psi\rangle = \sum_s \langle\psi|s\rangle\langle s|q_j\rangle\langle q_j|\psi\rangle \; = \\ &= \sum_s \langle s|q_j\rangle\langle q_j|\psi\rangle\langle\psi|s\rangle = \mathrm{Tr}\Big\{P_j|\psi\rangle\langle\psi|\Big\} \end{aligned} \tag{9}$$

As the scalar products $\langle\ |\ \rangle \in \mathbb{C}$ are commuting numbers, the product could be re-ordered. The sum of the diagonal elements of a matrix is called trace. w_j is the trace of the product of the projectors $P_j = |q_j\rangle\langle q_j|$ and $|\psi\rangle\langle\psi|$.

The expected mean value of an observable Q can as well be computed by means of the trace:

$$\langle Q\rangle_\psi = \langle\psi|Q|\psi\rangle = \sum_s \langle\psi|Q|s\rangle\langle s|\psi\rangle = \sum_s \langle s|\psi\rangle\langle\psi|Q|s\rangle$$

$$\boxed{\langle Q\rangle_\psi = \mathrm{Tr}\{P_\psi Q\} \quad \text{with} \quad P_\psi \equiv |\psi\rangle\langle\psi|} \tag{10}$$

While this formulation at first seems (and actually is) more laborious than necessary, it will allow for a very useful generalization in the description of open systems.

In the last terms each of (9) or (10) it's no more visible that the trace was generated with the basis vectors $|s\rangle$. Actually this information is not needed, because the same trace is generated for arbitrary operators A with any arbitrary system of vectors $|t\rangle$, provided they form a complete system $\sum_t |t\rangle\langle t| = 1$:

$$\begin{aligned}\mathrm{Tr}\{A\} &= \sum_t \langle t|A|t\rangle = \sum_{t,s} \langle t|s\rangle\langle s|A|t\rangle \ = \\ &= \sum_{t,s} \langle s|A|t\rangle\langle t|s\rangle = \sum_s \langle s|A|s\rangle\end{aligned} \tag{11}$$

We mention two further properties of the trace, which often are useful. First, the trace remains unchanged if arbitrary operators A, B, C are cyclically permuted under the trace:

$$\begin{aligned}\mathrm{Tr}\{ABC\} &= \sum_{s,t} \langle s|AB|t\rangle\langle t|C|s\rangle \ = \\ &= \sum_{s,t} \langle t|C|s\rangle\langle s|AB|t\rangle = \mathrm{Tr}\{CAB\}\end{aligned} \tag{12}$$

Note, that the trick does only work for cyclical permutations,

$$\mathrm{Tr}\{ABC\} \neq \mathrm{Tr}\{BAC\} \ . \tag{13}$$

Second, the identity

$$\mathrm{Tr}\Big\{|a\rangle\langle b|\Big\} = \sum_s \langle s|a\rangle\langle b|s\rangle = \sum_s \langle b|s\rangle\langle s|a\rangle = \langle b|a\rangle \tag{14}$$

is remarkable. In particular, the trace of the projector $P_\psi = |\psi\rangle\langle\psi|$ is equal to the norm $\langle\psi|\psi\rangle$ of the state, onto which it is projecting.

Until now we assumed, without explicit mention, that there is no uncontrolled interaction in-between the system S and it's environment. Systems, for which this assumption is correct, are called closed. Conversely, open systems are characterized by the fact, that in-between them and their environment there are interactions, which at best are partially controlled. To introduce the concept of decoherence, we need to extend our analysis to open quantum systems.

4 Open Quantum Systems and Density Operators

In the sequel we consider an open quantum system S, which is part of a closed quantum system S_W, see figure 1. S_W is composed from the two partial systems S and S_R. W signifies "world", meaning the quantum system consisting of the complete universe. We assume that this system is closed, and don't ponder the question (which is likewise difficult from physical as from philosophical point of view), whether the universe really is a closed system (better phrased: the

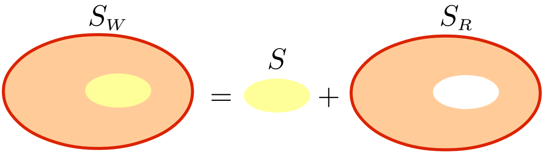

Fig. 1 : The system $S_W = S + S_R$

question, whether there does exist a closed system at all). S is the quantum system, which we want to investigate and to describe. S_R is the "rest of world". The state functions $|\psi_W\rangle$ of the closed system S_W are elements of the Hilbert space

$$\mathcal{H}_W = \mathcal{H} \otimes \mathcal{H}_R \ , \tag{15}$$

which is the direct product of the Hilbert spaces $\mathcal{H}$ and $\mathcal{H}_R$. Let $|s\rangle$ be an orthonormal basis of the Hilbert space $\mathcal{H}$, and $|r_R\rangle$ be an orthonormal basis of the Hilbert space $\mathcal{H}_R$, such that any vector $|\psi\rangle \in \mathcal{H}$ can be expanded in the series

$$|\psi\rangle = \sum_s |s\rangle\langle s|\psi\rangle = \sum_s c_s|s\rangle \ , \tag{16}$$

and any vector $|\psi_R\rangle \in \mathcal{H}_R$ can be expanded in the series

$$|\psi_R\rangle = \sum_r |r_R\rangle\langle r_R|\psi_R\rangle = \sum_r d_{Rr}|r_R\rangle \ . \tag{17}$$

The tensor product of these both vectors is

$$|\psi\rangle \otimes |\psi_R\rangle = \sum_s \sum_r c_s d_{Rr}\, |s\rangle \otimes |r_R\rangle \ \ \in \mathcal{H}_W \ . \tag{18}$$

The scalar product of this product-vector and the product-vector

$$|\phi\rangle \otimes |\phi_R\rangle = \sum_s \sum_r e_s f_{Rr}\, |s\rangle \otimes |r_R\rangle \ \ \in \mathcal{H}_W \tag{19}$$

is defined by

$$\begin{aligned} &\langle\psi| \otimes \langle\psi_R|\phi\rangle \otimes |\phi_R\rangle = \langle\psi|\phi\rangle\langle\psi_R|\phi_R\rangle \ = \\ &= \sum_{s,s'} \sum_{r,r'} c^*_s d^*_{Rr} e_{s'} f_{Rr'} \ \underbrace{\langle s|s'\rangle}_{\delta_{ss'}} \underbrace{\langle r|r'\rangle}_{\delta_{rr'}} = \sum_s \sum_r c^*_s d^*_{Rr} e_s f_{Rr} \ . \end{aligned} \tag{20}$$

Thus for the computation of the tensor product, first the partial products in the systems $\mathcal{H}$ and $\mathcal{H}_R$ are computed.

Not every state vector in $\mathcal{H}_W$ can be written as the direct product of a vector in $\mathcal{H}$ and a vector in $\mathcal{H}_R$. Let's compare the two vectors

$$|\phi_W\rangle = |\phi\rangle \otimes |\phi_R\rangle = \sum_s \sum_r c_s d_{Rr} \, |s\rangle \otimes |r_R\rangle \ \in \mathcal{H}_W \tag{21a}$$

$$|\psi_W\rangle = \sum_s \sum_r c_{Wsr} \, |s\rangle \otimes |r_R\rangle \ \in \mathcal{H}_W \ . \tag{21b}$$

(21a) is a product vector, which can be written as the direct product of the vectors $|\phi\rangle \in \mathcal{H}$ and $|\phi_R\rangle \in \mathcal{H}_R$. If for any of the coefficients of (21b)

$$c_{Wij} \neq c_{Wji} \qquad \text{and/or} \qquad c_{Wii}c_{Wjj} \neq c_{Wij}c_{Wji} \ , \tag{22}$$

then the vector $|\psi_W\rangle \in \mathcal{H}_W$ does not equal the direct product of any two vectors in $\mathcal{H}$ and in $\mathcal{H}_R$. In this case, the vectors of the partial systems are said to be "entangled" in the vector of the total system. Schrödinger, who coined this notion, considered the appearance of entangled state vectors in composite systems to be the essential difference in-between classical theory and quantum theory. [11]

> If a composed system is described by an entangled state vector, then no state vectors can be assigned to the partial systems. (23)

A simple example for an entangled vector is

$$|\psi_W\rangle = c_{W11} \, |1\rangle \otimes |1_R\rangle + c_{W22} \, |2\rangle \otimes |2_R\rangle \ . \tag{24}$$

This vector can not be written as the direct product of vectors

$$\sum_{s=1}^{2} c_s \, |s\rangle \qquad\qquad \sum_{r=1}^{2} d_{Rr} \, |r_R\rangle \tag{25}$$

of the partial systems S and S_R, because in the direct product

$$\sum_{s=1}^{2}\sum_{r=1}^{2} c_s d_{Rr}\,|s\rangle\otimes|r_R\rangle = c_1 d_{R1}\,|1\rangle\otimes|1_R\rangle + c_1 d_{R2}\,|1\rangle\otimes|2_R\rangle + \\ + c_2 d_{R1}\,|2\rangle\otimes|1_R\rangle + c_2 d_{R2}\,|2\rangle\otimes|2_R\rangle \tag{26}$$

there inevitably will be terms which are mixed in the indices 1 and 2 (because c_1, d_{R1}, c_2, d_{R2} all must be different from zero), which don't exist in (24).

Open quantum systems are almost always entangled with the rest of the world. Consequently they can not be described by state vectors, see (23). Exactly this is the difference in-between open and closed quantum systems. This induces a practical problem. If we want to compute by the usual methods the expectation value

$$\langle Q\rangle_\psi = \langle\psi|Q|\psi\rangle \overset{(10)}{=} \mathrm{Tr}\{|\psi\rangle\langle\psi|\,Q\} \tag{27a}$$

of an observable Q in the state $|\psi\rangle$ of system S, then we get stuck already from the outset, as the state $|\psi\rangle$ of system S isn't defined at all, if S and S_R are described by an entangled overall state. In case of entanglement, only the combined state function $|\psi_W\rangle$ of the entangled systems is defined. It is defined “in principle”, but it is never known explicitly, and thus can't be used in computations.

In the following, we will derive an “effective” state function $|\chi\rangle$ of system S, by means of which the expectation value

$$\langle Q\rangle_{\psi_W} = \mathrm{Tr}\{|\chi\rangle\langle\chi|\,Q\} \tag{27b}$$

of the observable Q can be computed even if the system S is entangled with the environment, and even if measurements are confined to system S.

For this purpose we must define upfront, how scalar-products and projectors of entangled states are formed. The projector onto the entangled state (21b) is

$$\begin{aligned}|\psi_W\rangle\langle\psi_W| &= \sum_s\sum_r c^*_{Wsr}c_{Wsr}\,|s\rangle\otimes|r_R\rangle\langle s|\otimes\langle r_R|\\ &= \sum_s\sum_r c^*_{Wsr}c_{Wsr}\,|s\rangle\langle s|\otimes|r_R\rangle\langle r_R|\ .\end{aligned} \tag{28}$$

The scalar product of the vector (21b) and the vector

$$|\phi_W\rangle = \sum_s\sum_r d_{Wsr}\,|s\rangle\otimes|r_R\rangle\ \in\mathcal{H}_W \tag{29}$$

is

$$\langle\psi_W|\phi_W\rangle = \sum_{s,s'}\sum_{r,r'} c^*_{Wsr}d_{Ws'r'}\ \underbrace{\langle s|s'\rangle}_{\delta_{ss'}}\underbrace{\langle r_R|r'_R\rangle}_{\delta_{rr'}} = \sum_s\sum_r c^*_{Wsr}d_{Wsr}\ . \tag{30}$$

Thus to compute the overall product, first the partial products in $\mathcal{H}$ and in $\mathcal{H}_R$ are computed.

Let's compute the expectation value $\langle Q\rangle_{\psi_W}$ of an observable Q, which is exclusively a property of the partial system S, i.e. the operator Q is acting only in Hilbert space $\mathcal{H}$. Assume that the state of system S is entangled with the state S_R of the rest of the world, composing the state

$$|\psi_W\rangle = \sum_s\sum_r c_{Wsr}\,|s\rangle\otimes|r_R\rangle\ \in\mathcal{H}_W \tag{31}$$

of the universe S_W. This state can not be written as the direct product of a state vector of the system S and a state vector of the system S_R. Therefore neither the system S nor the system S_R is in a defined state. We define the operator for the overall system as the direct product

$$Q_W = Q\otimes 1_R\ . \tag{32}$$

The operator 1_R is acting only in the Hilbert space $\mathcal{H}_R$. It is the “identity operator”, which — see (8) — leaves unchanged any state function, onto which it is acting. We make the plausible assumption, that the expectation value of the observable Q, which is measured in the system S, is identical to the expectation value of the observable Q_W, which is measured in the system S_W. As the system W is closed, the expectation value can be computed by means of the projector $|\psi_W\rangle\langle\psi_W|$ and the trace:

$$\langle Q\rangle_{\psi_W} \overset{(10)}{=} \mathrm{Tr}_W\Big\{|\psi_W\rangle\langle\psi_W|\,Q_W\Big\} \tag{33}$$

Inserting the operator (32), and computing the trace with the orthonormal system $|s\rangle\otimes|r_R\rangle$, results into

$$\begin{aligned}\langle Q\rangle_{\psi_W} &= \sum_s\langle s|\sum_r\langle r_R|\psi_W\rangle\langle\psi_W|1_R|r_R\rangle\,Q\,|s\rangle\\ &= \mathrm{Tr}\Big\{\mathrm{Tr}_R\{|\psi_W\rangle\langle\psi_W|\}\,Q\,\Big\}\ .\end{aligned}$$

The trace, which is to be computed in the system R (the rest of the world), is called the density operator ρ. It is converted such, that only state functions of the system S are showing up in it:

$$\begin{aligned}\rho \equiv \mathrm{Tr}_R\{|\psi_W\rangle\langle\psi_W|\} &= \sum_r\langle r_R|\psi_W\rangle\langle\psi_W|r_R\rangle\\ \overset{(28)}{=} \sum_{r',s,r} c^*_{Wsr}c_{Wsr}|s\rangle\langle s|\,&\underbrace{\langle r'_R|r_R\rangle\langle r_R|r'_R\rangle}_{\delta_{rr'}}\\ = \sum_s w_s|s\rangle\langle s|\ \ \text{with}\ \ w_s &\equiv \sum_r c^*_{Wsr}c_{Wsr} \geq 0\in\mathbb{R}\ .\end{aligned} \tag{34}$$

Thus the expectation value of the observable Q in the open system is:

$$\langle Q\rangle_{\psi_W} = \mathrm{Tr}\{\rho\,Q\}\ \ \text{with}\ \begin{cases}\rho = \sum_s w_s|s\rangle\langle s|\\ w_s = \sum_r c^*_{Wsr}c_{Wsr} \geq 0\in\mathbb{R}\end{cases} \tag{35}$$

This result for the open system should be compared to the result

$$\langle Q\rangle_\psi \overset{(10)}{=} \mathrm{Tr}\{P_\psi Q\} \quad \text{with} \quad P_\psi = |\psi\rangle\langle\psi|$$

for the closed system! $|s\rangle\langle s|$ is a projector, which is acting in the system S. Therefore also the density operator ρ, being the weighted sum of these projectors, is an operator, which is acting in the system S. Only deeply buried in the weighting factors w_s, the density operator is shaped by the entanglement of the systems S and S_R.

Comparison of (27b) and (35) results into

$$|\chi\rangle\langle\chi| = \sum_s \sum_r c^*_{Wsr} c_{Wsr} \, |s\rangle\langle s| = \sum_s w_s \, |s\rangle\langle s| \ , \tag{36}$$

and consequently the effective state function

$$|\chi\rangle = \sum_s \sqrt{w_s} \, |s\rangle e^{i\varphi_s} \quad \text{with} \left\{ \begin{array}{l} \varphi_s \in \mathbb{R} \\ \varphi_s \text{ not defined} \end{array} \right. \tag{37}$$

can be assigned to the open system S. As $|\chi\rangle$ has been determined by detour via the projectors (36), the phase factors φ_s are not defined because of

$$|s\rangle\langle s| = |s\rangle e^{-i\varphi_s} \, \langle s| e^{i\varphi_s} \quad \text{for arbitrary } \varphi_s \in \mathbb{R} \ .$$

A state with un-defined phase is called a “mixture”, in contrast to a “pure state”

$$|\psi\rangle = \sum_s |s\rangle\langle s|\psi\rangle = \sum_s c_s |s\rangle \ , \tag{38}$$

whose phases are well-defined by the complex coefficients $c_s = \langle s|\psi\rangle \in \mathbb{C}$. This is a significant insight: If the state function of the universe can not be written as the direct product of a state function of the open system S and a state function of the rest of the world, then the effective state of the system S is not a pure state, but a mixture. This is the regular case. Only if the evaluated system is effectively isolated from the rest of the world, it can be described approximately (but never exactly!) by a pure state.

Aside from the weighting factors w_s, there are exclusively quantities of the system S in (35). All quantities of the system S are measurable and computable. But how can we know the w_s? Without these factors, the result (35), while being mathematically perfectly correct, would be completely useless. There is a simple answer to this question in the special case that the environment, with which the system S gets entangled, is a well constructed measurement instrument. Let's assume that S is described by the state vector $|\psi\rangle$, and that the measurement instrument is constructed to measure the observable Q, i. e. the measurement result will be one of the eigenvalues q_i , and S get's prepared in the related eigenstate $|q_i\rangle$ of the measuring instrument.

Then we should first expand $|\psi\rangle$ with respect to the $|q_i\rangle$:

$$|\psi\rangle = \sum_j a_j \, |q_j\rangle \tag{39}$$

With the Copenhagen interpretation, exclusively classical physics are valid for the measurement instrument. But now we want to understand how the system S behaves when it is getting entangled to an environment, which is described by quantum theory. Thus we now should have a look at v. Neumann's theory of measurement, in which quantum theory is (though only "in principle") applied to the instrument. It has been shown in equation (4a), how v. Neumann describes the entanglement as the 1. aspect of the measurement process:

$$\left.\begin{array}{r} |m_0\rangle \\ \sum_j a_j \, |q_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j \, |q_j\rangle \, |m_j\rangle$$

Comparing that with

$$|\psi_W\rangle \overset{(31)}{=} \sum_s \sum_r c_{W\,sr}\, |s\rangle \otimes |r_R\rangle \ ,$$

we see that

$$\begin{aligned} &\text{if } |s\rangle \text{ are the eigenfunctions of the environment,} \\ &\text{then } \sum_r c_{W\,sr} = a_s \quad \text{and} \quad w_s \overset{(36)}{=} \sum_r |c_{W\,sr}|^2 = |a_s|^2 \ . \end{aligned} \tag{40}$$

Thus finding the coefficients w_s in (36) is simple, if the environment is a measuring instrument. In other cases, we must guess to what type of measuring instrument the environment is similar, expand the system's state function accordingly, and achieve thereby at least an acceptable guess for the coefficients w_s .

As we encode *all* our knowledge about the evaluated open system in the density operator ρ, we should better write $\langle Q\rangle_\rho$ instead of $\langle Q\rangle_{\psi_W}$ in (35):

$$\boxed{\langle Q\rangle_\rho = \mathrm{Tr}\{\rho\, Q\} \quad \text{with} \quad \begin{cases} \rho = \sum_s w_s |s\rangle\langle s| \\ w_s \geq 0 \in \mathbb{R} \text{ determined} \\ \text{by best guess according} \\ \text{to (40).} \end{cases}} \tag{41}$$

5 PVM and POVM

The acronym PVM codes for Projection Valued Measure, and the acronym POVM codes for Positive Operator Valued Measure. As these notions are often encountered in the mathematically oriented literature, I will now give a short explanation.

If the state of a closed system is described by $|\psi\rangle$, then the expectation value of the operator Q is

$$\begin{aligned}\langle Q\rangle_\psi &\overset{(10)}{=} \mathrm{Tr}\{P_\psi Q\} = \sum_k \langle q_k|\psi\rangle \underbrace{\langle\psi|Q|q_k\rangle}_{q_k\langle\psi|q_k\rangle} = \\ &= \sum_k w_k q_k \quad \text{with } w_k \equiv \big|\langle q_k|\psi\rangle\big|^2 \geq 0\ . \qquad (42a)\end{aligned}$$

If the state of an open system is described by the density operator

$$\rho = \sum_k w_k |q_k\rangle\langle q_k|\ ,$$

then the expectation value of the operator Q is

$$\begin{aligned}\langle Q\rangle_\rho &\overset{(41)}{=} \mathrm{Tr}\{\rho\, Q\} = \sum_{k,k'} w_k \underbrace{\langle q_{k'}|q_k\rangle\langle q_k|Q|q_{k'}\rangle}_{q_{k'}\delta_{kk'}} = \\ &= \sum_k w_k q_k \quad \text{with } w_k \overset{(35)}{=} \sum_r \big|c_{Wkr}\big|^2 \geq 0\ . \qquad (42b)\end{aligned}$$

The only difference of (42b) versus (42a) is that the projection operator P_ψ has been replaced by the density operator ρ, while the results are identical. In either case the coefficients w_k are reflecting the probability, that a single measurement of the observable Q will have the result q_k. As for any reasonable probabilities, the w_k sum up to unity:

$$\sum_k w_k = 1 \qquad (43)$$

But only the coefficients $w_k = \big|\langle q_k|\psi\rangle\big|^2$ of the closed system (42a) can be computed. The coefficients w_k of the open system (42b) must be found by guessing.

In the mathematical analysis of the system, we may be more interested in the values of the probabilities w_k than in the measured values q_k. If the system is closed, and it's state function is $|\psi\rangle$, then the w_k are simply the expectation values of the projectors $P_{q_k} = |q_k\rangle\langle q_k|$:

$$\langle P_{q_k}\rangle_\psi = \langle\psi|P_{q_k}|\psi\rangle = \langle\psi|q_k\rangle\langle q_k|\psi\rangle \overset{(42a)}{=} w_k \tag{44}$$

This is a map from the set of state functions $|\psi\rangle$ onto the real numbers w_k . A "measure" is in mathematical terminology a generalized form of a map from some set onto the real numbers. In this case the map is specified by the projectors P_{q_k} . Hence (44) is called a projection-valued measure = PVM.

We would like to generalize the PVM to the open quantum system. (42a) could be generalized to (42b) by replacing the projector P_ψ by the density operator ρ . This method of generalization can not immediately be transferred to (44), because the state function $|\psi\rangle$ of the closed system is an indispensable part of (44), while no state function is defined for the open system.

But remember the identity-operator 1 defined in (7). This operator leaves unchanged any state function on which it is acting. Furthermore any arbitrary state function $|\phi\rangle$ is an eigenfunction of the operator 1 with eigenvalue 1 :

$$1|\phi\rangle \overset{(8)}{=} 1|\phi\rangle \tag{45}$$

This property (i. e. the independence from the state functions $|\phi\rangle$) makes the identity-operator suitable for the sought measure:

$$\langle\phi|W_k|\phi\rangle = w_k \quad \forall|\phi\rangle \tag{46}$$

This construction will work, if the operators W_k (written as capitals, while the probabilities w_k are written as small characters) are a decomposition

$$\sum_k W_k = 1 \tag{47}$$

of the identity-operator 1, because of

$$\sum_k W_k|\phi\rangle \overset{(47)}{=} 1|\phi\rangle \overset{(45)}{=} 1|\phi\rangle \overset{(43)}{=} \sum_k w_k|\phi\rangle \ .$$

The measure (i. e. the map) (46) from the set of arbitrary (and actually unknown) state functions $|\phi\rangle$ of the open quantum system onto the real numbers w_k is positive (because all w_k are ≥ 0), and it is operator-valued (because the projectors P_ψ of (44) have been generalized to the operators W_k). Hence (46) is called a positive operator-valued measure = POVM. It generalizes the PVM (44), which is applicable only in case of closed systems, to the case of open systems.

The definition of the POVM (46) is of course important for the mathematical analysis of the problem. Regarding the practical task of the physicist, however, who is trying not only to analyze but to solve the problem, i. e. to actually find out the values of the w_k, the definition of the operators W_k and the POVM (46) is obviously irrelevant.

Still many physicists say that they change from a PVM description of measurements to a POVM description, when handling open quantum systems. But this is imprecise wording. What they want to point out is that they change from (42a) to (42b), i. e. that they base their computations of expectation values on density operators but not on state functions. This change is of course indispensable, if open quantum systems shall be handled appropriately.

6 Decoherence

Due to the undefined phase, a mixture can not generate interference effects. It can't neither interfere with itself, nor with other state functions. The loss of well-defined phase relations also becomes visible in the disappearance of off-diagonal elements of matrices:

We compare the matrix representations of the projector P_ψ and the density operator ρ, using the same basis $|s\rangle$ as applied in the definition of ρ in (35):

$$(P_\psi)_{ss'} = \langle s|\psi\rangle\langle\psi|s'\rangle \overset{(38)}{=} c_s c^*_{s'} \tag{48a}$$

$$(\rho)_{ss'} = \sum_{s''} w_{s''}\, \underbrace{\langle s|s''\rangle}_{\delta_{ss''}} \underbrace{\langle s''|s'\rangle}_{\delta_{s''s'}} = w_s \delta_{ss'} \tag{48b}$$

The density matrix (48b) is a diagonal matrix, all off-diagonal elements are zero. In contrast, in the projector-matrix the off-diagonal elements usually are different from zero.

The entanglement of the system S with the rest of the world produces the result, that the effective state functions $|\chi\rangle$ loose a significant property of the state functions of closed quantum systems — namely the capability to produce interference phenomena. In the experimental observation of mesoscopic objects (medium-sized molecules), the detection of the gradual loss of interference capability (caused by gradually increased coupling to the environment) is possible, see e. g. [12].

Using the keyword "gradual", we are alluding to an overly simplification in our previous delineation: At the start of this letter, we considered a closed system. And now we considered a system which is completely entangled with it's environment, with all off-diagonal elements of the density matrix (48b) being zero. But inbetween, there still is the important range of gradual transition between these extremes in case of more or less strong coupling of S and S_R.

How fast will a state decohere, if a system, which was closed at the beginning, is exposed to interactions with the environment? Joos and Zeh [13] tried to estimate the speed of decoherence. For that purpose they considered quantum objects, which at time t_0, when the interaction with the environment is switched on, can be found with finite probability at different spots $\boldsymbol{x}, \boldsymbol{x}'$ in three-dimensional position space. If these objects are exposed to scattering by electromagnetic radiation or by gas molecules of the environment, then these scattering events are gradually destroying the off-diagonal elements in the density matrices of these objects, i. e. they are destroying the phase relations inbetween the state function's components localized at different positions.

The density matrix (48b), whose components were computed by means of the basis vectors $|s\rangle$, is in this case replaced by a density matrix, whose components are computed by means of the vectors $|t\boldsymbol{x}\rangle$ of the time-dependent continuous position basis. We won't try to reproduce the computation of Joos and Zeh, but merely state their result:

$$\begin{aligned}
(\rho)_{xx'}(t) &= \int \mathrm{d}\boldsymbol{x}''\,\langle t\boldsymbol{x}|t\boldsymbol{x}''\rangle\langle t\boldsymbol{x}''|t\boldsymbol{x}'\rangle \\
&= (\rho)_{xx'}(t_0)\exp\{-(t-t_0)(\boldsymbol{x}-\boldsymbol{x}')^2\Lambda\} \qquad (49)\\
0 < \Lambda &\sim \frac{N}{V}\,k^2\,v
\end{aligned}$$

It's plausible, that the decoherence rate Λ is proportional to the velocity v of the scattering particles, proportional to the square k^2 of their wave number, and proportional to their number N per volume

diameter of system S	10 000 nm	100 nm	10 nm
cosm. background rad.	10^{-8}	10^{-20}	10^{-26}
room temperature	10^{-5}	10^{-2}	10^{-8}
sunlight (on earth)	10^{7}	10^{3}	10^{-1}
air	10^{22}	10^{18}	10^{16}
laboratory vacuum	10^{9}	10^{5}	10^{3}

Table 1: Decoherence rate $\Lambda\,/(\mathrm{nm}^{-2}\mathrm{s}^{-1})$

V. The decoherence of the delocalized quantum objects takes place remarkably fast, i. e. exponentially with $(t-t_0)(\boldsymbol{x}-\boldsymbol{x}')^2\Lambda$. In table 1 on the previous page the rates of decoherence are listed, which Joos and Zeh [13] found for quantum systems S of different sizes due to different kinds and strengths of coupling to the environment. Apparently the decoherence due to scattering of gas molecules is significantly more efficient than the decoherence due to scattering of photons. But even if the entanglement with the environment is merely effected by the cosmic background radiation, this effect is significant for macroscopic objects.

We emphasize that (49) is describing the decoherence of the quantum object S, but clearly not it's localization. The different diagonal elements of the density matrix are specifying different spots $\boldsymbol{x}$ as the positions of this object. The values of the different diagonal elements are not changed, i. e. we get for all diagonal elements $(\rho)_{xx}(t)\overset{(49)}{=}(\rho)_{xx}(t_0)$. Only the off-diagonal elements tend to zero. The decoherence does not produce a collapse of the quantum object S to a certain position, but only destroys the capability of interference of state components with different position coordinates. If in a doubleslit-experiment a molecule, which is running through the apparatus, is loosing it's capability for interference due to coupling to the environment, then no interference figure is observed behind the doubleslit. This does not at all mean, that the molecule is localized and crossing only one of the two slits. It stays to be delocalized over the area of both slits, exactly as in the case without decoherence (the diagonal elements of it's density matrix have not been changed by decoherence). Just it's two state components, which are localized at the two slit positions, are not any more capable to produce interference (the off-diagonal elements of it's density matrix have disappeared due to decoherence).

We end this section with a citation of Heisenberg. In the winterterm 1955/56, Heisenberg read the Gifford-Lectures at the University St. Andrews in Scotland. In the tenth lesson, titled “Language and Reality”, he remarked [5, chap. X]:

“[In the case of quantum theory] we have at first no simple guide for correlating the mathematical symbols with concepts of ordinary language; and the only thing we know from the start is the fact that our common concepts cannot be applied to the structure of the atoms. Again the obvious starting point for the physical interpretation of the formalism seems to be the fact that the mathematical scheme of quantum mechanics approaches that of classical mechanics in dimensions which are large as compared to the size of the atoms. But even this statement must be made with some reservations. Even in large dimensions there are many solutions of the quantum-theoretical equations to which no analogous solutions can be found in classical physics. In these solutions the phenomenon of the interference of probabilities would show up, [. . . which] does not exist in classical physics. Therefore, even in the limit of large dimensions the correlation between the mathematical symbols, the measurements, and the ordinary concepts is by no means trivial. In order to get to such an unambiguous correlation one must take another feature of the problem into account. It must be observed that the system which is treated by the methods of quantum mechanics is in fact a part of a much bigger system (eventually the whole world); it is interacting with this bigger system; and one must add that the microscopic properties of the bigger system are (at least to a large extent) unknown. This statement is undoubtedly a correct description of the actual situation, since the system could not be the object of measurements and of theoretical investigations — it would in fact not belong to the world of phenomena — if it had no interactions with such a bigger system of which the observer is a part. The interaction with the bigger system with its undefined microscopic properties then introduces a new statistical element into the description — both the quantum-theoretical and the classical one — of the system under consideration. In the limiting case of the large dimensions this statistical element destroys the effects of the interference of probabilities in such a manner that now the quantum-mechanical scheme really approaches the classical one in the limit. Therefore, at this point the correlation between the mathematical symbols of quantum theory and the concepts of ordinary language is unambiguous ... ”

Heisenberg had by 1955 a clear understanding of the cause and the effect of decoherence, as proved by this quote. The entanglement of the evaluated system's state with it's environment results into loss of interference capability (the non-diagonal elements of the density matrix disappear). But the result is not a unique classical state. Instead “the interaction [with the environment] introduces a new statistical element into both the quantum-theoretical and the classical description”: Not only one, but many diagonal elements of the density matrix are different from zero, i. e. in the example (49) the object can be found with finite probability at many different spots in position space, if it's position is measured. This is a classical probability. As the interference capability is lost, one may assume that the object “really has” a well-defined unique location, which the observer just does not know. For that type of probability there are appropriate notions available in human language, while no words can be found in ordinary language for the probability amplitude of quantum theory, which is capable of interferences.

7 Decoherence and the “Measurement Problem”

Some people claim, that the “measurement problem of quantum theory” could be solved by decoherence. Such claims are not justified. To clarify this issue, we symbolize a measurement in v. Neumann's model as sketched in figure 2 on the facing page: First the system S, which is to be investigated, and the measurement device S_M are brought into contact:

$$\left.\begin{array}{r} |m_0\rangle \\ \sum_j a_j\,|q_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j\,|q_j\rangle\,|m_j\rangle \tag{50a}$$

Clearly S must be open with respect to S_M, because otherwise no measurement would be possible. But S_M (which possibly could be e. g. the eyes of a human being), being a macroscopic system, will inevitably be open versus S_R (the rest of the world), because it is impossible to shield a macroscopic object completely (or even approximate completely) against the scattering of gas molecules or electromagnetic radiation from the rest of the world. Therefore the state of the measurement device and the state of the rest of the world S_R will entangle (with $|r_0\rangle$ being the state of S_R before the entanglement):

$$\left.\begin{array}{r} |r_0\rangle \\ \sum_j a_j\,|q_j\rangle\,|m_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j\,|q_j\rangle\,|m_j\rangle\,|r_j\rangle \tag{50b}$$

This overall state function of $S_W = S + S_M + S_R$ is entangled, i.e. it can not be written as the direct product of state functions of the partial systems. And the effective state function of the partial system $S+S_M$ is due to decoherence no more capable of interference. But decoherence can not replace the collapse, which didn't yet take place in (50b)! The human observer reads off from the display of

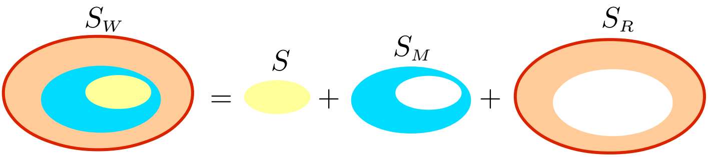

Fig. 2 : The system $S_W = S + S_M + S_R$

the measurement device some certain, unique result q_k, but not a superposition of different values q_j. Thus (50b) could be accepted as an appropriate description only in the Everett interpretation. Without the Everett interpretation, a reduction of state

$$\sum_j a_j \left|q_j\right\rangle \left|m_j\right\rangle \left|r_j\right\rangle \xrightarrow{\text{2. aspect}} \left|q_k\right\rangle \left|m_k\right\rangle \left|r_k\right\rangle \qquad (50c)$$

must follow.

If one is accepting the Everett interpretation, then one does not need a solution of a "measurement problem", because the observer does anyway observe just one unique measurement result with each component of his consciousness. Also if one decides to follow the Copenhagen interpretation, then there is no collapse-problem, for which a solution is required, because then from the outset all measurement devices are described by classical physics. Decoherence then just is, what it's name says: The interesting fact, that the effective state vector of the system S, computed by "tracing out" from (50b) $= \sum_j a_j \left|q_j\right\rangle \left|m_j\right\rangle \left|r_j\right\rangle$ the factors related to S_M and S_R, is a mixture with no interference capability. But that interesting fact does not supply a solution for the measurement problem of the other interpretations of quantum theory, as it does not trigger a "collapse" of the state function, i. e. it does not explain the step from (50b) to (50c).

8 The preferred Basis

While thus the fact of decoherence of open quantum systems does not contribute anything to the solution of the "measurement problem" (which does exist only for some of the interpretations of quantum theory), another long-standing mysterious issue could be clarified due to the decoherence concept: The problem of the "preferred basis". The case is as follows.

It's not at all clear from start on, why a measurement apparatus S_M, which is used for the measurement of the observable Q of a system S, combines with the system S according to v. Neumann's theory of measurement to the superposition-state

$$\left.\begin{array}{r} |m_0\rangle \\ \psi = \sum_j a_j\,|q_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a_j\,|q_j\rangle\,|m_j\rangle\ , \tag{51a}$$

and then collapses by

$$\sum_j a_j\,|q_j\rangle\,|m_j\rangle \xrightarrow{\text{2. aspect}} |q_k\rangle\,|m_k\rangle \tag{51b}$$

to a certain value q_k. Couldn't just as well with $|q'_j\rangle \neq |q_j\rangle$ and with $|m'_j\rangle \neq |m_j\rangle$ an entanglement

$$\left.\begin{array}{r} |m_0\rangle \\ \psi = \sum_j a'_j\,|q'_j\rangle \end{array}\right\} \xrightarrow{\text{1. aspect}} \sum_j a'_j\,|q'_j\rangle\,|m'_j\rangle \tag{52a}$$

happen, and then collapse by

$$\sum_j a'_j\,|q'_j\rangle\,|m'_j\rangle \xrightarrow{\text{2. aspect}} |q'_k\rangle\,|m'_k\rangle \tag{52b}$$

to the eigenvalue $q'_k \neq q_k$ of a quite different observable $Q' \neq Q$? Of course, the measurement apparatus has been constructed such, that it measures the quantity Q, but not some different quantity Q'. But that is a statement in the framework of classical physics. If — following v. Neumann — the measurement device is considered as a quantum system, then it's state

$$|m\rangle = \sum_j b_j\,|m_j\rangle = \sum_j b'_j\,|m'_j\rangle \tag{53}$$

can be expanded with equal right in a series with respect to the basis functions $|m_j\rangle$ (which correlate with the eigenfunctions $|q_j\rangle$ of the observable Q), or in a series with respect to the basis functions $|m'_j\rangle$ (which correlate with the eigenfunctions $|q'_j\rangle$ of the observable Q'). It is a *classical* property of the measurement apparatus, not to measure just any one of the quantities $Q', Q'', \ldots$ compatible with quantum theory, but reliably and stably the certain quantity Q. How does the device acquire this classical property?

To make clear that this is not only a problem for v. Neumann's measurement theory, but for the Copenhagen interpretation of quantum theory as well, we rephrase this question still more general: How does it come, that some quantum systems constantly and stably are displaying certain classical properties? A particular striking example are chiral molecules. These might for example be organic molecules, forming a tetraeder with a carbon atom in the center, and four different ligands. We name $|R\rangle$ the state, in which a certain chiral, and therefore optically active molecule is rotating the polarization plane of light clockwise. Accordingly the left-rotating state is named $|L\rangle$. The right-rotating molecule is the mirror image of the left-rotating molecule. Therefore in the simplifying sketch of figure 3 on the next page, the potential energy of the left-rotating molecule, displayed as a function of some axis in position space, is the mirror image of the potential energy of the right-rotating molecule.

If an infinite amount of energy was required, to transform a right-rotating molecule into a left-rotating one, and vice versa (left sketch in figure 3), then the both potential-wells would be completely decoupled. The Schrödinger equation of the right- resp. left-rotating molecule then would be

$$H_0\,|R\rangle = E_0\,|R\rangle \qquad \text{resp.} \qquad H_0\,|L\rangle = E_0\,|L\rangle\ . \tag{54}$$

H_0 does not combine the potential-wells of the right-rotating and the left-rotating molecule:

$$\begin{aligned}\langle L|\,H_0\,|R\rangle &= E_0\,\langle L|R\rangle = 0\\ \langle R|\,H_0\,|L\rangle &= E_0\,\langle R|L\rangle = 0\end{aligned} \tag{55}$$

But in reality, only finite energy is required, to transform a chiral molecule into it's enantiomer. Thus the height of the potential barrier between the two energy wells is finite, as displayed in the right sketch of figure 3. Therefore H_0 must be completed by an interaction term H_I, and the Schrödinger equation of the chiral molecule becomes

$$(H_0 + H_I)\,|\psi\rangle = E\,|\psi\rangle\ . \tag{56}$$

$|R\rangle$ and $|L\rangle$ are not eigenstates of the parity operator P (the parity operator inverts the three coordinate axes of position space). Instead $|R\rangle$ and $|L\rangle$ are converted into another by the parity transformation. The eigenfunctions of the parity operator are the symmetric and antisymmetric combinations of $|R\rangle$ and $|L\rangle$:

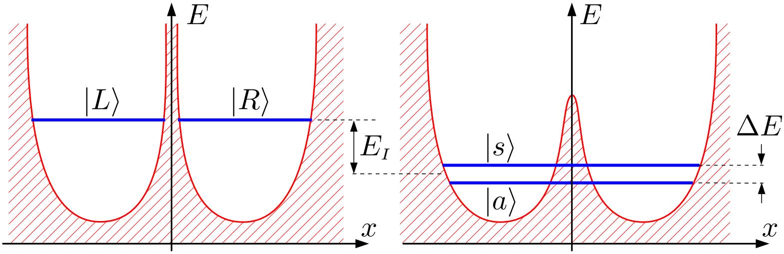

Fig. 3 : Energy eigenvalues of a chiral molecule

$$P\,|R\rangle = |L\rangle \qquad\qquad P\,|L\rangle = |R\rangle$$

$$P\,|s\rangle = +1\,|s\rangle \qquad \text{with} \quad |s\rangle \equiv \sqrt{\tfrac{1}{2}}\Big(|R\rangle + |L\rangle\Big) \tag{57a}$$

$$P\,|a\rangle = -1\,|a\rangle \qquad \text{with} \quad |a\rangle \equiv \sqrt{\tfrac{1}{2}}\Big(|R\rangle - |L\rangle\Big) \tag{57b}$$

Here the normalization

$$\langle s|s\rangle = \langle a|a\rangle = \tfrac{1}{2}\Big(\underbrace{\langle R|R\rangle}_{1} \pm \underbrace{\langle R|L\rangle}_{0} \pm \underbrace{\langle L|R\rangle}_{0} + \underbrace{\langle L|L\rangle}_{1}\Big) = 1 \tag{58}$$

was chosen. Due to the mirror symmetry of the potential in the right sketch of figure 3, the parity operator and the Hamilton operator of the chiral molecule commute.

$$[P, H] = [P, (H_0 + H_I)] = 0 \tag{59}$$

Therefore the eigenfunctions of H are identical to the eigenfunctions (57) of the parity operator:

$$H\,|s\rangle = E_s\,|s\rangle \qquad\qquad H\,|a\rangle = E_a\,|a\rangle \tag{60}$$

The energy of the antisymmetric state is

$$\begin{aligned}
\langle a|\,H|a\rangle &= \langle a|\,(H_0 + H_I)\,|a\rangle \;= \\
&= \tfrac{1}{2}\Big(\underbrace{\langle R|\,H_0|R\rangle}_{E_0} + \underbrace{\langle L|\,H_0|L\rangle}_{E_0} - \underbrace{\langle R|\,H_0|L\rangle}_{0} - \underbrace{\langle L|\,H_0|R\rangle}_{0} + \\
&\quad + \underbrace{\langle R|\,H_I|R\rangle}_{E_I} + \underbrace{\langle L|\,H_I|L\rangle}_{E_I} - \underbrace{\langle R|\,H_I|L\rangle}_{\Delta E/2} - \underbrace{\langle L|\,H_I|R\rangle}_{\Delta E/2}\Big) \;= \\
&= E_0 + E_I - \tfrac{1}{2}\Delta E
\end{aligned} \tag{61a}$$

For the symmetric state, by the same method the energy

$$\langle s|\,H|s\rangle = E_0 + E_I + \tfrac{1}{2}\Delta E \tag{61b}$$

is found. Typically, E_I is negative, while ΔE is positive. Thus we find the energy levels as indicated in blue in figure 3.

Chiral organic molecules usually are synthesized in biological systems by means of chiral enzymes. Therefore they are not created in the symmetric or antisymmetric states $|s\rangle$ or $|a\rangle$, but in the chiral states $|L\rangle$ or $|R\rangle$. We investigate by means of the Schrödinger equation the evolution in time of a chiral molecule, whose state is $|L\rangle$ at time $t = 0$:

$$\psi(t) = l(t)\,|L\rangle + r(t)\,|R\rangle \ , \ \ |l|^2(t{=}0) = 1 \ , \ \ |r|^2(t{=}0) = 0 \tag{62}$$

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}\,H\psi$$

$$|L\rangle\,\frac{\partial l}{\partial t} + |R\rangle\,\frac{\partial r}{\partial t} = -\frac{i}{\hbar}(H_0 + H_I)\Big(l\,|L\rangle + r\,|R\rangle\Big)$$

Multiplying these equations from left by $\langle L|$ resp. by $\langle R|$, we get the coupled equations

$$\frac{\partial l}{\partial t} = -\frac{i}{\hbar}\Big(l\,E_0 + l\,E_I + r\,\Delta E/2\Big) \tag{63a}$$

$$\frac{\partial r}{\partial t} = -\frac{i}{\hbar}\Big(r\,E_0 + r\,E_I + l\,\Delta E/2\Big)\ . \tag{63b}$$

It is easy to check by insertion, that these equations are solved — respecting the boundary conditions (62) — by

$$l(t) = C_l\exp\{-\frac{i}{\hbar}(E_0 + E_I)t\}\ \cos\Big(\frac{t\Delta E}{2\hbar}\Big) \tag{64a}$$

$$r(t) = C_r\exp\{-\frac{i}{\hbar}(E_0 + E_I)t\}\ \sin\Big(\frac{t\Delta E}{2\hbar}\Big) \tag{64b}$$

$$C_r = iC_l \quad , \quad |C_l|^2 = |C_r|^2 = 1\ .$$

$|l|^2$ resp. $|r|^2$ is the probability to observe the molecule in the left-rotating resp. right-rotating configuration. This probability is oscillating with the frequency

$$\frac{\Delta E}{\hbar} = 2\,\frac{\langle R|\,H_I|L\rangle}{\hbar} \approx \frac{1\,\mu\mathrm{eV}}{\hbar} \approx 1\,\mathrm{GHz} = \frac{1}{1\,\mathrm{ns}}\ . \tag{65}$$

As ΔE typically is of order $1\,\mu$eV, the right- and left-rotating forms of chiral molecules should typically be stable for not much longer than about 1 ns. If this was true, then it would be an exceedingly formidable experimental objective, to demonstrate optical activity at all. As is well-known, this is not true. Actually, chiral molecules, except for the very smallest, are stable in the right- or left-rotating form, and do not change this form in months and years. Why don't they? What is wrong with our computation?

The wrong result is caused by the fact, that we considered the chiral molecule as a closed system, and ignored any interactions with the environment. But the sugar molecules, whose optical activity is measured in the beginners practical training, are solved in water. Thus the sugar molecules are permanently interacting with the water molecules in their neighborhood. Due to entanglement with the environment, the pure state function $\psi(t) =$ (62) of the chiral molecule is replaced by a mixture. The Hamilton-operator's expectation value for this mixture can easily be computed, as the molecule's Hilbert space is spanned (as far as optical activity is concerned) by two vectors only, i. e. $|L\rangle$ and $|R\rangle$:

$$\begin{aligned}
\langle H\rangle_\rho &\overset{(41)}{=} \mathrm{Tr}\{\rho\, H\} = \langle L|\rho H|L\rangle + \langle R|\rho H|R\rangle \\
&= \langle L|\rho|L\rangle\langle L|H|L\rangle + \langle L|\rho|R\rangle\langle R|H|L\rangle + \\
&\quad + \langle R|\rho|L\rangle\langle L|H|R\rangle + \langle R|\rho|R\rangle\langle R|H|R\rangle \\
&= \rho_{ll}H_{ll} + \rho_{lr}H_{rl} + \rho_{rl}H_{lr} + \rho_{rr}H_{rr} \\
&\overset{(61)}{=} \underbrace{(\rho_{ll} + \rho_{rr})}_{=\,\mathrm{Tr}\{\rho\}\,=1}(E_0 + E_W) + \underbrace{(\rho_{lr} + \rho_{rl})}_{\approx\,0}\,\frac{\Delta E}{2}
\end{aligned} \tag{66}$$

In (75) we will prove, that the trace of any density operator is 1. And we know that the non-diagonal elements of the density matrix will decohere, i. e. they tend towards zero. Thus, if the molecule's state is entangled with the environment, it's energy becomes

$$\langle H\rangle_\rho \approx E_0 + E_W \ . \tag{67a}$$

This should be compared with the energy of the closed system:

$$\langle H\rangle_\psi \overset{(61)}{=} E_0 + E_W \pm \tfrac{1}{2}\Delta E \quad \text{if } \psi = |s\rangle \text{ or } \psi = |a\rangle \tag{67b}$$

Obviously, entanglement with the environment results into

$$\Delta E \xrightarrow{\text{entanglement with the environment}} 0 \ . \tag{68}$$

$\Delta E \approx 0$ does mean according to (64), that the molecule, once it's configuration is left- resp. right-rotating at $t = 0$, will keep that configuration forever, or at least for very long time. This is caused by the fact, that decoherence is completed within *much shorter time* than the 1 ns, after which an isolated molecule would typically switch to the enantiomer configuration according to estimation (65). In table 1 on page 25, the rate of decoherence of an object of size 10 nm due to scattering of air molecules is indicated as $10^{16}\text{nm}^{-2}\text{s}^{-1}$. While we should think of objects typically 10× smaller than the assumed 10 nm, when considering how the structure of a chiral molecule can be fixed, this factor probably is more than balanced by the much higher density of scattering water molecules as compared to the density of scattering air molecules.

The structure of other, non-chiral molecules is stabilized due to decoherence as well. And also larger aggregates of molecules (that is to say solids) get their geometrical stability thanks to entanglement with their environment. Due to entanglement, a measurement apparatus, once it has been constructed appropriately for the measurement of an observable Q, will preserve this structure durably, and will not suddenly mutate into an apparatus for the measurement of some different observables $Q', Q'', \ldots$

This effect is completely contrary to intuition! We are disposed to expect, that a molecule or a solid, whose exact form shall durably be preserved, should be shielded as perfect as possible against any "disturbance" from the environment. But the exact opposite is true: Just the permanent, uncontrolled interactions with the environment guarantee the geometrical constancy of the object. Large molecules, and the more so macroscopic solids, are stabilized in eigenstates of the position operator, because these states are *less robust* against entanglement with the environment than the eigenstates of the parity-operator and the Hamilton-operator.

From this point of view, it is sometimes correctly stated, that decoherence can explain the "appearance of the classical world out of the quantum world". In a startling — though comprehensible — manner, diffusely wafting clouds of quantum mist are transformed into dimensionally stable, classical objects due to entanglement with their environment.

9 Further Properties of the Density Operator

Density operators and projectors have many properties in common. Because of

$$\Big(|a\rangle\langle b|\Big)^{+} = \Big(\langle b|\Big)^{+}\Big(|a\rangle\Big)^{+} = |b\rangle\langle a| \ , \tag{69}$$

a density operator is hermitean, same as any projector, because it equals it's transposed complex-conjugate. Therefore all eigenvalues of projectors and of density operators are real. A projector has only one eigenfunction, namely the state vector, onto which it is projecting. The eigenvalue of this eigenfunction is 1:

$$P_\psi|\psi\rangle = |\psi\rangle \underbrace{\langle\psi|\psi\rangle}_{1} = 1\,|\psi\rangle \tag{70}$$

Any vector $|s\rangle$ of any basis is an eigenfunction of the density operator with eigenvalue w_s:

$$\rho|s\rangle = \sum_{s'} w_{s'}|s'\rangle \underbrace{\langle s'|s\rangle}_{\delta_{ss'}} = w_s|s\rangle \tag{71}$$

The expectation value of a projector is ≥ 0 in any state. This is called "non-negative definite":

$$\langle\phi|P_\psi|\phi\rangle = \langle\phi|\psi\rangle\langle\psi|\phi\rangle = |\langle\psi|\phi\rangle|^2 \geq 0 \tag{72}$$

The same holds for the density operator:

$$\langle\phi|\rho|\phi\rangle = \sum_s w_s\,\langle\phi|s\rangle\langle s|\phi\rangle = \sum_s w_s\,|\langle s|\phi\rangle|^2 \geq 0 \tag{73}$$

A projector's trace is

$$\mathrm{Tr}\{P_\psi\} = \mathrm{Tr}\Big\{|\psi\rangle\langle\psi|\Big\} \overset{(14)}{=} \langle\psi|\psi\rangle = 1\ . \tag{74}$$

We will demonstrate in two steps, that the same is true for the density operator.

$$\mathrm{Tr}\{\rho\} = \sum_s w_s\,\mathrm{Tr}\Big\{|s\rangle\langle s|\Big\} \overset{(14)}{=} \sum_s w_s\,\langle s|s\rangle = \sum_s w_s \tag{75a}$$

Now we assume, that the vector $|\psi_W\rangle$ is normalized to 1. Therefore

$$1 = \langle\psi_W|\psi_W\rangle \overset{(30)}{=} \sum_s\sum_r c^*_{Wrs}c_{Wrs} \overset{(35)}{=} \sum_s w_s\ . \tag{75b}$$

If one of the coefficients w_s is 1, then ρ degenerates to a projector

$$w_k = 1 \quad \overset{(75b)}{\Longleftrightarrow} \quad w_s = 0 \; \forall s \neq k \ , \tag{76}$$

because then ρ is idempotent. This is the defining property of a projector:

$$\rho\,\rho = |k\rangle \underbrace{\langle k|k\rangle}_{1} \langle k| = |k\rangle\langle k| = \rho \tag{77}$$

But if at least two coefficients w_s are different from zero, then $w_s < 1$ for all w_s. In this case, the density operator isn't a projector, because it is not idempotent:

$$\rho\,\rho = \sum_s \sum_{s'} w_s w_{s'}\, |s\rangle \underbrace{\langle s|s'\rangle}_{\delta_{ss'}} \langle s'| = \sum_s \underbrace{w_s^2}_{<w_s}\, |s\rangle\langle s| \neq \rho \tag{78}$$

If the density operator's eigenfunctions $|s\rangle$ are time-dependent, then it's partial derivative with respect to time is

$$\frac{\partial\rho}{\partial t} = \sum_s w_s \Big(\frac{\partial|s\rangle}{\partial t}\, \langle s| + |s\rangle\, \frac{\partial\langle s|}{\partial t} \Big) \ . \tag{79}$$

The Schrödinger equation and it's adjoint equation are

$$i\hbar\,\frac{\partial|s\rangle}{\partial t} = H|s\rangle \qquad\qquad -i\hbar\,\frac{\partial\langle s|}{\partial t} = \langle s|H \ . \tag{80}$$

From this follows

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= \sum_s w_s \frac{i}{\hbar}\Big(-\, (H|s\rangle)\langle s| + |s\rangle(\langle s|H)\Big) \\
\frac{\partial\rho}{\partial t} &= \sum_s w_s \frac{i}{\hbar}\Big(-\, H|s\rangle\langle s| + |s\rangle H\langle s| + \\
&\qquad + |s\rangle\langle s|H - |s\rangle H\langle s|\Big) = -\frac{i}{\hbar}[H,\rho] \ ,
\end{aligned} \tag{81}$$

resp. in case of a projector

$$\frac{\partial P_\psi}{\partial t} = -\frac{i}{\hbar}[H, P_\psi] \ . \tag{82}$$

This should be compared to the time-derivative of an operator Q in the Heisenberg-picture:

$$\frac{\mathrm{d}Q(t)}{\mathrm{d}t} = +\frac{i}{\hbar}[H, Q] + \frac{\partial Q(t)}{\partial t} \ . \tag{83}$$

The last term is zero, if the observable $Q(t)$ depends on time only canonically, but not explicitly. Obviously

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{\mathrm{d}P_\psi}{\mathrm{d}t} = 0 \tag{84}$$

for density operators and for projectors, as the canonical time-dependencies and the explicit time dependencies of these operators mutually cancel.

Even though they are hermitean operators, projectors and density operators are no observables: There exists no measurement device, which displays as result of a measurement the eigenvalue 1 of a projector or the eigenvalue w_k of a density operator, and prepares at the same time the system S in the eigenstate $|\psi\rangle$ of the projector resp. in the eigenstate $|k\rangle$ of the density operator.

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