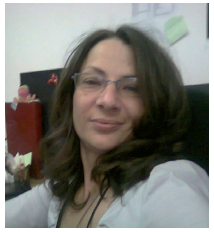
Key advancements in the understanding of the fundamental and universal Quantum Mechanics now lead the way towards realizing the long outstanding resolution to the idea that "Quantum Mechanics is capable of yielding its own interpretation". One seemingly simple consideration today opens new doors to significant progress and sensibility, and that is the the consideration of the quantum mechanical view of the decomposition of System into subsystems. Progress in the understanding of subsystems and how they conspire to make a whole is presented in terms of Quantum Correlations Relativity, the Parallel Occurrence of Decoherence, Preferred Local Structures for Bipartite Decompositions of a two-mode Open System, and the discovery of a limitation of the Nakajima-Zwanzig Projection Method in Open Systems Theory. Ultimately, we can now impose a limitation on, and forcefully question the long term viability of the Everett Interpretation.



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978-3-659-43118-0

Quantum Structures

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A View of the Quantum World

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Impressum / Imprint
Bibliografische Information der Deutschen Nationalbibliothek: Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über http://dnb.d-nb.de abrufbar.

Bibliographic information published by the Deutsche Nationalbibliothek: The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

Coverbild / Cover image: www.ingimage.com

Verlag / Publisher:
LAP LAMBERT Academic Publishing
ist ein Imprint der / is a trademark of
AV Akademikerverlag GmbH & Co. KG
Heinrich-Böcking-Str. 6-8, 66121 Saarbrücken, Deutschland / Germany
Email: info@lap-publishing.com

Herstellung: siehe letzte Seite /
Printed at: see last page
ISBN: 978-3-659-43118-0

Preface

Quantum mechanics provides a striking and counterintuitive observation in that it is easier to describe a quantum whole than its constituent parts. In other words, there is more uncertainty about quantum subsystems than about the total system composed of the quantum subsystems. This observation suggests that there is more to the idea of ”structure” (decomposition into parts, subsystems) in the quantum world than there is in the classical world.

For example, we can smash a rock into little bits, and each of those bits continues to follow classical physics, but ultimately when we smash those bits to the quantum scale we no longer see ”material” so much as we see something that is better described as ”pure behavior”. And this behavior is so fast and fleeting that we have only statistical methods with which to continue to presume that there is ”material stuff”. Odd as this is, classically, Quantum Mechanics is so accurate that we have to presume that the statistical methods have a lock on something very real. In experiments and in math it is possible to select and or to describe different and equivalent possible views of the same thing. The maths of quantum physics are at a point where they have captured the lessons of many different experiments and we can most readily describe these views in terms of mathematical decomposition ”structures” that achieve the whole.

Ultimately questions arise such as: Is there a unique fundamental structure of a composite quantum system (is one view any more ”real” or ’better” than any other)? How do classical structures (and intuition) appear from the quantum substrate? Can the structural variations available in the quantum world be of any practical use that is not known to classical physics? These are the main questions raised in this book. Some of the answers that we provide are so far only partial. Nevertheless, the results suggest that the topic of ”quantum structures” will be of significant interest to fundamental physics going forward.

The bulk of the results presented here have been obtained by the authors over the last seven years. Emphasis is placed on the appearance of ”structure” in different contexts and particular attention is given to the distinction between the classical and quantum mechanical concept of structure. The contents are arranged so as to provide a coherent and self contained reading. We have endeavored to include enough supplemental material to be ”reader-friendly”, while of course providing references for more detailed investigation of the topics covered.

We benefited much from discussions and encouragement that came from Allen Francom, Nate Harshman, David Steglet, Stephen P. King, Hitoshi Kitada and Dejan Raković. Some lucid observations provided by Allen Francom in a few last years have constantly enriched our inspiration and significantly influenced our thinking and the view of the quantum world.

Niš/Kragujevac, Summer 2013

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M. Arsenijević
M. Dugić

Abbreviations

BP – *Brownian particle*
ChM – *Chemical model* [of molecule]
CM – *Center of mass*
DISD – *Decoherence-induced suppression of decoherence*
EM – *Electromagnetic* [field]
ER – *Entanglement relativity*
lhs –*Left hand side* [of an equation]
LOCC – *Local operations and classical communication*
PFP – *Protein folding problem*
POD – *Parallel occurrence of decoherence*
QBM – *Quantum Brownian motion*
QCM – *Quantum chemistry model* [of molecule]
QCR – *Quantum correlations relativity*
QDR – *Quantum discord relativity*
QRF – *Quantum reference frame*
RF – *Reference frame*
rhs–*Right hand side* [of an equation]
SSM – *Solid-state model* [of molecule]

Contents

Chapter 1

Introduction

In non-relativistic physics, "system" is defined by the set of its degrees of freedom (x_i) and the related conjugate momentums (p_i), as well as by the set of the parameters (such as the mass, electric charge etc.). If the system is not elementary, it's said to be "composite", i.e. to be decomposable into parts (subsystems), which define the system's *structure*. Realistic systems, ranging from mesons to the Universe as a whole, are–composite.

In classical physics, "structure" is pre-defined and assumed to be basic. Subsystems of a composite system can be further decomposed ("fine-graining"), or grouped ("coarse-graining"), while the other variations of the system's structure are often regarded as physically artificial–a mathematical artifact.

However, in the quantum (non-relativistic) theory, the things look different. Solution to the quantum hydrogen atom (HA) Schrödinger equation is a cornerstone of the quantum theory that provides an outstanding observation. Actually, the classically paradoxical discrete energy-spectrums, which are experimentally observed, refer precisely to the atomic *internal* degrees of freedom (denoted R).

Only recently some elaborate attempts of describing HA as "electron+proton" ($e+p$) system have been made (Tomassini et al 1998, Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008, Jeknić-Dugić et al 2012). The conclusions are classically non-describable. Actually, as distinct from the atomic "center-of-mass+relative position" ($CM+R$) structure, the $e+p$ structure is endowed by quantum entanglement and *cannot* provide a proper theoretical explanation of the experimental evidence of the discrete atomic spectra[1].

On the other hand, the atomic CM and R systems appear *directly* accessible in the *realistic* physical situations such as e.g. atomic cooling, Bose condensation, interference, atomic lithography etc. The atomic CM and R formal subsystems are exactly decoupled from each other and (for the atom considered as a "closed" quantum system) can have the quantum states of their own–independent of each other. This is an important observation, which suggests that we can "directly" observe the (sub)systems only if there is the (sub)systems' *individuality*. However, the choice of such "preferred" degrees of freedom (i.e. of the preferred structure) of a composite system is not established by any general rule or condition. Is there such a rule or condition? If there is such a rule or condition, what might be its/their kinematic or dynamic quantum-mechanical basis? In other words: what constitutes a "system" accessible for an observer? These are the main questions of interest for us that are occasionally posed in the contemporary physics-research papers, see e.g. (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008, Harshman 2012a, Fel'dman and Zenchuk 2012, Lychkovskiy 2013).

These questions are of *universal* interest and importance in quantum theory, independently of the model of the composite system, which can be open or isolated, finite- or infinite-dimensional. This is of interest not only for the foundations of quantum theory but also for certain applications as well as for some interpretational reasons. The fact that this topic is as yet weakly appreciated may be a consequence of the classical prejudice and intuition, as well as of the widespread scientific attitude, which is described by Zurek's (Zurek 2003):

"*Quantum mechanics has been to date, by and large, presented in a manner that reflects its historical development. That is, Bohr's planetary model*

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[1] See eq.(21) below. An up to date presentation can be found in (Jeknić-Dugić et al 2012).

of the atom is still often the point of departure, Hamilton-Jacobi equations are used to "derive" the Schrödinger equation, and an oversimplified version of the quantum-classical relationship (attributed to Bohr, but generally not doing justice to his much more sophisticated views) with the correspondence principle, kinship of commutators and Poisson brackets, the Ehrenfest theorem, some version of the Copenhagen interpretation, and other evidence that quantum theory is really not all that different from classical–especially when systems of interest become macroscopic, and all one cares about are averages–is presented."

In different applications of quantum theory, numerous "one-particle" (i.e. noninteracting particles) models–which include the "virtual particles"–have been developed in order to avoid the difficulties in description of the many-particle systems. However, there is a *caveat*[2]: there is not any guarantee that the results can be straightforwardly interpreted in terms of the "original" constituent particles. It seems that this subtle point remained virtually unnoticed until recently (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008, Stokes et al 2012, Fel'dman and Zenchuk 2012, Harshman 2012a, Jeknić-Dugić et al 2012, Dugić et al 2013, Arsenijević et al 2013a,b, Lychkovskiy 2013). Presence of quantum correlations and related lack of classical individuality of quantum subsystems precludes a straightforward transfer of the results between the different structures of the composite system. Having this in mind, careful analysis of the composite system's structures and their behaviors becomes an emerging need of the modern quantum (non-relativistic) theory. This way comes both a fresh insight into well known methods and their results as well as emergence of a new methodological basis of quantum theory. As a matter of fact, we are yet to start working in that direction. So, the main purpose of this book is to try to overcome the classical prejudice, and to promote a fresh view of the quantum world.

The contents of this book is based mainly (but not exclusively) on the authors'

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[2] See also the arguments in (Zeh 2005).

contributions that are made in approximately the last seven years. It tackles all of the above-posed questions and carefully emphasizes subtlety of the topic of quantum structures. In Chapter 2 we provide a general conceptual basis for the remainder of the book. In Chapter 3, we introduce relativity of the concept of "quantum [non-classical] correlations" in composite quantum (closed or open) systems. Both the quantum entanglement and the quantum discord relativity are presented in detail. In Chapter 4 we give some details regarding the different molecule structures in use in the different fields. We emphasize a new qualitative proposal of interest for resolving the long-standing problems known as the Hund's paradox (Hund 1927) in chemistry, and the Levinthal paradox (or the "protein folding" problem), (Levinthal 1968), in the foundations of the macro-molecules dynamics (such as e.g. molecular recognition). In Chapter 5 we highlight some experimental evidence, which clearly stresses physical importance of the "non-fundamental" structure of the atomic and molecule species. Chapter 6 is one of the central parts of this book. It tackles the above-posed questions regarding the Universe as the isolated (closed) quantum system. There we present a recently obtained result of the "parallel occurrence of decoherence" for a specific model of the quantum Brownian motion. Physically, the results are striking: the model-Universe hosts some mutually irreducible and, physically and information-theoretically, mutually independent (autonomous), simultaneously evolving-in-time structures, which are endowed by the decoherence-induced quasi-classical structures. Some interpretational aspects of our findings, as well as the important issues raised by the "quantum reference frame", are the subject of Chapter 8. In Chapter 7, we provide a few models, which strongly suggest the following answer to the above questions for *open* systems: environment singles out the "preferred" (i.e. directly accessible for an observer) structure of the composite system. This finding can be described (see also Harshman 2012a) by the condition of the minimum quantum correlations in the preferred structure. Chapter 9 collects the questions, the offered answers and their subtleties in one place. Regarding application of our results, we hope for prospects anticipated in (Fel'dman and Zenchuk 2012): "*Using different bases, we may choose the preferable behavior of quantum correlations which allows a given quantum system to be more flexible in applications*."

To ease the exposition, we provide Supplement, which completes and partially, technically, extends what is told in the body text.

Chapter 2

The transformations of variables

Transformations of variables are ubiquitous in mathematical methods and manipulations. They are so common that sometimes are not explicitly distinguished. For instance, the equality:

$$\cos(\alpha+\beta)\sin(\alpha-\beta) = \sin\alpha\cos\alpha - \sin\beta\cos\beta \tag{1}$$

involves a linear transformation of the set $\{\alpha,\beta\}$ into the set $\{u,v\}$, where $u=\alpha+\beta$ and $v=\alpha-\beta$. In the spirit of our considerations, eq.(1) reads as:

$$\cos u \sin v = f_1(\alpha)g_1(\beta) + f_2(\alpha)g_2(\beta); \tag{2}$$

$f_1(\alpha)=\sin\alpha\cos\alpha$, $f_2(\alpha)=-1$, $g_1(\beta)=1$, $g_2(\beta)=\sin\beta\cos\beta$, while $\alpha,\beta\in[0,2\pi]$.

Product of two Gaussian functions, $F(x_1)=\exp\{-x_1^2/2\}$ and $F(x_2)=\exp\{-x_2^2/2\}$:

$$F(x_1)F(x_2) = F(x_-)F(x_+), \tag{3}$$

for the new variables $x_\pm=(x_1\pm x_2)/\sqrt{2}$ and $x_i\in(-\infty,\infty), i=1,2$. As it can be easily shown: for Gaussian functions, in general, there are also the sums like in eq.(2)–there is more than one term on at least one side of eq.(3).

The linear *canonical* transformations are of general use in physics. For a pair of one-dimensional systems described by the respective position and momentum variables, (x_1, p_1) and (x_2, p_2), one can define the center of mass (CM) and the "relative position" (R) degrees of freedom:

$$X_{CM} = \frac{m_1 x_1 + m_2 x_2}{M}, \quad r_R = x_1 - x_2, \tag{4}$$

where $m_i, i = 1, 2$, are the masses and $M = m_1 + m_2$. The new degrees of freedom, X_{CM} and r_R, define the respective conjugate momentums, $P_{CM} = p_1 + p_2$ and $p_R = (m_2 p_1 - m_1 p_2)/M$. Typical physical interactions are distance dependent, $V(|x_1 - x_2|)$ for the pair of systems 1 and 2. Then the transformations of variables, $\{x_1, x_2\} \to \{X_{CM}, r_R\}$, give rise to the variables separation. The total Hamiltonian function, H, does not involve any coupling of the new variables:

$$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|x_1 - x_2|) = H = \frac{P_{CM}^2}{2M} + \frac{p_R^2}{2\mu} + V(|r_R|), \tag{5}$$

where $\mu = (m_1^{-1} + m_2^{-1})^{-1}$ is the "reduced mass". Separation of the new variables (of the CM and the R formal systems) is at the root of exact solvability of the classical two-body problem[3].

Mathematical spirit of the transformations of variables can blur their physical contents. The transformations of variables are often considered as a purely mathematical tool, a mathematical artifact not having any physical meaning. This classical prejudice is going to be challenged, and then removed, in the quantum mechanical context, starting from the next section.

2.1 Classical physics prejudice on the transformations of variables

Let us start with the "obviously" correct observations. Center of mass for the pair "the Earth and the Venus" is an empty point in space, not a physical object. That is, for the classical, macroscopic bodies, the transformations of variables are simply mathematical artifacts[4]. For this reason, the results

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[3] Which is illustrated in Chapter 1 by the hydrogen atom.

[4] Sometimes it is said that the "relative positions" in eq.(4) do not have the same physical

presented via the "artificial" (the new) variables (X_{CM} and r_R), are typically transformed and presented via the "realistic" (the original) variables (x_1 and x_2).

As we show in Section 8.2, this classical interpretation of the transformations of variables is quantum mechanically sound. However, its extrapolation may be misleading. As an illustration, we borrow from (Dieks 1998):

"*This suggests the following necessary condition for factorizations to correspond to physically real systems. The factor Hilbert spaces should carry a representation of the space-time group... in the same way as the factor spaces of the original factorization, with the usual identification of generators of the space-time group and dynamical variables.*"

It is suggested above that the [linear canonical] transformations not preserving the space-time symmetry are not physically "real". The new degrees of freedom are required to be describable by the exactly the same physics (symmetries and the particles interactions) as the original ones. However, the later is not fulfilled already for the $CM + R$ system, the rhs of eq.(5), which, in turn, is the standard quantum mechanical model of the hydrogen atom as well as of the whole of atomic physics and quantum chemistry (see Chapter 5 for some phenomenological facts). Requiring the same symmetry rules for the "new" variables is mathematically misleading–the symmetry rules for the new variables *cannot be chosen* but are (uniquely) defined (induced) by the symmetry rules for the original ones (Anderson 1993, 1994, Harshman 2012b, Manzano et al 2013).

So we conclude: Every set of the physical degrees of freedom is formally *equal* to any other–i.e. it's subject of the same formalism. On the other hand, physical *reality* of the degrees of freedom is a separate issue that, as we show starting from Chapter 3, is a bit more subtle than in the classi-

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meaning as the original degrees of freedom. To this end, it is important to stress: *all the variables linked mutually via some proper variables transformations* have the same *mathematical meaning*. They are all vectors in the same vector space thus providing the *universal mathematical basis* of the physical considerations.

cal physics context[5]. To this end, *phenomenology* plays substantial role–the purely theoretical analysis is not sufficient (see Section 8.2).

2.2. Classifications of the canonical transformations

In the remainder of this book, we stick to the *linear canonical transformations* (LCTs)[6].

For a composite system $\mathcal{C}$ defined by the conjugate variables, x_i, p_j, where the commutator $[x_i, p_j] = \imath\hbar\delta_{ij}$, the LCTs are formally defined:

$$\xi_m = \sum_i c_{im} x_i + \sum_n d_{jm} p_j, \pi_n = \sum_i c'_{in} x_i + \sum_n d'_{jn} p_j \tag{6}$$

while $[\xi_m, \pi_n] = \imath\hbar\delta_{mn}$. The constants appearing in eq.(6) are mutually constrained; for an example, see eq.(127) below. In a slightly different form, one can introduce analogous expressions for the finite-dimensional systems (e.g. the qubit systems) or regarding the Fock space (e.g. via the Bogoliubov transformations)–see Supplement.

Def.2.1: *By* structure *of a composite system it is assumed the set of the composite system's degrees of freedom.*

This descriptive terminology should ease the exposition as well as to support physical intuition. e.g. In eq.(6) appear two structures, $\mathcal{S} = \{x_i, p_j\}$ and $\mathcal{S}' = \{\xi_m, \pi_n\}$, that refer to one and the same composite system, $\mathcal{C}$, and are mutually related by some LCTs.

2.2.1 Some classifications of the LCTs and structures

We introduce a few criteria for classification of the LCTs (and of the related structures) of interest for our considerations. All of them apply to the finite- as well as the infinite-dimensional (the continuous variable), open or closed, classical or quantum systems.

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[5] Of course, mathematical consistency, as described above, is required.

[6] For non-canonical transformations see e.g. (Lychkovskiy 2013).

While an LCT *induces* a structure, we will use the same terminology for both LCTs and structures.

(A) If no "new" variable, in eq.(6), can be expressed by more than one "old" ("original") variable, we refer to such transformations (and the related structures) as *trivial*. Otherwise they are *nontrivial*. Regarding the trivial LCTs, we distinguish the particles re-ordering or permutations, grouping of the particles (the "coarse graining" of the composite system's structure). In a simplified form, the later can be illustrated[7]:

$$1 + 2 + 3 \rightarrow 1 + (2 + 3) \equiv 1 + S, \tag{7}$$

where the bipartite system $S = 2 + 3$; if the 2 system represents the electron and the 3 system represents the proton, then S may be the hydrogen atom. So for the total system, $\mathcal{C}$, the following two structures are distinguished above: $\mathcal{S} = \{1, 2, 3\}$, which is tripartite, and the bipartite structure $\mathcal{S}' = \{1, S\}$. An example of non-trivial LCTs is given by eq.(4).

(B) LCTs are *global* if they target *all* degrees of freedom of a composite system. Otherwise, they are *local* (non-global). As it can be easily shown, global/local character for a pair of structures is not transitive. If $\mathcal{S}_2$ is local relative to both, $\mathcal{S}_1$ and $\mathcal{S}_3$, $\mathcal{S}_1$ and $\mathcal{S}_3$ may still be global to each other. Similarly, if $\mathcal{S}_2$ is global relative to both, $\mathcal{S}_1$ and $\mathcal{S}_3$, $\mathcal{S}_1$ and $\mathcal{S}_3$ may still be local to each other. This relation for a pair of structures is symmetric: if $\mathcal{S}_1$ is global (or local) relative to $\mathcal{S}_2$, then also $\mathcal{S}_2$ is global (local) to $\mathcal{S}_1$.

(C) If the "fine graining" (i.e. splitting into smaller parts) of a structure $\mathcal{S}$ can lead to a structure $\mathcal{S}'$, then the $\mathcal{S}$ structure is said to be *reducible* to the $\mathcal{S}'$ structure. Otherwise, the $\mathcal{S}$ structure is said to be *irreducible* to the $\mathcal{S}'$ structure. By definition, two structures having the same set of the degrees of freedom are mutually reducible. In eq.(7), the $\mathcal{S}'$ structure is reducible to the $\mathcal{S}$ structure, but not the other way around–reducibility is not symmetric.

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[7] We simplify notation: instead of the degrees of freedom, we simply use the particles labels .

Reducibility is transitive yet: if $\mathcal{S}_3$ is reducible to $\mathcal{S}_2$, and $\mathcal{S}_2$ is reducible to $\mathcal{S}_1$, then $\mathcal{S}_3$ is reducible to $\mathcal{S}_1$.

Below, we provide some illustrative examples.

Example 1. Let us consider a composite system $\mathcal{C}$ consisting of three particles, 1, 2 and 3. We are interested in the following structures of $\mathcal{C}$: $\mathcal{S} = \{1, 2, 3\}$, $\mathcal{S}_1 = \{1, 3, 2\}$, $\mathcal{S}_2 = \{1, S\}$ and $\mathcal{S}_3 = \{S', 3\}$, where the bipartite systems, $S = 2 + 3$ and $S' = 1 + 2$. These structures are obtained from each other by the trivial operations of grouping the systems, or decomposing, or reordering/permutations. In the set of the structures, only $\mathcal{S}_2$ and $\mathcal{S}_3$ are mutually global structures, while the other are mutually reducible: $\mathcal{S}_i \to \mathcal{S}_1, i = 2, 3$. The global transformation:

$$\mathcal{S}_2 = \{1, S\} \to \mathcal{S}_3 = \{S', 3\} \tag{8}$$

is characteristic for quantum teleportation. The composite system's state is endowed by entanglement–"entanglement swapping"; for some details see Section 3.1.

Example 2. Consider a composite system consisting of four subsystems. To be specific, let us consider two electrons, formally presented as $1e, 2e$, and two protons, $1p, 2p$. The structures of interest are: $\mathcal{S} = \{1e, 2e, 1p, 2p\}$, $\mathcal{S}_1 = \{1e, 1p, 2e, 2p\}$, $\mathcal{S}_2 = \{1H, 2e, 2p\}$, $\mathcal{S}_3 = \{1H, 2H\}$, $\mathcal{S}_4 = \{1CM, 1R, 2CM, 2R\}$ and $\mathcal{S}_5 = \{CM, R\}$; CM and R, cf. eq.(4), represent the center-of-mass and the "relative particle", while e.g. the $1H$ represents the hydrogen atom composed of the $1e$ and $1p$, symbolically $1H = 1e + 1p$. By definition, eq.(4), the CM and R "systems" do not consist of (cannot be separated into) the "original" systems (the electrons and protons), and *vice versa*. The $\mathcal{S}_3$ structure refers to a pair of the hydrogen atoms, each atom being presented as a pair "electron and proton" ($H = e + p$). The $\mathcal{S}_4$ structure represents a pair of the hydrogen atoms, each of which decomposed as $CM + R$. The $\mathcal{S}_5$ represents a pair $CM + R$ for the total $\mathcal{C}$ system.

We strongly emphasize: $\mathcal{S}_3 = \{1H, 2H\} \neq \mathcal{S}'_4 = \{1H, 2H\}$, where the later is obtained by grouping in the $\mathcal{S}_4$ structure, $H = CM + R$. This non-equality is a consequence of the fact that the hydrogen atoms are differently *built* starting from the smaller "pieces"–from the e and p, or from the CM and R systems, respectively. On the other hand, if the atom's structures are not specified, then formally the structure $\{1H, 2H\}$ can be differently decomposed also as (is reducible to) $\mathcal{S}_1$, $\mathcal{S}_4$ or $\mathcal{S}_5$.

In quantum chemistry, the $\mathcal{S}$ structure is considered to be the most fundamental [non-relativistic] definition of the hydrogen molecule. To this end, more precisely, the bipartite structure $\mathcal{S}' = \{E, P\}$ is considered, where $E = 1e+2e$ and $P = 1p + 2p$. On the other hand, the $\mathcal{S}_3$ structure is of interest in some condensed-matter considerations. There, the hydrogen molecule is considered as a pair of electrically neutral, oscillating particles (the atoms, $1H$ and $2H$). The $\mathcal{S}_5$ is of interest in investigating the large-molecules interference/decoherence effects as well as in the Stern-Gerlach-like experiments. All these structures are physically realistic in the respective physical situations–see Chapter 5 for details.

Regarding Example 2: the structures follow from each other, e.g., as

$$\mathcal{S} \overset{re-order}{\longrightarrow} \mathcal{S}_1 \overset{grouping}{\longrightarrow} \mathcal{S}_2 \overset{grouping}{\longrightarrow} \mathcal{S}_3 \overset{non-trivial}{\longrightarrow} \mathcal{S}_4 \overset{non-trivial}{\longrightarrow} \mathcal{S}_5. \tag{9}$$

The $\mathcal{S}_2$ structure is local relative to both, $\mathcal{S}_{1,3}$, while $\mathcal{S}_1$ is global relative to $\mathcal{S}_3$. There is a chain of reducibility: $\mathcal{S}_3 \to \mathcal{S}_2 \to \mathcal{S}_1$. For certain definitions of the relative positions, R [e.g. $R = 1R \bigcup 2R$]: the $\mathcal{S}_3$ structure is global relative to both $\mathcal{S}_{4,5}$, but $\mathcal{S}_4$ is local relative to $\mathcal{S}_5$. The structures $\mathcal{S}_i, i = 3, 4, 5$, are mutually irreducible.

It is important to emphasize: every structure $\mathcal{S}$ uniquely determines the sets of the structures of the composite system that are global/local, reducible/irreducible relative to $\mathcal{S}$.

2.2.2 Mutually irreducible global structures

Instead of delving into the mathematical subtleties of the LCTs forming the symplectic group for a composite system, we proceed with the less formal yet physically more intuitive presentation.

In this section, we consider the *mutually global and irreducible* structures, which cannot be obtained from each other via the trivial LCTs. By excluding the trivial transformations, this kind of structures are mutually global if they do not have even a single degree of freedom in common. In Example 2: the $\mathcal{S}_{4,5}$ structures are of the kind relative to all other structures, as well as to each other.

For a set of such structures, the following are direct implications of eq.(6):

(1) For every bipartite structure of a composite system, $\mathcal{C} = A+B$, the A subsystem is defined if and only if the B subsystem is defined. The subsystems A and/or B may have their own structures.

(2) Subsystems belonging to different (not necessarily bipartite) structures are mutually irreducible. To this end, the transformations eq.(4) are paradigmatic: the CM or R systems cannot be decomposed into the original systems 1 and 2, and *vice versa*.

(3) Subsystems belonging to different structures mutually do not interact. Therefore there is not any correlation and hence there is no information flow between them.

(4) Every structure is defined by its own "elementary" particles and their interactions. The symmetry rules for one structure are in a unique (the LCTs-defined) relation with the symmetry rules for any other structure (Anderson 1993, 1994, Harshman 2012b, Manzano et al 2013).

Now, for the mutually global and irreducible structures, we provide:

Lemma 2.1 *Subsystems belonging to different structures are mutually information-theoretically separated. There is not any information flow between them.*

Proof: Without loss of generality, let us consider bipartite structures, $\mathcal{S}_1 = A + B$ and $\mathcal{S}_2 = D + E$; each subsystem, A, B, D or E may be a composite system itself. The probability distributions for e.g. A and D, denoted[8] respectively $\rho(x_A)$ and $\rho(x_D)$, are not mutually related. The $\rho(x_D) = \rho(x_D(x_A, x_B))$ cannot be used to derive $\rho(x_A)$: integrating $\rho(x_D)$ over x_B does not provide $\rho(x_A)$: $\int \rho(x_D) dx_B \neq \rho(x_A)$. The only way to obtain $\rho(x_A)$ via integrating over x_B is to use the total system's, $\mathcal{C}$'s, probability density, $\rho_C \equiv \rho(x_A, x_B) = \rho(x_D, x_E)$: $\rho(x_A) = \int \rho_C dx_B$. On the other hand, presenting $\rho_C = \rho(x_A, x_D)$ cannot help as the linear dependence of x_A and x_D makes the integration $\int \rho(x_A, x_D) dx_B$ ill defined. So, knowledge about one subsystem (e.g. about the A system), *in principle*, does not provide any information about a subsystem (e.g. the D system) belonging to an alternate structure. Finally, due to the above point (3), there is not exchange of information or correlation between subsystems, which belong to different structures–which completes the proof. Q.E.D.

Of course, subsystems belonging to the *same* structure (e.g. A and B) may in principle provide description of each other. Due to correlation between the subsystems, a local measurement performed on one subsystem may provide some information regarding the other subsystem. Regarding quantitative measures of correlations, see Sections 3.1 and 3.2.

Everything told above equally refers to the "closed" as well as to the "open" quantum systems.

2.3 Quantum mechanical structures

It is essential, yet probably trivial, to note: every composite quantum system $\mathcal{C}$ is defined by *unique* Hilbert state space, $\mathcal{H}_C$, Hamiltonian, H, and quantum state in every instant in time.

The "coarse-graining" and the "fine-graining" operations formally do not preserve the number of the composite system's degrees of freedom. Of course,

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[8] In order to simplify notation, we do not use the rigorous form, $\rho(x, x') \equiv \langle x|\rho|x'\rangle$.

the degrees of freedom as stil there, but "buried" in the degeneracy of the coarse-grained state. LCTs induce re-factorization of the composite system's Hilbert state space, $\mathcal{H}_C$

$$\Pi_{i=1}^{\otimes N}\mathcal{H}_i = \mathcal{H}_C = \Pi_{\alpha=1}^{\otimes N'}\mathcal{H}_\alpha, \tag{10}$$

where $\mathcal{H}_i$ is a factor space pertaining to the original, while $\mathcal{H}_\alpha$ pertains to the new structure of the composite system. For bipartite decompositions, which is our main subject, $\mathcal{C} = A + B$, or $\mathcal{C} = D + E$, eq.(10) reads as:

$$\mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_C = \mathcal{H}_D \otimes \mathcal{H}_E. \tag{11}$$

Needless to say, tensor product (as well as scalar product) of states belonging to the factor spaces of the different factorizations, is not defined.

The composite system's Hamiltonian, H, has different forms for the different structures, e.g.:

$$\sum_{i=1}^{N}\frac{p_i^2}{2m_i} + V(\{x_i\}) = \sum_{\alpha=1}^{N}\frac{\pi_\alpha^2}{2\mu_\alpha} + V(\{\xi_\alpha\}). \tag{12}$$

For the bipartite structures introduced above, the Hamiltonian reads, in general, as:

$$T_A + V(x_A) + T_B + V(x_B) + V_{AB} = T_D + V(x_D) + T_E + V(x_E) + V_{DE}, \tag{13}$$

where "V" denotes the possible classical external fields for the subsystems, while the double-subscript terms represent the interactions.

It is worth repeating: for a composite system, the Hilbert state space and the set of the observables, including the system's Hamiltonian, are *unique*. According to the Schrödinger law, [normalized] quantum state of the system is [up to arbitrary phase] also *unique* in every instant in time. The same applies to the open systems not describable by the Schrödinger law. An open system's state is defined by the tracing out operation, e.g. $\rho_A(t) = tr_B \rho_C(t)$, which implies unique density matrix for every subsystem in every instant in time.

2.4 Quantum relativity of "system" and "locality"

Quantum structures point out, that the very basic physical concept of "system" is *relative.* Lemma 2.1, Section 2.2.2, exhibits that subsystems belonging to certain different structures are mutually physically and information-theoretically separated. In practice this means that the concept of "system" is *structure dependent* (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008): a system belonging to one structure can be unobservable for an observer that belongs to some alternative structure.

An open composite system is determined by the set of the observables accessible to measurement and manipulation (the "preferred" observables). In principle, every observable of a composite system can be measured. In practice, it is usually the case that only some observables can be easily measured (Zanardi 2001). In effect, experimenter acquires only small fraction of information about the composite system. Most of the remaining degrees of freedom (subsystems) remain undetermined or poorly known.

Every structure is uniquely defined by a tensor product factorization eq.(10). The orthonormalized bases and observables *adapted* to a factorization are *structure specific.* e.g. For the $\mathcal{H}_1 \otimes \mathcal{H}_2$ factorization, an orthonormalized basis $\{|m\rangle_1 \otimes |n\rangle_2\}$ as well as an observable $A_1 \otimes I_2$ are structure specific. It is important to stress: the observable $A_1 \otimes I_2$ and its measurement are *local* only for the $\mathcal{H}_1 \otimes \mathcal{H}_2$ factorization. Relative to some alternative structure, the observable $A_1 \otimes I_2$ is a "collective" observable whose measurement is non-local (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008). e.g. Measurement of the atomic CM position is a one-particle observable, $x_{CM} \otimes I_R$, for the $\mathcal{H}_{CM} \otimes \mathcal{H}_R$ factorization. However, regarding the alternate $e+p$ structure, its measurement is collective–eq.(4) emphasizes that the CM position is determined by the positions of *both* e and p.

Therefore, measurement of the CM's position (or momentum) affects both e and p, but only *partially*–the R system remains unaffected by the measurement. On the other hand, simultaneous measurement of both the CM and R systems is equivalent to a simultaneous measurement of both the e and p, and *vice versa*. Such measurements are the measurements performed on the atom as a whole. Thereby the concept of "collective" ("composite") observables and measurements also become relative (structure dependent). So we may say, that the atomic CM system is not more "collective" than the atomic electron. Needless to say: every observable local to a structure is an observable of the total system $\mathcal{C}$.

Hence, in formal terms, "locality" (of a subsystem, observable or of a measurement, or of any action exerted on the composite system $\mathcal{C}$) is defined by the tensor product structure of the Hilbert state space and by the corresponding "one-particle" observables. Phenomenological aspects of these findings are presented and discussed in Chapter 5.

Finally, the structure-induced notion of locality as described above does not incorporate the relativistic notion of locality, which is of interest for the Bell inequalities tests. Relativistic locality can be introduced once the tensor-product structure (i.e. the structure-induced locality) is defined. For approaches that unite the structure-induced locality and the relativistic locality see e.g. (Zanardi et al 2004, Harshman and Ranade 2011).

Chapter 3

Quantum Correlations Relativity

In quantum teleportation (Bennett et al 1993), three qubits are specifically prepared. A qubit 1 is in unknown state $|u\rangle_1$, while the pair $2+3$ is in a Bell state, e.g. $|\Phi^-\rangle_{23} = \frac{1}{\sqrt{2}}(|0\rangle_2|1\rangle_3 - |1\rangle_2|0\rangle_3)$. The total system's quantum state can be presented in the different forms for the following structures[9]:

$$\begin{aligned}
\mathcal{S} = 1 + (2+3): &\quad |\Psi\rangle_{123} = |u\rangle_1 \frac{1}{\sqrt{2}}(|0\rangle_2|1\rangle_3 - |1\rangle_2|0\rangle_3) \\
\mathcal{S}_1 = 1 + 2 + 3: &\quad |\Psi\rangle_{123} = \frac{1}{\sqrt{2}}(|u\rangle_1|0\rangle_2|1\rangle_3 - |u\rangle_1|1\rangle_2|0\rangle_3) \\
\mathcal{S}_2 = 2 + 1 + 3: &\quad |\Psi\rangle_{123} = \frac{1}{\sqrt{2}}(|0\rangle_2|u\rangle_1|1\rangle_3 - |1\rangle_2|u\rangle_1|0\rangle_3).
\end{aligned} \tag{14}$$

However, quantum teleportation is *not* possible due to any of the structures presented in eq.(14), but rather to the $\mathcal{S}_3 = (1+2)+3$ structure for which:

$$|\Psi\rangle_{123} = \frac{1}{2}[|\Psi^-\rangle_{12}|u_1\rangle_3 + |\Psi^+\rangle_{12}|u_2\rangle_3 + |\Phi^+\rangle_{12}|u_3\rangle_3 + |\Phi^-\rangle_{12}|u_4\rangle_3]. \tag{15}$$

The states $\{|\Psi^\pm\rangle, |\Phi^\pm\rangle\}$ form the so-called Bell basis, while the $|u_i\rangle$ states are not mutually orthogonal (for further details see (Benett et al 1993) or (Nielsen and Chuang 2000)).

The structures are related by the trivial transformations of variables as fol-

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[9] We omit the tensor-product symbol.

lows:

$$\mathcal{S} \overset{decomposing}{\longrightarrow} \mathcal{S}_1 \overset{grouping}{\longrightarrow} \mathcal{S}_3. \tag{16}$$

So, a simple redefinition of the composite system's structure provides entanglement swapping from the pair $2+3$ to the pair $1+2$, for the quantum state $|\Psi\rangle_{123}$ in an instant in time. A composite measurement on the subsystem 1+2 and the classical communication between Alice and Bob allow teleportation of the unknown state $|u\rangle$ from qubit 1 to qubit 3.

This dependence of the form of a quantum state on the composite system's structure can be easily demonstrated for the hydrogen atom, which is a *continuous variable* (CV) system.

Hydrogen Atom (HA) is defined as a pair "electron+proton" $(e+p)$ that mutually interact via Coulomb interaction. Introducing the atomic CM and R variables (while neglecting the spin) provides separation of variables and the exact solution to the quantum HA model. Relation of the two structures is of the kind considered in Section 2.2, see also eq.(4).

Formally, the Hamiltonian, H, of the atom reads as:

$$\frac{\vec{p}_e^{\,2}}{2m_e} + \frac{\vec{p}_p^{\,2}}{2m_p} - \frac{e^2}{4\pi\epsilon_\circ|\vec{r}_e - \vec{r}_p|} = H = \frac{\vec{p}_{CM}^{\,2}}{2M} + \frac{\vec{p}_R^{\,2}}{2\mu} - \frac{e^2}{4\pi\epsilon_\circ|\vec{r}_R|} \tag{17}$$

where we borrow notation from eq.(4). Due to non-interaction between the CM and R systems, the state for the $CM+R$ structure of the atom can be assumed to be tensor product:

$$CM + R : |\psi\rangle_{atom} = \quad |\chi\rangle_{CM}|nlm_lm_s\rangle_R; \tag{18}$$

in eq.(18), we employ the standard notation of quantum theory for the hydrogen atom.

However, due to the Coulomb interaction between the electron and the proton, one should expect entanglement:

$$e + p : \quad |\psi\rangle_{atom} = \sum_i c_i |i\rangle_e |i\rangle_p. \tag{19}$$

This entanglement can be estimated to be weak as follows. Let us apply the standard *adiabatic approximation* to the pair $e + p$. In the zeroth order of approximation, the proton is "frozen" in a spatial position $\vec{r}_p^{\circ}$. Then the atomic Hamiltonian, the lhs of eq.(17), reduces to the electron's effective Hamiltonian and the related Schrödinger equation:

$$\left\{ \frac{\vec{p}_e^{\,2}}{2m_e} - \frac{e^2}{4\pi\epsilon_\circ |\vec{r}_e - \vec{r}_p^{\circ}|} \right\} |\phi_n\rangle_e = E_{en} |\phi_n\rangle_e. \tag{20}$$

where $\vec{r}_p^{\circ}$ is a c-number, not a dynamical variable. It is obvious that eq.(20) is of the same form as for the R system–cf. the rhs of eq.(17). So, the solutions to the rhs of eq.(17) and eq.(20) are formally the same. With some simplification of notation, the state of the atom is of the form (Gribov and Mushtakova 1999, Atkins and Friedman 2005):

$$\sqrt{1 - \kappa^2} |\phi_n\rangle_e |\vec{r}^{\circ}\rangle_p + |O(\kappa)\rangle_{ep}, \tag{21}$$

where $\kappa \equiv (m_e/m_p)^{3/4} \ll 1$–of the order of the standard adiabatic parameter in quantum molecules theory (see Section 4.2.2). As distinct from eq.(18), the small term on the rhs of eq.(21) reveals the presence of entanglement for the atomic $e + p$ structure. Hence quantum dynamics for the two structures ($e + p$ and $CM + R$) of the hydrogen atom are *not* mutually equivalent, while eq.(18) is known to be in accordance with experimental observations.

3.1 Quantum entanglement relativity

From eqs. (14)-(21) we can respectively write:

$$|u\rangle_1 \frac{1}{\sqrt{2}} (|0\rangle_2 |1\rangle_3 - |1\rangle_2 |0\rangle_3) = |\Psi\rangle_{123} =$$

$$\frac{1}{2}[|\Phi\rangle_{12}|u_1\rangle_3 + |\Phi\rangle_{12}|u_1\rangle_3 + |\Phi\rangle_{12}|u_1\rangle_3 + |\Phi\rangle_{12}|u_1\rangle_3] \tag{22}$$

and:

$$\sqrt{1-\kappa^2}|\phi_n\rangle_e|\vec{r}^{\circ}\rangle_p + |O(\kappa)\rangle_{ep} = |\psi\rangle_{atom} = |\chi\rangle_{CM}|nlm_l\rangle_R. \tag{23}$$

In the position representation, eq.(23) [with a slight change in notation] reads:

$$\sqrt{1-\kappa^2}\phi_n(\vec{r}_e - \vec{r}_p^{\circ})\delta(\vec{r}_p - \vec{r}_p^{\circ}) + \kappa\Phi_O(\vec{r}_e, \vec{r}_p) = \chi(\vec{r}_{CM})\varphi_{nlm_l}(\vec{r}_R). \tag{24}$$

The expressions eq.(22) and eq.(24) are instances of the general quantum mechanical *rule*–of the so-called *Entanglement Relativity* (Vedral 2003, Caban et al 2005, Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008, Zanardi 2001, Ciancio et al 2006, De la Torre et al 2010, Harshman and Wickramasekara 2007, Jeknić-Dugić and Dugić 2008, Terra Cunha et al 2007). For a composite system $\mathcal{C}$ that can be decomposed as $S + S'$ or as $A + B$, Entanglement Relativity (ER) establishes for an instantaneous state, $|\Psi\rangle$, e.g.

$$|\xi\rangle_S|\phi\rangle_{S'} = |\Psi\rangle = \sum_i c_i|i\rangle_A|i\rangle_B. \tag{25}$$

For every set (e.g. an orthonormalized basis) of the tensor-product states, there is infinitely many entangled states–the number of entangled states in a Hilbert space is incomparably larger than the number of the tensor-product states. Hence the tensor product states are rare (”improbable”) in the Hilbert state space and for the most of the practical purposes–but see eq.(3)–this possibility can be neglected. So, ER implies that there is entanglement for practically every state $|\Psi\rangle$ of a composite system. Of course, a state can have entanglement for both structures of the composite system; some subtleties regarding the finite-dimensional systems can be found in (Harshman and Ranade 2011). Nevertheless, amount of entanglement for a quantum state is not an LCTs invariant.

From eqs. (22)-(25), we directly realize: "quantum entanglement" is not a feature of a composite system, or of a system's state, but is a *feature of the composite system's* structure.

3.2 Quantum discord relativity

"Quantum discord" is a common name for a number of mutually different measures of non-classical (quantum) correlations in composite quantum systems (Olivier and Zurrek 2001, Henderson and Vedral 2001, Modi et al 2012, Xu and Li 2012). For closed systems, "discord" coincides with "entanglement". For open quantum systems, there are quantum correlations that are not identical with entanglement. Total amount of non-classical correlations is measured by "discord".

If a composite (e.g. bipartite) quantum system carries the total correlation I, then the non-classical correlation can be quantified by subtracting the classical correlation, denoted J, from the total I. Of course, operationally, information is acquired by performing a quantum measurement, e.g. on one subsystem of the composite system. On this basis, one tries to conclude about the amount of non-classical correlations in the composite system.

Two systems, S and S', constitute a bipartite system $\mathcal{C} = S + S'$. A quantum measurement performed on S' and defined by a projector, $\Pi_{S'i}$, provides the final state of the composite system: $\rho_S|_{\Pi_{S'i}} = I_S \otimes \Pi_{S'i} \rho I_S \otimes \Pi_{S'i}$. Then the maximum classical correlations can be defined as:

$$J^{\leftarrow}(S|S') = \mathcal{S}_{vn}(S) - \inf_{\{\Pi_{S'i}\}} \sum_i |c_i|^2 \mathcal{S}_{vn}(\rho_S|_{\Pi_{S'i}}) \geq 0, \tag{26}$$

where $\mathcal{S}_{vn}$ represents von Neumann entropy, $\mathcal{S}_{vn}(\rho) = -tr\rho \ln \rho$, for instantanoeus state ρ.

The total correlation in the system is defined as the mutual information, $I(S : S') = \mathcal{S}_{vn}(S) + \mathcal{S}_{vn}(S') - \mathcal{S}_{vn}(S, S') \geq 0$ that, according to the above described idea, provides the following measure, termed "one-way discord", of quantum correlations in the composite system $\mathcal{C}$ (Olivier and Zurek 2001):

$$D^{\leftarrow}(S|S') = I(S:S') - J^{\leftarrow}(S|S') \geq 0. \tag{27}$$

The arrows appearing in eq.(27) emphasize that the measurement is performed on S'. If the measurement is performed on S, then the roles of S and S' in eq.(27) are mutually exchanged. Then the one-way discord $D^{\leftarrow}(S'|S) = D^{\rightarrow}(S|S')$ in full analogy with eq.(27). The closely related measure is the "two-way discord", $D^{\leftrightarrow}(S, S') = max\{D^{\leftarrow}(S|S'), D^{\leftarrow}(S'|S)\}$, which tends to be larger than one-way discord.

The one-way discord $D^{\leftarrow}(S|S')$ equals zero if and only if the composite system's state, ρ_C, is of the form (Modi et al 2012, Xu and Li 2012), (and the references therein):

$$\rho_C = \sum_k p_k |k\rangle_S\langle k| \otimes \rho_{S'k}, \quad {}_S\langle k|k'\rangle_S = \delta_{kk'}, \sum_k p_k = 1, \tag{28}$$

while the two-way discord equals zero if and only if the composite system's state is of the form (Modi et al 2012, Xu and Li 2012), (and the references therein):

$$\rho'_C = \sum_{kl} p_{kl}|k\rangle_S\langle k| \otimes |l\rangle_{S'}\langle l|,_S \langle k|k'\rangle_S = \delta_{kk'},_{S'} \langle l|l'\rangle_{S'} = \delta_{ll'}, \sum_{k,l} p_{kl} = 1. \tag{29}$$

Apparently, the state ρ'_C, eq.(29), is a special case of ρ_C appearing in eq.(28): commutativity of all $\rho_{S'k}$ in eq.(28) gives rise to ρ'_C in eq.(29).

Let us now consider an alternate structure (Dugić et al 2013), $\mathcal{C} = A + B$.

By definition, mixed states are "mixtures" of pure states: in eq.(29), the pure states $|k\rangle_S|l\rangle_{S'}$ are "mixed" with the probability distribution $\{p_{kl}\}$. So, we can use ER, Section 3.1. As it can be easily shown, only if for every $|k\rangle_S|l\rangle_{S'}$ there exists some $|\alpha\rangle_A|\beta\rangle_B$ [such that ${}_A\langle\alpha|\alpha'\rangle_A = \delta_{\alpha\alpha'}$ and ${}_B\langle\beta|\beta'\rangle_A = \delta_{\beta,\beta'}$] the state eq.(29) obtains the form: $\rho'_C = \sum_{\alpha,\beta} p'_{\alpha\beta}|\alpha\rangle_A\langle\alpha|\otimes|\beta\rangle_B\langle\beta|, \sum_{\alpha,\beta} p_{\alpha\beta} = 1$, for which the two-way discord for the $A+B$ structure $D^{\leftrightarrow}(A,B)=0$. In all other cases, the state ρ'_C is not of the form of eq.(29) for the alternate $(A+B)$ structure. So, a change of the composite system's structure induces a change in two-way discord: two-way discord that equals zero for one structure (e.g. for $1+2$) becomes nonzero for an alternate structure (for $A+B$).

Entanglement Relativity, Section 3.1, states:

$$|k\rangle_S |l\rangle_{S'} = \sum_{\alpha,\beta} c^{kl}_{\alpha\beta} |\alpha\rangle_A |\beta\rangle_B. \tag{30}$$

Substituting eq.(30) into eq.(29) gives:

$$\rho'_C = \sum_{k,l,\alpha,\beta} p_{kl} |C^{kl}_{\alpha\beta}|^2 |\alpha\rangle_A\langle\alpha| \otimes |\beta\rangle_B\langle\beta| \\ + \sum_{k,l,\alpha\neq\alpha',\beta\neq\beta'} p_{kl} C^{kl}_{\alpha\beta} C^{kl*}_{\alpha'\beta'} |\alpha\rangle_A\langle\alpha'| \otimes |\beta\rangle_B\langle\beta'|. \tag{31}$$

In order for eq.(31) takes the form of eq.(29) also for the $A+B$ structure, the following conditions should be satisfied:

$$\sum_{k,l} p_{kl} C^{kl}_{\alpha\beta} C^{kl*}_{\alpha'\beta'} = 0, \forall\alpha \neq \alpha', \forall\beta \neq \beta', \tag{32}$$

Analogous analysis of the state ρ_C, eq.(28), gives rise to the following conclusion: in order for one-way discord equals zero also for the alternate structure $(A+B)$, the following conditions must be fulfilled:

$$\sum_{k,l} p_k \omega^k_l C^{kl}_{\alpha\beta} C^{kl*}_{\alpha'\beta'} = 0, \forall\alpha \neq \alpha', \forall\beta, \beta', \tag{33}$$

while $p_k \geq 0, \omega^k_l \geq 0, \sum_k p_k = 1 = \sum_l \omega^l_k, \forall l$. Both conditions, eq.(32) and eq.(33), represent the sets of the simultaneously fulfilled equalities. For the continuous variable systems, the number of such equalities is infinite. However, this does not mean that these conditions can never be fulfilled.

Actually, the number of the normalization and orthogonality conditions for the states $|k\rangle_S|l\rangle_{S'}$ as well as for $|\alpha\rangle_A|\beta\rangle_B$ is also infinite. So, we cannot conclude that these conditions, or at least one of them, is never fulfilled. Nevertheless, for every combination of the coefficients $C^{kl}_{\alpha\beta}$ satisfying eq.(32) or eq.(33), there is an infinite number of variations of the coefficients p_k and ω^k_l, or p_{kl}, respectively, that do not satisfy eq.(32) and eq.(33). In practice, it means one may forget about the states fulfilling the conditions eq.(32) and/or eq.(33).

In effect, virtually every change in structure of a bipartite quantum system gives rise to a change in quantum discord: e.g. if quantum discord is zero for one structure, it is almost certainly non-zero for arbitrary alternative structure of the composite system

$$\rho_S \otimes \rho_{S'} = \sum_i \lambda_i \rho_{Ai} \otimes \rho_{Bi}. \tag{34}$$

Eq.(34) exhibits quantum discord relativity (QDR, (Dugić et al 2013)). Bearing in mind that "quantum discord" is more general than "entanglement", we find Quantum Correlations Relativity (QCR): *there is quantum correlation for practically every state of a composite quantum system.* Or the other way around: "quantum correlation" does not concern of a composite system, or of any of its possible states, *but concerns the composite system's structure.*

3.3 Some mathematical remarks

Considerations in Section 3.2 are based on ER, which is a *universal* rule–a corollary of the universally valid quantum mechanics–applicable for finite- as well as infinite-dimensional, open or closed systems and for every kind of LCTs.

The task of estimating amount of non-classical correlations in a composite system for different structures can be reduced to the following task:

T. *Starting from a given form of a composite system's state, provide a form* *of the state for some alternate structure of the composite system.*

Regarding the trivial LCTs (of grouping or decomposing or permutations of the constituent particles), it is straightforward (although probably sometimes tedious) to provide the alternate forms of the state–cf. eqs. (14) and (15).

However, regarding the non-trivial LCTs, and particularly those distinguished in Section 2.2.2, for the *closed* systems the task **T** coincides with providing the Schmidt canonical form (for a fixed instant in time) of the state. To this end, we are not aware of any *algebraic* recipe. Typically, obtaining Schmidt form of the state assumes a representation (e.g. the position representation). The methods are proposed that do not provide any analytical solutions: numerical analysis may be helpful for Gaussian states of the continuous variable systems, see e.g. (Ciancio et al 2006). For an example regarding the spin-chain systems see (Fel'dman and Zenchuk 2012).

Finally, regarding the mixed states (of interest for *open* systems), the task **T** is an instance of the so-called "quantum separability (QUSEP)" problem, which is thoroughly investigated for the finite-dimensional systems. The QUSEP problem is known to be computationally an NP-Hard problem (Gharibian 2010). Also for the finite-dimensional systems, it appears that calculating quantum discord is NP-Complete (Huang 2013).

So there is not a universal method for solving the task **T**. This is an open issue pointed out by our considerations.

3.4 Some physical remarks

It seems unavoidable to conclude, that QCR constitutes the core of the most, if not all, of the problems (Zeh 1993, 2005, Primas 1994) appearing in the "one-particle" methods in solid state physics, nuclear physics and quantum chemistry. Nevertheless, introducing quantum correlations into consideration can be useful as we emphasize below.

There is a simple idea for *avoiding decoherence* (Jeknić-Dugić and Dugić 2008). Decoherence is expected to reduce amount of quantum correlations in a composite system. If decoherence ruins quantum correlations for the $S+S'$ structure, this is *not expected* to be the case for an alternate structure $A+B$. So, quantum engineers can avoid decoherence (that is unfolding in the $S+S'$ structure) by simply targeting the observables of the alternate, the $A+B$, structure.

QCR implies: manipulating the composite system $\mathcal{C}$ can be virtually independent of the $\mathcal{C}$'s *initial preparation.* No matter of the initial state of $\mathcal{C}$, there is always a possibility to use quantum correlations. e.g. If the initial state is tensor product for the $S+S'$ structure, one can use quantum correlations by operationally targeting the observables of an alternate $A+B$ structure. Accessibility of a composite system's observables is a subtle an issue to be discussed in Chapters 5 and 7. So, keeping in mind this subtlety, in principle, one may forget about the problems posed by the initial state preparation for bipartitions of a composite quantum system.

QCR changes our *intuition* about the composite *quantum* systems. The universally valid quantum mechanics does not *a priori* select a preferred structure of a composite system. All structures can be formally treated on the equal footing thus challenging the classical prejudice of Section 2.1. The place of the classical intuition, Section 2.1, in the quantum mechanical context is a subject of Chapters 7 and 8, and particularly of Section 8.2.

Finally, the following consequences of QCR will be presented in the remainder of this book: the so-called parallel occurrence of decoherence (Section 6.3.3), a limitation of the Nakajima-Zwanzig projection method in open quantum systems theory (Section 6.3.4), and the preferred structure of open system (Chapter 7).

Chapter 4
Quantum Molecule Structures

There are different ways of defining "molecule" as a physical system. We distinguish (in somewhat simplified terms) a few typical models of interest in physics and chemistry.

Chemical model (ChM). In chemistry, "molecule" is often defined as "*An electrically neutral entity consisting of more than one atom*"[10]. Physically, it is a set of atoms mutually linked[11] by chemical bonds. If the atoms are point-like (unstructured) particles, "molecule" is simply a chain or a lattice of point-like oscillators. Spatial distribution of atoms defines the molecule geometrical shape (molecule configuration)–the very basic concept of stereochemistry.

Solid state model (SSM). If internal atomic excitations are added to every atomic position introduced in the ChM, then one obtains another definition (model) of "molecule". This "molecular excitons" model is typical for solid state physics and applications.

Quantum chemistry model (QC). In quantum chemistry, "molecule" is defined as a set of the atomic nuclei and the electrons in mutual interaction via the Coulomb electrostatic field.

Taking the spin into consideration complicates the analysis. So, in order to exhibit the structural relations between the different models, we will ignore the molecule spin.

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[10] IUPAC Recommendations 1994; doi:10.1351/pac199466051077.

[11] Phenomenologically inspired boundary conditions.

4.1 Mutual relations of the molecule structures

The chemical model (ChM) is simply a set of point-like atoms, $\mathcal{S}_{ChM} = \{1, 2, 3, ...\}$–internal atomic degrees of freedom are ignored. Chemical bonds typically enter the picture through a definite geometric shape (a configuration) of a molecule. Hence it is reasonable to assume that the $\mathcal{S}_{ChM}$ represents a set of harmonic oscillators–the chemical bonds provide the effective harmonic field for every oscillator (which is defined by its mass, spatial equilibrium-position and frequency). The assumption of existence of the atomic equilibrium-positions is classical in its spirit. There is not a quantum mechanical reason to think so, for an isolated molecule (Hund 1927). Therefore, in the quantum mechanical context, the ChM model is not physically complete. For large molecules (such as bio-polymers), the ChM model raises the following foundational problems: why, and how, large molecules obtain different configurations (Hund 1927, Giulini et al 1996), and how can be described transitions between the molecule configurations (a variant of the celebrated protein folding problem, see (Levinthal 1968)).

For the ChM, the molecule Hilbert state space is tensor product of the individual oscillators Hilbert spaces:

$$\mathcal{H}_{ChM} = \otimes_i \mathcal{H}_i, \tag{35}$$

while the Hamiltonian reads as:

$$H_{ChM} = \sum_i (\frac{\vec{p}_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 \vec{r}_i^2) + \sum_{i \neq j} V_{ij}. \tag{36}$$

Non-harmonic corrections are neglected in eq.(36). For non-interacting oscillators, $V_{ij} = 0, \forall i, j$

The solid-state model (SSM) enriches the ChM description. If the excitations are denoted by "ex", then the molecule structure reads as: $\mathcal{S}_{SSM} = \{1, 1ex, 2, 2ex, 3, 3ex, ...\}$. Detailed physical nature of "exciton" is here of secondary importance. Here we assume the excitations are well spatially defined–joined with the respective oscillator equilibrium-positions. "Coarse graining" of the $\mathcal{S}_{SSM}$ structure can provide a bipartite structure, $\mathcal{S}'_{SSM} = \{\mathcal{S}_{ChM}, Ex\}$, where the exciton system $Ex = \{1ex, 2ex, 3ex, ...\}$. Quantum mechanically, the exciton system can be analysed independently of the lattice vibrations: the excitation transfer from one to another cell of the lattice is allowed and numerous interesting physical effects may occur.

For the SSM structure, the Hilbert state space acquires the form:

$$\mathcal{H}_{SSM} = \mathcal{H}_{ChM} \otimes_i \mathcal{F}_i, \tag{37}$$

where $\mathcal{F}_i$ represents the Fock space for the ith excitation. The Hamiltonian reads[12]:

$$H_{SSM} = H_{ChM} + H_{ex}. \tag{38}$$

As we emphasize below, the quantum chemistry model (QCM) is the most fundamental model of "molecule". As a kind of generalization of the standard definition of "atom", in quantum chemistry (Gribov and Mushtakova 1999, Atkins and Friedman 2005), "molecule" is defined as a set of the atomic nuclei (denoted n) and of the atomic electrons (e)–the $\mathcal{S}_{QCM} = \{1e, 1n, 2e, 2n, ...\}$ structure; compare to the $\mathcal{S}$ structure in Example 2, Section 2.2.1. The ith atomic nucleus brings some electrostatic charge, $Z_i e$, and there is the electrostatic Coulomb interaction between the molecule's constituents.

Let $\mathcal{H}_{ei}$ represents the Hilbert state space of the ith electron, and $\mathcal{H}_{n\alpha}$ represents the Hilbert state space of the αth atomic nucleus. Then the molecule Hilbert state space factorizes as:

$$\mathcal{H}_{QCM} = \otimes_i \mathcal{H}_{ei} \otimes_\alpha \mathcal{H}_{n\alpha}. \tag{39}$$

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[12] Coupling between the molecule vibrations and excitations is typically provided by applying some external field to the molecule.

The molecule Hamiltonian reads as:

$$H_{QCM} = \sum_i \frac{\vec{p}^{\,2}_{ei}}{2m_e} + \sum_{i\neq j} V_{ij} + \sum_\alpha \frac{\vec{p}^{\,2}_{n\alpha}}{2m_\alpha} + \sum_{\alpha\neq\alpha'} V_{\alpha\alpha'} + \sum_{i,\alpha} V_{i\alpha}. \qquad (40)$$

In eq.(40): the double-script terms refer to the Coulomb interactions; the Latin letters refer to the electrons while the Greek letters refer to the atomic nuclei.

A molecule of a given chemical kind is a unique entity that, as a quantum system, is described by the unique Hilbert state space, unique Hamiltonian and unique quantum state in every instant in time. With this in mind, the indices that appear in eqs. (35)-(40) emphasize the structures of a single molecule, not the different molecules. Below, we point out relations between the different structures of a single molecule.

By grouping the electrons one can obtain the structural change, $\mathcal{S}_{QCM} \to \mathcal{S}_{SSM}$. This can be achieved by joining Z_i electrons with the ith atomic nucleus, so as to obtain the ith electrically neutral atom. e.g. For the hydrogen molecule, the structure $\mathcal{S}_{QCM} = \{1e, 1p, 2e, 2p\}$ can be transformed by grouping[13] to obtain $\{(1e, 1p), (2e, 2p)\} = \{1H, 2H\}$–cf. the point (C) in Section 2.2.1. The next step may be to introduce the atomic CM and R systems: $H = CM + R$. Then the hydrogen molecule is described by the following structure: $\{(1CM, 1R), (2CM, 2R)\}$. The R-system's excitations can be described in the Fock-space representation, eq.(37)-(38). Finally, by neglecting the atomic excitations, one obtains the ChM model (structure) of the molecule.

This chain of transformations can be shortly presented as follows:

$$\mathcal{S}_{QCM} \longrightarrow \mathcal{S}_{SSM} \overset{negl-excit}{\longrightarrow} \mathcal{S}_{ChM}. \qquad (41)$$

Eq.(41) can be readily presented in the Hilbert state space structure terms.

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[13] Of course, we assume the bound states–otherwise we have free particles.

Regarding the Hamiltonian, eq.(41) can be presented as follows[14]:

$$\begin{aligned} &H_{QCM} \overset{grouping}{\longrightarrow} H_{group} = \sum_{\alpha} [T_{n\alpha} + \sum_{q_\alpha=1}^{Z_\alpha} (T_{eq_\alpha} + V^{en}_{\alpha q_\alpha}) + \sum_{q_\alpha, q'_\alpha(\neq q_\alpha)=1}^{Z_\alpha} V^{e}_{q_\alpha q'_\alpha}] \\ &+H' \overset{nontriv}{\longrightarrow} \sum_{\alpha} [T_{CM\alpha} + m_{CM\alpha}\omega_\alpha^2 x_{CM\alpha}^2/2 + T_{R\alpha} + V_{R\alpha}] \overset{excit}{\longrightarrow} \\ &H_{SSM} = \sum_{\alpha} [T_{CM\alpha} + m_{CM\alpha}\omega_\alpha^2 x_{CM\alpha}^2 + H_\alpha^{ex}] \overset{negl-excit}{\longrightarrow} H_{ChM}. \end{aligned} \tag{42}$$

In eq.(42), "α" enumerates the atoms, while H' contains interactions between the constituents of the different atoms. There are exactly decoupled CM and R systems for every atom, while the H' is the origin for the (effective) harmonic potentials for the atoms. The terms in eq.(42) are simplified since we do not take into account the electrons that are shared by the neighbor atoms. Of course, there may be some corrections to the exact harmonic potential that are not made explicit in eq.(42). Stating eq.(42) in the more rigorous form does not alter our main observations.

Compare the H_{group} from eq.(42) with the H_{QCM} eq.(40). For the QCM structure, all the electrons, by definition, are subject to the Pauli exclusion principle. However, for the H_{group}, the Pauli exclusion principle applies exclusively to the electrons belonging to the same atom.

Quantum state of Z electrons in the QCM structure is the following Slater determinant:

$$|\Psi\rangle_{molecule} = \frac{1}{\sqrt{Z!}} \begin{vmatrix} |\Psi_1\rangle_1 & |\Psi_2\rangle_1 & ...|\Psi_Z\rangle_1 \\ |\Psi_1\rangle_2 & |\Psi_2\rangle_2 & ...|\Psi_Z\rangle_2 \\ & & \\ \dots & & \\ |\Psi_1\rangle_Z & |\Psi_2\rangle_Z & ...|\Psi_Z\rangle_Z \end{vmatrix} \tag{43}$$

However, for the electrons-system of the αth atom, the Slater determinant

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[14] See Supplement for some details.

reads as:

$$|\Phi\rangle_\alpha = \frac{1}{\sqrt{Z_\alpha !}} \begin{vmatrix} |\Psi_1\rangle_1 & |\Psi_2\rangle_1 & ...|\Psi_{Z_\alpha}\rangle_1 \\ |\Psi_1\rangle_2 & |\Psi_2\rangle_2 & ...|\Psi_{Z_\alpha}\rangle_2 \\ \\ \dots & & \\ |\Psi_1\rangle_{Z_\alpha} & |\Psi_2\rangle_{Z_\alpha} & ...|\Psi_{Z_\alpha}\rangle_{Z_\alpha} \end{vmatrix} \tag{44}$$

For noninteracting atoms, the total electrons system state is simply tensor product:

$$|\Phi\rangle_{molecule} = \otimes_\alpha |\Phi\rangle_\alpha, \quad Z = \sum_\alpha Z_\alpha. \tag{45}$$

The point to be emphasized is that:

$$|\Psi\rangle_{molecule} \neq |\Phi\rangle_{molecule}. \tag{46}$$

Correlations of identical particles are so specific, that $\sum_i c_i |\Phi_i\rangle_{molecule} \neq |\Psi\rangle_{molecule}$, where $|\Phi_i\rangle_{molecule}$ is of the form of eq.(45) for every index i.

Needless to say, eq.(43) is reducible to eq.(45). So, $\mathcal{S}_{QCM}$ is the most general and the most fundamental [non-relativistic] model of molecule.

Of course, this generality of the QCM structure does not imply that the QCM structure is reducible onto the other structures *in the sense* of the point (C) of Section 2.2.1. To this end, only the SSM structure, eq.(37), is reducible to the QCM structure via decomposing the atoms, and is also reducible to the ChM structure by neglecting the electrons system.

It is important to stress: *a huge amount of information is lost* in transition from the QCM to the SSM structure. Already at the first step of grouping, certain electrons correlations are lost, cf. eq.(46). By introducing the atomic CM and R systems, correlation of the electrons and the atomic nuclei is lost. Thereby, as distinct from the QCM structure, for the SSM structure there is no hope for obtaining the molecule configuration change (transformation) via influencing the atomic internal degrees of freedom–some external action that could couple the CM and the R degrees of freedom is needed. So, the following question is in order: *to what extent the conclusions obtained for one molecule structure can be applied to another structure?* A partial answer will be given in Section 4.3.

4.2 The protein folding problem

Protein molecules are large–of the mass in the interval $10^4 - 10^9$ a.m.u. (atomic mass units). There is really a huge number of the possible geometric shapes for proteins. Interestingly, biochemists claim that there exists a special, globular shape, the so-called ”native” shape of a molecule, that is biologically active. Non-globular (”degenerate” shape) protein configurations are biologically inactive, ”dead”, or even toxic. Transition from the non-native to the native form (conformation) is the protein folding problem (PFP).

In living organisms, protein molecules are suspended in water. Therefore, it is expected that their dynamics is non-trivially influenced by interaction with the solvent molecules. For a single molecule, the structures considered in Section 4.1 are global, while for a molecule suspended in a solution, the structures are local (the transformations of variables do not include the solvent-molecules degrees of freedom).

PFP is fairly described by the so-called Levinthal paradox (Levinthal 1968): If a single protein molecule is going to be folded by sequentially sampling of all possible conformations[15], it would take an astronomical amount of time to do so, even if the conformations were sampled at a rapid rate (on the nanosecond or picosecond scale). Based upon the observation that proteins fold much faster than this, Levinthal then proposed that a random conformational search does not occur, and the protein must, therefore, fold through a series of meta-stable intermediate states. This kinetic picture of the protein folding is at the core of the modern approach (Dill and Chan 1997).

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[15] For simplicity, we further interchange the use of [molecule] ”shape”, ”configuration” and ”conformation”. Terminological subtlety is of no importance for our considerations.

PFP traditionally refers to the ChM molecule structure, Section 4.1. A molecule is imagined as a random coil that should fold in a sequence of some well defined conformation changes. The quantum mechanical counterpart does not seem to be much more useful for resolving the PFP. In the next section we briefly review some classical approaches, and emphasize the kinetic nature of the problem. In Section 4.2.2 we briefly describe a new, quantum-decoherence based paradigm that refers to the quantum chemistry molecule structure.

4.2.1 The statistical-thermodynamic approach

The ChM structure is of interest. The point-like-atoms' equilibrium-positions form a three-dimensional lattice. Regarding the large molecules, "conformation" is a lattice with the fixed (average) distance between the adjacent atoms and the fixed (average) angles between the adjacent lattice segments. For every change of conformation it is assumed *not* to change the distances and the angles–conformal transformations.

Protein folding is defined as a series of local rotations that sequentially change the molecule's shape. Even for small protein molecules, the number of combinations of local rotations is huge. It is not expectable that a molecule quickly find the native conformation–the Levinthal paradox.

The most of the current research on protein folding considers an ensemble of molecules suspended in a solution at fixed temperature. Related methods provide powerful means for determining conformations even for the very large protein molecules. Some computational methods are based on the assumption that the native state is very stable–it can be imagined as a minimum of the configuration-energy landscape. While all of these methods can provide *existence* of the native conformation (as well as, in general, some metastable conformations), the PFP problem, as stated by Levinthal, is more subtle–it's *kinematic*. As (Dill and Chan 1997) strongly emphasize: the PFP is *not* merely about existence of the (meta)stable conformations, but rather about the possible configuration transitions within the classical configuration space of a *single* molecule.

Even the kinetic approach does not challenge the basic strategy stemming from the classical ChM molecule structure: for a single molecule it is supposed that there is a *pathway* ("trajectory") in the molecule conformation space, while in every instant in time a molecule has a definite geometrical form. In addition, internal degrees of freedom of molecule are neglected, and are sometimes treated as un-necessary complication. The approach (Dill and Chen 1997) is still in a purely qualitative form.

4.2.2 A quantum decoherence approach

Quantum mechanical approach introduces the atomic internal degrees of freedom into consideration. To this end, the results that can be obtained for the SSM or QCM structure are in principle not achievable on the basis of the ChM structure. So, partial answer to the above question (cf. Section 4.1) reads as: there is a lot of information about the folding mechanism that are inaccessible within the ChM-based approach.

To see richness of the SSM and QCM structures compared to the ChM structure, we recall and extend what is told in Section 4.1. Both the SSM and especially the QCM structure provide a basis for the electrons-system-mediated change of conformation. To this end, it is well known that the molecule fluorescence and phosphorescence are phenomena closely related to protein folding. On the other hand, quantum mechanical approach, in principle, does not allow a definite pathway in the configuration space of the molecule. This may be a hint for avoiding the Levinthal paradox.

However, there is more subtlety to the quantum mechanical approach to PFP. Ever since Hund's remark (Hund 1927), it is a foundational issue of the whole of chemistry: how do the definite, the classical-like, stable molecule configurations appear from the quantum mechanical substrate? Furthermore, if quantum mechanics can provide protein conformation as a classical-like stable characteristic, one can wonder if it may happen that, after all, the configuration transitions are inevitably classical–i.e. that follow some special pathways in the configuration space?

In the remainder of this section we offer answers to both questions, *in* the context of the QCM molecule structure. The answers are due to the process of quantum decoherence: *both* configuration stability and transitions can be naturally [but purely qualitatively] described (Jeknić-Dugić 2009a). This way both, the Hund's and the Levinthal paradox, are resolved.

The QCM structure is defined by eq.(40). Here we apply the standard adiabatic approximation to the following variation of the QCM structure: $\mathcal{S}'_{QCM} = \{E, N\}$, where E stands for the electrons, and the N for the system of atomic-nuclei. This bipartition helps us straightforwardly to introduce the CM and R degrees of freedom for the later: $N = CM_N + R_N$. The set of the relative atomic-nuclei positions, $\vec{\rho}_{ij} = \vec{r}_i - \vec{r}_j$ can be further decomposed. Actually, the set $\{\vec{\rho}_{ij}\}$ can be divided into two subsets, which define the rotational (Rot_N) degrees of freedom and the internal, the conformation (K_N), degrees of freedom.

So, a molecule is defined by the following factorization of the Hilbert space:

$$\mathcal{H} = \mathcal{H}_E \otimes \mathcal{H}_{CM_N} \otimes \mathcal{H}_{Rot_N} \otimes \mathcal{H}_{K_N}. \tag{47}$$

The related form of the molecule Hamiltonian[16]:

$$\begin{aligned} H_{QCM} = \sum_i \frac{\vec{p}^2_{ei}}{2m_e} + \sum_{i \neq j} V_{ij} + T_{CM_N} + T_{Rot_N} + T_{K_N} + \\ V_{E,CM_N} + V_{E,Rot_N} + V_{E,K_N} + V_{Rot_N,K_N}. \end{aligned} \tag{48}$$

where, as usually, the double subscripts distinguish the interaction terms; the T denoting the kinetic energy terms and the index E standing for the total electrons system.

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[16] See Supplement for details.

Compared with the standard QCM structure, $E + N$, our approach has the following virtues. First, cf. Section 4.3 below, it can be directly compared with the ChM and the SSM structures. Second, there are at least three different channels of the environmental (the solvent) influence on K_N–the last two interaction terms in eq.(48) provide the possible "channels" for influencing the molecule conformation. Third, one can easily apply the standard adiabatic approximation to the structure eq.(47). Fourth, on this basis, one can define the electrons positions to be measured from the CM_N system as the reference system. Classically, the $\vec{r}_{CM_N}$ is a c-number, not a dynamical variable; so, rigorously, the electrons variables presented formally as the operators acquire the form: $\hat{\vec{r}}_{ei} - \vec{r}_{CM_N}\hat{I}$. The quantum mechanical reference frames will be considered in Chapter 8. Due to the presence of the electrons, the CM_N and R_N systems are in mutual interaction[17].

The following masses are implicit in the kinetic-energy terms in eq.(48): the electron mass m_e, the CM_N mass M, the rotational moment of inertia ${I_{Rot_N}}$[18], and the "reduced masses" $\mu_{K_N i}$. Now it is easy to show that the adiabatic parameter $\kappa = max\{m_e/M, m_e/I_{Rot_N}, m_e/\mu_{min}\} \sim m_e/\mu_{min} < 10^{-3}$, where μ_{min} is the minimum "reduced mass"–of the order of the minimum nucleus-mass. Physically it means that, like for the standard QCM structure, $E + N$, one can adiabatically cut off the electrons system from the rest of the molecule.

In the zeroth order of approximation, when dynamics of the non-electronic degrees of freedom is "frozen", the Hamiltonian eq.(48) reduces to the electrons-system's Hamiltonian:

$$H_E = \sum_i \frac{\vec{p}_{ei}^{\,2}}{2m_e} + \sum_{i \neq j} V_{ij} + V(CM_N) + V(E, Rot_N) + V(E, K_N) +$$
$$V(Rot_N, K_N) \approx \sum_i \frac{\vec{p}_{ei}^{\,2}}{2m_e} + \sum_{i \neq j} V_{ij} + V(Rot_N) + V(K_N). \qquad (49)$$

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[17] This coupling is absent for the atomic CM and R of the *total* atom.

[18] Properly expressed in the mass units.

The terms on the rhs of eq.(49) represent the effective external classical fields for the electrons system[19]. We assume that the CM_N system will not affect the electrons, at least as long as adiabatic approximation is satisfied.

The electrons-system Hamiltonian eq.(49) gives rise to the zeroth order Schrödinger equation:

$$H_E|\phi_n(K_N)\rangle_E = E_n(K_N)|\phi(K_N)\rangle_E. \tag{50}$$

In eq.(50), we keep only dependence on the conformation, K_N, since it defines spatial configuration of the positively charged atomic nuclei. Tentatively neglecting the Rot_N and CM_N systems, the zeroth order form of the molecule quantum state reads as:

$$|\phi_n(K_N)\rangle_E \otimes |K\rangle_N + |O(\kappa)\rangle, \tag{51}$$

Just like in eq.(21), there is entanglement–for the E and K_N systems.

Now dynamics of the K_N system is adiabatically defined by the effective (”average”) Hamiltonian (Gribov and Mushtakova 1999):

$$H_{K_N} =_e \langle\phi_n(E_n(K_N))|H_{QCM}|\phi_n(E_n(K_N))\rangle_e. \tag{52}$$

Intuitively, eq.(52) describes what the K_N system can ”see” of the fast electrons-system dynamics. Without delving into details, we emphasize: the energy eigenvalue for the fixed quantum number n, $E_n(K_N)$, represents an effective potential-energy (hyper)surface for the configuration system. It is usually assumed that there are certain depressions (the local minimums) in the potential energy landscape that would correspond to the phenomenologically observed stable conformations (Gribov and Mushtakova 1999, Atkins and Friedman 2005). Of course, the number of such local minimums (the stable conformations) is enumerable $(K_{N1}, K_{N2}, ...)$ for every n.

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[19] The fixed atomic nuclei positions enter as the fixed parameters in eq.(49).

Conformation dynamics generated by the Hamiltonian eq.(52) is usually imagined as conformational *vibrations* (oscillations) in the vicinity of a local minimum of the conformation-energy hypersurface. Given that the weak V_{K_N,Rot_N} interaction can be considered as a perturbation, the *exact* form of the molecule state is of the form[20]:

$$|\Phi\rangle_{molecule} = |\phi_n(K_N)\rangle_E |K\rangle_N |\chi\rangle_{Rot_N} |\phi\rangle_{CM_N} + |O(\kappa)\rangle_{E,K_N,Rot_N,CM_N}. \tag{53}$$

So, if one deals with the first (the dominant) term on the rhs of eq.(53), the adiabatic method guarantees that he will obtain the results with an error not larger than $\kappa^{3/4} \ll 1$.

But this is strange, since neither the exact state eq.(53) nor its dominant term are eigenstates of the molecule Hamiltonian eq.(48). In the dominant term, the conformation state $|K\rangle_N$ is the molecule-conformation eigenstate. Bearing in mind that $[H_{QCM}, K_N] \neq 0$, one may say that the adiabatic approximation provides a partial answer to the Hund's paradox (Hund 1927). Nevertheless, the adiabatic "mechanism" is not sufficient for this purpose (Gribov and Magarshak 2008, Dugić and Jeknić-Dugić 2009a).

On the other hand, for the stable classical-like conformations, one may wonder if *any quantum-mechanical mechanism can provide the finite-time conformational transitions*–the Levinthal paradox (Levinthal 1968)?

Interestingly enough, the following plausible stipulations provide a coherent and rather general background for answering both questions. The stipulations are phenomenologically inspired: typical experimental investigations are performed on an ensemble of molecules in a solution (e.g. in water). In this new context both the Hund's and the Levinthal paradoxes are resolved (Jeknić-Dugić 2009a)[21].

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[20] Integrating over the electronic degrees of freedom in eq.(52) turns all the electrons-system's couplings [appearing in eq.(48)] with the rest into the external fields, and the only remaining interaction term is the V_{K_N,Rot_N} term.

[21] http://www.verticalnews.com/premium-newsletters/Journal-of-Physics-Research-/2009-03-31/71094PR.html.

Stipulation 1. *For every* stationary *state of the composite system "[ensemble of] molecules + solution", the solution acts as a decoherence-inducing environment for the molecule conformation system K_N.*

Stipulation 2. Non-stationary *state of the "[ensemble of] molecules + solution" system does not preserve molecular conformations. Every non-stationary state terminates by a stationary state.*

If there is not any severe external influence on the "molecules+environment" system, then we say the system is in stationary state. "Non-stationary" means the opposite, i.e. the different ways the composite system can be disturbed, e.g., by heating, by intense illuminating, by adding new solvent (this can change the solution pH value) etc. Both "stationary" and "non-stationary" are *phenomenologically* inspired. By definition, "stationary state" is a state (or, physically, a set of states) that follows from some kind of the environment relaxation. For large environment, this can be thermodynamic equilibration.

The stipulations do not prejudice either the decoherence mechanism or the asymptotic ($t \to \infty$) relaxation into a (possibly unique) stationary state of the open system, K_N. The initial and the final (non-asymptotic) stationary states may be physically totally different, *except* in that that they should provide the occurrence of decoherence for the K_N system.

Stipulation 1 establishes: arbitrary initial state of the molecule conformation quickly becomes a mixture of conformations:

$$\rho_{K_N} = tr_{E,CM_N,Rot_N}\rho_{molecule} = \sum_i p_i |k_i\rangle_{K_N}\langle k_i|. \tag{54}$$

Every "stationary state" is described by eq.(54). Of course, the sum in eq.(54) can sample different sets of conformations for different stationary states.

Now, according to Stipulation 2, external influence does *not* preserve the states in the form of eq.(54). Even more, one can expect that external influence (giving rise to "non-stationary state") provides a time dependent state

$\rho'_{K_N}(t)$, such that:

$$[\rho'_{K_N}(t), \rho'_{K_N}(t')] \neq 0, \quad t \neq t'. \tag{55}$$

Totally independently of the non-stationary state dynamics[22], relaxation into another stationary state provides [Stipulation 1] the final conformation-system state, ρ''_{K_N}, of the general form of eq.(54)[23]. Therefore, the total dynamics of the open system can be described as follows:

$$\rho_{K_N} = \sum_i p_i |k_i\rangle_{K_N} \langle k_i| \rightarrow \rho'_{K_N} = \sum_i \pi_i |\chi_i\rangle_{K_N} \langle \chi_i| \rightarrow \rho''_{K_N} = \sum_i q_i |k'_i\rangle_{K_N} \langle k'_i|, \tag{56}$$

where: $\sum_i p_i = 1 = \sum_i q_i$, $|\chi_i\rangle = \sum_j c_{ij}|k_j\rangle$, and $[\rho, \rho'] \neq 0 \neq [\rho', \rho'']$, but $[\rho, \rho''] = 0$. The final state (ρ'') can mix the conformations that are not present in the initial state (ρ), while the statistical weights for the common conformations need not be equal for the initial (ρ) and the final (ρ'') state; i.e. $p_i \neq q_i$ for at least some index i.

This possibility of appearance of the new conformations, as well as of the different probabilities for the common conformations for the initial and the final conformation-system state, is the *decoherence-based model of the conformation transitions* in large molecules.

So, Stipulation 1 provides an answer to the Hund's paradox. On the other hand, both Stipulation 1 and Stipulation 2 provide a general basis for the conformational transitions, eq.(56). The time needed for such transitions is of the order of the "decoherence time" thus not leaving room for the Levinthal paradox.

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[22] Except if one assumes nonrealistic scenario that the external influence preserves the conformation-system state.

[23] This is a direct consequence of the fact that decoherence is a quantum measurement performed by the environment on the open system. The final state is a mixture of the measured-observable eigenstates. Here it's the molecule conformation that is measured.

4.2.3 Overview

The approach presented in Section 4.2.2 is purely qualitative. But this is, as yet, unavoidable–the composite system of interest is too complicated. This is also the case with the classical-physics approach (Dill and Chen 1997).

As distinct from the classical models, the model of Section 4.2.2 does not leave room for the classical pathways in the molecule configuration space, while there are different "channels" for the conformation transitions. The adiabatic approximation provides the local minimums on the energy hypersurface as the preferred, the decoherence-distinguished stable conformations–an answer to the Hund's paradox. The fast decoherence process dissolves the Levinthal paradox.

From the quantum mechanical point of view, while the occurrence of decoherence is expected for the conformation system (Stipulation 1), a rigorous proof of this expectation is virtually intractable. To this end, a part of the difficulties[24] will be presented and discussed in Chapters 6 and 7. Here we finish our considerations by comparing the approach of Section 4.2.2 with some similar models/approaches in the literature.

(Gelin et al 2011) derive a master equation for a molecular aggregate in contact with the heat bath. Their model is similar to the model of Section 4.2.2, yet with simplification of identical constituents of the aggregate. Adiabatic approximation is implicit to their model, which couples the aggregate's CM system (but not the conformational system) with the environment. In effect, they obtain a basis for the CM-system's quantum Brownian-like motion, while the internal degrees of freedom remain purely quantum mechanical. This result is a consequence of a number of approximations, notably of the assumption that all the constituents are mutually identical (chemically and physically). Due to the absence of solutions to the master equation, they do not tackle either the Hund's or the Levinthal paradox.

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[24] The main difficulty is the fact that the protein molecules in the living biological cells are far from the thermodynamic equilibrium.

In a recent paper (Luo and Lu 2011), the authors consider the quantum mechanical transitions of the protein conformations for the different temperature regimes. The QCM molecule structure is of interest. This approach regards the thermodynamic description (Section 4.2.1) while assuming existence of the definite (the initial and the final) conformation. So, they don't even tempt to answer the Hund's paradox.

On the other hand, recent papers (Trost and Hornberger 2009, Bahrami et al 2012) consider the Hund's paradox for the quantum-mechanical counterpart of the ChM structure, but exclusively for the *small*-molecules chirality, while leaving the configuration transitions issue (and the Levinthal paradox) intact. Complexity of the occurrence of decoherence for small molecules suggests virtual intractability of the same issue for the large molecules (Stipulation 1). A similar quantum mechanical approach to Hund's problem can be found in (Jona-Lasinio and Claverie 1986, Amann 1991). Therein, interaction with the environment is *designed* so as to provide decoherence, while the microscopic and structural considerations are completely left out. The authors don't even try to describe the configuration transitions.

4.3 Quantum structures in context

Probably the main lesson of Section 4.2.2 is a need for a proper selection of the degrees of freedom (of a subsystem of a composite system)–the conformation K_N system can be compared with the molecules conformation-systems for the ChM and SSM models. This is achieved by performing the proper LCTs in conjunction with adiabatic approximation. Notice that the LCTs are applied *locally* to the system of atomic nuclei by introducing the CM_N and R_N subsystems, and then by the "fine graining" of the R_N system to introduce the Rot_N and K_N subsystems: $\{1n, 2n, ...\} \to \{CM_N, R_N\} \to \{CM_N, Rot_N, K_N\}$.

There is a chain of the molecule-structure transformations (compare to eqs.

(41), (42))[25]:

$$\mathcal{S}_{QCM} = \{1e, 1n, 2e, 2n, ...\} \overset{electrons-grouping}{\longrightarrow} \{1E, 1n, 2E, 2n, ...\} \overset{nontrivial}{\longrightarrow} \{1CM, 1R, 2CM, 2R, ...\} \overset{introd-excit}{\longrightarrow} \mathcal{S}_{SSM} = \{1CM, 1ex, 2CM, 2ex, ...\} \overset{negl-excit}{\longrightarrow} \mathcal{S}_{ChM} = \{1, 2, ...\}. \quad (57)$$

Every step in eq.(57) is subject to quantum correlations relativity, Section 3.2. So, there is not direct transition of conclusions from one to another structure. Nevertheless, due to the small mass ratio m_e/m_n, the atomic center of mass is close to the atomic nucleus position (e.g. $1n \approx 1\text{CM} \approx 1$ for the structures appearing in eq.(57)). Bearing this (i.e. eq.(53)) in mind, we can hope, that Section 4.2.2 provides a qualitatively useful description of the conformation stability and transitions also for the ChM and SSM structures. However, this conclusion does not directly apply to the electrons system–cf. eq.(46)–as well as to channelling the conformation transitions.

From eq.(53) we can see, that the external influence exerted on the electrons system E, or on the rotational degrees of freedom Rot_N, can also influence the molecule conformation K_N system. The details regarding the preferred configuration states (the configuration "pointer basis") as well as a scenario regarding the electrons-system mediated configuration transitions can be found in (Jeknić-Dugić 2009a,b).

On the other hand, from eq.(42), the only way indirectly to influence conformation for the SSM structure, is, to externally induce interaction between the $\{CM_\alpha\}$ and the excitation systems (Caspi and Ben-Jacob 2000). Even this possibility is absent for the ChM model, for which the only way to change conformation is directly to target the conformation system (Jona-Lasinio and Claverie 1986, Amann 1991).

Our considerations do not exhaust the list of the possible molecule struc-

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[25] Of course, $1E + 1n = 1CM + 1R = 1CM + 1ex$ are the different decompositions of the one and the same atom denoted 1.

tures[26], neither the list of the possible ways to manipulate the molecule degrees of freedom. Similarity of the effects as well as the quantum correlations relativity, Section 3.2, suggest that the realistic experimental situations are hardly structurally as clear and neat as our (idealized) theoretical formulations.

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[26] Subtlety of the molecular structures are also presented in (Michal Svrček, 2012). Regarding the foundations and limits of the adiabatic approximation, see (Gribov and Magarshak 2008, Dugić and Jeknić-Dugić 2009a).

Chapter 5

Realistic Physical Structures

It is a universal physical fact: of a composite system, only a fraction of the degrees of freedom is practically accessible (Giulini et al 1996, Zurek 2003, Schlosshauer 2004, Nielsen and Chuang 2000). The classical, macroscopic bodies are described by their spatial shape and orientation. In formalism, those are the "collective" variables of the center of mass and the Euler angles. Internal degrees of freedom are not directly observable and provide a basis for the macroscopic-bodies temperature and radiation.

Quantum mechanical systems (atoms, molecules etc.) are also described by the center-of-mass and the relative-positions degrees of freedom. These degrees of freedom are presented by eq.(4) and by the rhs of eq.(5). Manipulating these degrees of freedom makes them realistic in the operational physical sense. Bearing Chapters 2 and 3 in mind, in this chapter, we provide a fresh view of some well known experimental situations and we highlight *operational reality* of the CM and R degrees of freedom.

5.1 Relativity of "local operations"

The concept of "structure" assumes locality of the subsystems degrees of freedom. Manipulating the subsystems degrees of freedom assumes their (local) accessibility.

"Locality" is structure dependent, Section 2.4 (not necessarily incorporating the relativistic locality). "Local operation" assumes *non-disturbance of the* *rest*, which is a part of the same structure of the composite system. In quantum information science, "local operations" are presented e.g. by the so-called "local operations and classical communication" (LOCC) procedures. Formally, local operations are defined by the "single-particle" operators of the form $A \otimes I$. e.g. The center of mass position, X_{CM}, eq.(4), takes the form $X_{CM} \otimes I_R$ relative to the $CM + R$ structure, *but* for the $1+2$ structure, it takes the form $(m_1/M)x_1 \otimes I_2 + (m_2/M)I_1 \otimes x_2$. So for the $CM + R$ structure, X_{CM} is a local, while for the $1+2$ structure, it is a "collective" ("composite") observable. Direct measurement of X_{CM} is supposed not to disturb the R system, while partially disturbing both the 1 and 2 systems. On the other hand, X_{CM} can be indirectly measured by directly measuring x_1 and x_2, and then, according to eq.(4), to calculate X_{CM}. However, due to eq.(4), such measurement provides information also about the R system and is therefore not local. The told equally refers to arbitrary observable of the composite system. For instance, x_1 can be indirectly measured by directly measuring X_{CM} and r_R. Therefore, the concept of "local observable/operation" as well as of the "composite observable/measurement" is structure dependent–the electron's position $\vec{r}_e$ in the hydrogen atom is a collective observable *relative* to the atomic $CM + R$ structure. Formally, there is nothing "more local" regarding the electron's position, $\vec{r}_e$, than regarding the CM position, $\vec{R}_{CM}$.

Whether an observable is accessible to measurement in a given physical situation is a separate question (Zanardi 2001, Harshman 2012a). Here we adopt the following:

Def.5.1 "Accessibility" *of an observable of a system assumes a measurement procedure, which does not make use of any indirect measurement, i.e. measurement of other observables of the system.*

Inaccessibility of a macroscopic-system center-of-mass is at the root of the classical prejudice on the transformations of variables, Section 2.1. e.g. For the classical systems, the formal CM system pertains to an empty point in space, not to a physical object[27].

The most of the realistic quantum measurements employ detection of quantum particles. e.g. In atomic and molecule spectroscopy, the photon field is accessible (directly measured, detected). This detection provides an (indirectly acquired) information about the atomic (molecule) internal energy and state. This is a local operation relative to the atomic $CM + R$ structure, but is a global operation relative to the $e + p$ structure. Mechanism of quantum measurements, even the simplest ones, is not yet known. So Def.5.1 does *not* refer to such details. Rather, Def.5.1 assumes, that measurement of an observable does not assume or reveal the values of the observables[28] of any other system. Hence ”accessibility” requires locality of measurement but is more stringent: it also requires absence of information about any other observable.

Accessibility (direct measurement) of the hydrogen-atom's electron's and the proton's positions, $\vec{r}_e$ and $\vec{r}_p$, provides indirect measurement of the atomic CM and R positions. This is, of course, a local operation relative to the atomic $e + p$ structure, but is a global operation relative to the $CM + R$ structure. So we emphasize the following universal physical fact: accessibility of an observable of a quantum system is a matter of a *specific physical situation*, which is defined by the choice of the ”apparatus” and of its initial state. An example of accessibility, which is determined by the environment characteristics, can be found in Section 7.3.

The concept of locality now emphasizes subtlety of the concept of ”multi-particle entanglement (correlation)” (Brus 2002, Facchi et al 2006, Wichterich 2011, Bellomo et al 2011). Consider a system $\mathcal{C}$ of N non-identical particles. Its Hilbert state space $\mathcal{H} = \otimes_i^N \mathcal{H}_i$ and the state $|\Psi\rangle = \sum_{i_1,i_2,\dots i_N} C_{i_1 i_2 \dots i_N} \otimes_{j=1}^N |\phi_{i_j}\rangle_j$; $|\phi_{i_j}\rangle_j$ is the ith state of the jth particle. A bipartition $\mathcal{C} = A + B$

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[27] You cannot move a pair of apples by hitting their center of mass. In order to measure the apples CM position, you need to perform measurement of the apples' positions, and then to calculate the apples CM position.

[28] All but those that can be trivially linked with the measured one.

determines the factorization $\mathcal{H}_A \otimes \mathcal{H}_B$ and the state $|\Psi\rangle = \sum_i c_i |i\rangle_A |i\rangle_B$, which is given in the Schmidt canonical form. The point to be emphasized: bipartition $A + B$ is comparable with a pair of unstructured particles. In other words: there is no *a priori* more entanglement in the $A + B$ structure than in a state $|\Psi\rangle = \sum_i c_i |i\rangle_1 |i\rangle_2$ for a pair of unstructured particles 1 and 2. However, this similarity fades if the A's and B's structures are taken into consideration. In this case, the task of "multi-particle correlations" refers to the correlations of a numerous set of particles belonging to the different partitions (A and B, respectively).

Measurements of observables that are local *relative* to the structure of interest may reveal quantum correlations in *that* structure. So, e.g., measurement of an observable $\hat{A}$ that is sensitive to the A-block's structure is not necessarily useful for detecting entanglement for the $A+B$ partition (regarding the above Schmidt form, $|\Psi\rangle = \sum_i c_i |i\rangle_A |i\rangle_B$). Detecting "multi-particle" entanglement refers to entanglement between the *pairs of particles*, 1 and 2, which belong to A and B, respectively.

Hence, relativity of the concept of locality calls for caution: in order for the observable $\hat{A}$ be insensitive to the A's structure, it must be "collective observable" *relative* to the *constituent particles* of the A system. Whether the $\hat{A}$ observable pertains to another structure of the composite system $\mathcal{C}$ is irrelevant[29].

5.2 Manipulating the center of mass

The most of the realistic manipulations of the atomic species refer to the atomic $CM + R$ structure, see e.g. the rhs of eq.(58). In this section we are interested in actions that can be clearly expressed in terms of the atomic/molecule CM system–which includes the actions not affecting the

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[29] Plenty of the observables, e.g. the Hamiltonian, are "absolutely collective (non-local)", in the sense that they cannot be local for any partition. However, "insensitivity to structure" is subtle and poses the following question: are there "intensive" quantum observables, which are both "absolutely non-local" *and* structure insensitive?

atomic R system. Of course, such actions are precluded in the classical physics realm [see Footnote 27].

"*Two types of degrees of freedom have to be considered for an atom: (i) the internal degrees of freedom, such as the electronic configuration or the spin polarization, in the center-of-mass reference frame; and (ii) the external degrees of freedom, i.e. the position and momentum of the center of mass of the atom.*" (Cohen-Tanoudji and Dalibard 2006).

Electromagnetic forces and trapping (of charged or neutral particles), atomic laser and lithography, atomic interferometry, refer to the atomic CM system. For certain purposes, one can forget[30] about the internal degrees of freedom and consider an atom as a point-like particle with the total (center-of-mass) atomic mass M[31]. Temperature of an atomic gas (in thermal equilibrium) is defined by statistical distribution of the atomic-CM momentums (velocities)–the internal atomic structure is not of interest. Nevertheless, this picture is strict only for a gas of atoms on sufficiently high (e.g. room) temperature. For lower temperatures, the atomic CM system can be described e.g. by a wave packet (rather than by a point-like particle)–the quantum effects become relevant. This is still a particle-like description of the atoms in a gas. Temperature of the gas defines the average the de Broglie wavelength of the atomic CM systems–thus providing a quantitative criterion for the particle-like versus the wave-like behavior of the atomic CM systems. At sufficiently low temperature one can no longer distinguish the individual-atoms' center-of-mass systems from each other–e.g., in the Bose condensate, the CM systems of all atoms have the same wave-function.

Conceptually the same physical basis apply to the cooling of molecules: a molecule gas is cooled if the molecules center-of-mass systems are sufficiently slow in the laboratory reference frame (M. Zeppenfeld et al 2012)–there are no specific conditions that are imposed for the atomic internal degrees of

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[30] Of course, ignorance about some degrees of freedom is not equivalent with the locality of measurement, Section 5.1.

[31] See the ChM molecule model in Section 4.1.

freedom.

Experimental observation of diffraction and decoherence of *large molecules* is striking an effect (Hackermuller et al 2003, Hackermuller et al 2004). An obvious motivation for doing experiments with matter waves is the everyday experience that physical bodies do not at all spread out like waves; rather they have a well-defined position whenever they are observed. Of course, the center-of-mass position is of interest.

Micro- and nano-mechanical resonators are macroscopic systems–they can be seen with the naked eye. Nevertheless, center of mass of these systems can be modelled as a harmonic oscillator, which can undergo the quantum Brownian motion dynamics (Gröblacher et al 2013)[32]. Indirect observation of the CM dynamics can reveal non-Markovian characteristics of the environment, which monitors the CM system. Although the study is performed at room temperature, it can be directly applied to other mechanical resonators that operate close to the "quantum regime".

5.3 Manipulating the relative positions

In this section we consider the physical situations that can be clearly described in terms of the atomic/molecule R system–which includes the situations in which the corresponding CM system is not affected. Direct manipulating the internal degrees of freedom cannot be even defined in classical mechanics [see Footnote 27].

Typically, internal degrees of freedom are indirectly observed–e.g. by detecting the emitted radiation. This detection is all about the atomic/molecule *spectroscopy*. Atomic (molecule) excitation and de-excitation can be considered without taking the CM system into account. This, however, is not the only possibility. Accessibility (direct measurement, Def.5.1) of the "relative" degrees of freedom has recently been theoretically (Rau et al 2003, Dunningham et al 2004) and also experimentally (Maeda et al 2005) considered.

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[32] See Section 6.3.2 for some technical details.

In (Rau et al 2003), the authors come to the following conclusion:

"*Thus, we have a consistent definition of relative position that implies that relationships between objects, rather than coordinates and absolute variables, are fundamental in the quantum world.*"

Furthermore, they extend their observation for every pair of mutually conjugate observables: "*This suggests that some form of entanglement-driven localization might occur for any pair of relative conjugate observables.*". In (Dunningham et al 2004), physical reality of the relative position is claimed:

"*We have discussed how light scattering from delocalized quantum particles can lead to the emergence of 'classical' relative positions. This process occurs even though the absolute positions of the particles remain undefined and suggests that the natural spatial framework for such a system is relative position.*"

Furthermore, the authors (Dunningham et al 2004) claim non-disturbance of the particles CM system. That is, they consider a purely local action exerted on the R system.

In an experiment targeting the "atomic electron orbit", (Maeda et al 2005), the authors say:

"*Nonetheless, our intuitive picture of an atom is an electron moving in a Kepler orbit about an ionic core.... Using picosecond or femtosecond laser pulses, it is now straightforward to create wave packets of atoms of high principal quantum number n, in which the electrons move in Kepler orbits ... However, adding a small oscillating field at the orbital frequency can phase-lock the motion of the electron to the oscillatory field (5-11), such that the localization of the electron persists at least for thousands of orbits (11)–perhaps long enough to actually use these classical atoms in applications such as information processing (12).*"

While the phrases that describe the experimental findings are in terms of "electron orbits", the theoretical basis is clearly presented in terms of the atomic R degrees of freedom. Bearing in mind that, in the experiment, the atomic CM degrees of freedom are assumed to remain intact, with the aid of Section 5.1, we realize that the experiment is another instance of direct manipulation with the atomic R system.

Regarding the large-molecules species, the conformation K_N, Section 4.2.2, represents the internal degrees of freedom. These degrees of freedom are at the core of stereochemistry as well as of the foundations of the biopolymer dynamics, e.g., in the protein (un)folding and molecular recognition. Manipulation of the large-molecules conformation with light is by now a routine (Lendlein et al 2005).

5.4 Entanglement relativity in use

Entanglement relativity (or the more general quantum correlations relativity) is in direct use via "entanglement swapping" (Bennett et al 1993, Ma et al 2012), (and the references therein), and via "coarse graining" (Ragy and Adesso 2012) structural transformations. Entanglement swapping is formally a trivial kind of LCTs–regrouping of subsystems, Section 2.2.1, point (A). It is global, in the sense of Section 2.2.1, point (B). On the other hand, grouping ("coarse graining") or decomposing ("fine graining") the subsystems are also trivial but local kinds of LCTs.

In (Ma et al 2012), the authors consider an entanglement-based variant (Peres 2000) of the gedanken "delayed choice" experiment (Wheeler 1978). At first sight, it may seem that this is a delayed choice in the original Wheeler's spirit. However, this is not the case. The theoretical proposal (Peres 2000) as well as the experimental realization (Ma et al 2012) target entanglement [via entanglement swapping], rather than the individual qubits, in a system of four qubits. In the experiment it is clearly demonstrated: there is not individuality of the single qubits or of the pairs of qubits; see also (Dugić 2012). Rather, the effects due to entanglement of the different bipartitions of the system of four qubits are experimentally observed. In other words: the object of investigation is entanglement of different pairs of qubits, not the individual qubits. Depending on the choice of the pair of qubits to be measured, the remaining pair of qubits appears in entangled or in a separable pure state. Such a measurement in a later instant apparently changes the initially obtained record on entanglement of the pair of qubits. This intuitively paradoxical situation is described in the theoretical proposal (Peres 2000):

”*The point is that it is meaningless to assert that two particles are entangled without specifying in which state they are entangled, just as it is meaningless to assert that a quantum system is in a pure state without specifying that state [9]. If this simple rule is forgotten, or if we attempt to attribute an objective meaning to the quantum state of a single system, curious paradoxes appear: quantum effects mimic not only instantaneous action-at-a-distance but also, as seen here, influence of future actions on past events, even after these events have been irrevocably recorded.*”

However, once Entanglement Relativity is properly understood, the above quote can be re-phrased as follows: The point is that it is meaningless to assert that two particles are entangled without specifying the structure of interest. Even for a specified (pure) state of the system of qubits, entanglement may or may not be observed depending on the structure distinguished by the chosen (local to that structure) measurement to be performed in a later instant in time. Once again, we can say: entanglement is a structure-dependent, i.e., a relative notion.

”Coarse graining” of a composite system's structure is the ”particles grouping” kind of LCTs. Recently, a ”coarse grained” picture of the ”ghost imaging” technique has been analyzed (Ragy and Adesso 2012). The authors analyzed the nature of correlations in Gaussian light sources used for ghost imaging from a quantum informational perspective, combining a microscopic with an effective coarse-grained description. A transition from the microscopic modes a_i to the coarse grained two-mode boson operators, c_1, c_2, provides a striking observation. The findings are described as follows:

”*This reveals an interesting feature associated to the coarse-grained formalism* *put forward here. It actually indicates how the quantum nature of the light source becomes quenched as we diverge from the photon-counting regime and enter the classical limit of intensity correlations. For these high illuminations, the quantum correlations available for detection by our scheme tend to zero, and the physical model of the scheme does not require a quantum description of the light to be accurate.*"

So, the authors observe a transition from quantum to classical regime in the ghost imaging technique as a consequence of averaging of the coarse-grained structure of the light source. The authors properly interpret their finding–not yet emphasizing the quantum correlations relativity–, while not discussing a need to perform averaging of the field modes. So, this is not a solution to the problem of the transition from quantum to classical. Nevertheless, this is a very important contribution to this long-standing issue (Giulini et al 1996, Zurek 2003, Schlosshauer 2004): the observed transition is *not known for the original* (non-coarse-grained) degrees of freedom.

Both kinds of the LCTs considered are classical in spirit. In classical physics, the subsystems ("particles") are assumed to have individuality that is *not* jeopardized by the formally trivial LCTs of decomposing/(re)grouping the particles. Some groups of particles may be additionally charged by certain (local) boundary conditions to appear in bound states, like in the Chemical Model of molecules, Section 4.1. However, quantum correlations relativity, Section 3.2, substantially changes the picture as it is emphasized throughout this book. Bearing in mind the classical spirit of decomposing/(re)grouping systems, it is not surprising that this kind of LCTs is the main kind of structure transformations that are considered in the literature so far. Physical relevance of the more general ones (such as those to be presented in Chapters 6 and 7) is yet to be appreciated.

5.5 Outlook

The classically artificial, "collective", $CM + R$ structure proves itself operationally realistic in the quantum realm[33]. Laboratory manipulation makes these degrees of freedom *at least as realistic as the "fundamental" degrees of freedom of a composite quantum system.* If it were not so, we would have already been able more-or-less directly to observe the fundamental constituents of the matter.

Loss of individuality of quantum subsystems as well as quantum correlations relativity and relativity of locality, Section 2.4, provide a consistent view of this phenomenological fact. There is nothing "artificial", "collective" or "emergent" in the quantum center-of-mass and internal-degrees of freedom. Rather, physical situation defines a specific set of local degrees of freedom (and observables) that are operationally accessible. A set of such observables defines the local subsystems and related (composite system's) *operationally preferred* structure[34] (Zanardi 2001, Zanardi et al 2004, Harshman and Ranade 2011). Foundational issues on the operationally preferred structure of an open quantum system are subject of Chapter 7. Experimental confirmation of entanglement relativity gives rise to: (i) it changes our intuition on "structure", and (ii) it opens practical applications of quantum phenomena that are traditionally considered to be impossible in the classical physics realm.

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[33] Those subsystems are of general use, for the particles in bound states, as well as for the free particles.

[34] As stated in Chapter 2, we are exclusively interested in the composite systems allowing the tensor-product-structure variations.

Chapter 6

Parallel Occurrence of Decoherence

Quantum mechanics offers a stunning observation: a quantum whole carries less uncertainty than its parts. In favor of this observation is relativity of quantum locality and system as well as of quantum correlations. This is in sharp contrast with the classical intuition, which knows of "systems", their individuality and distinguishability, separability which became not only the goal but also a *means* for solving the quantum-to-classical-transition problem.

Quantum decoherence is currently the main candidate for establishing the quantum-to-classical transition (Giulini et al 1996, Zurek 2003, Schlosshauer 2004). The general task of the decoherence program (Schlosshauer 2004) starts as follows: "There is a system S that is in (unavoidable) interaction with its environment E. The composite system, $S + E$, is subject to the Schrödinger law."

This assumption on the pre-defined structure is the very basis of the standard, actually a *bottom-up*, approach to decoherence which is fairly presented by Zurek's (Zurek 2003):

"*In the absence of systems, the problem of interpretation seems to disappear. There is simply no need for 'collapse' in a universe with no systems. Our experience of the classical reality does not apply to the universe as a whole, seen from the outside, but to the systems within it.*"

The idea on predefined structure is classical in its spirit. Furthermore, in the decoherence context, it leads to a circular reasoning: stipulate a structure, and then use decoherence to justify the stipulation. However, bearing in mind relativity of "system" and "locality", Section 5.1, the following question appears:

(**Q**) What might be the physical consequences of the linear canonical transformations on the occurrence of decoherence?

Importance of this [as yet poorly posed] question can be seen from the following quote (Zurek 1998):

"*In particular, one issue which has been often taken for granted is looming big, as a foundation of the whole decoherence program. It is the question of what are the systems which play such a crucial role in all the discussions of the emergent classicality. (. . .) [A] compelling explanation of what are the systems–how to define them given, say, the overall Hamiltonian in some suitably large Hilbert space–would be undoubtedly most useful.*"

Intuitively, the LCT-induced change of structure may reveal non-trivial observations regarding the question of "what is 'system'?" (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008). In a sense, the question (**Q**) promotes a new *top-down* approach to describing composite quantum systems and decoherence.

However, the question (**Q**) is too general and imprecise. Not surprisingly, answer may depend on the number of the underlying assumptions and/or variations. To this end, we distinguish the following contexts of the question:

(1) LCTs refer to the closed, or to the open system;

(2) LCTs refer to a few- or to a many-particle system;

(3) Specific choice of the kind and/or of quantum state of the environment;

(4) Interpretation of quantum theory.

"Interpretation" is a subject of Chapter 8. In this Chapter we consider specific models that refer to the total (closed) system $\mathcal{C}$ by mainly following (Dugić and Jeknić-Dugić 2012). In Chapter 7, we will consider specific models of open bipartite systems.

6.1 The task

We are interested in global LCTs. More specifically: we are interested in a pair of mutually global and irreducible structures, Section 2.2.2.

This kind of structure variation means that LCTs intertwined degrees of freedom of the S and E system. Instead of the pair $S + E$, there appears a new structure $S' + E'$. We are interested in the continuous variable (CV) systems; a similar analysis regarding a finite-dimensional system can be found e.g. in (Fel'dman and Zenchuk, 2012), which is not devoted to the occurrence of decoherence for the different structures.

Since LCTs preserve the number of the degrees of freedom, equal dimensionality of S and S' implies equal dimensionality (complexity) of the respective environments, E and E'.

For the considered structures, there is a number of features of interest. To this end, we re-phrase the contents of Section 2.2.2: (i) the structures irreducibility implies that every structure is endowed by its own "elementary particles" and their interactions; (ii) the subsystems (e.g. S and S') belonging to different structures are information theoretically separated; (iii) There is neither correlation nor any information flow between the subsystems of the two structures. In this sense, the two structures appear autonomous relative to each other. Common for the two structures is the composite system's Hilbert space, the Hamiltonian and the unique quantum state in every instant in time.

Our task now reads as: for the proper LCTs, to investigate the occurrence of decoherence in the alternate structure $S' + E'$.

6.2 The obstacles

The above posed task faces some obstacles.

The first obstacle comes from Section 3: every change in the degrees of freedom typically gives rise to a change in correlation between subsystems–presence of correlations complicates analysis.

Derivation of the master equations for an open system S typically assumes (Breuer and Petruccione 2002, Rivas and Huelga 2011) both the initial tensor product state, $\rho_S \otimes \rho_E$, as well as that the environment is a thermal bath, i.e. $\rho_E = \rho_{th} = \exp(-\beta H_E)/Tr_B(\exp(-\beta H_E))$; H_E is the environment's Hamiltonian and $\beta = (k_B T)^{-1}$ is the standard "inverse temperature".

However, there is a direct consequence of the quantum correlations relativity, Section 3.2: the tensor-product state $\rho_S \otimes \rho_E$ bears correlations for the new structure, i.e. $\rho_S \otimes \rho_E \neq \rho_{S'} \otimes \rho_{E'}$. As a consequence, one directly observes: the new environment E' need not be in thermal state–worse, it's state need not be even stationary–see Lemma 6.1 below. Worse, non-factorized initial state for the "system+environment" (here: $S' + E'$) challenges both Markovianity as well as complete positivity of the open system's dynamics (Breuer and Petruccione 2002, Rivas and Huelga 2011, Rodriguez-Rosario and Sudarshan 2011, Brodutch et al 2012)[35].

On the other hand, LCTs typically introduce the new interaction terms. So, one can expect interactions of the constituent particles of the new environment E'. This, in general, poses significant technical difficulties in deriving master equation for the open system (Breuer and Petruccione 2002, Rivas and Huelga 2011, Breuer et al 2009, Laine et al 2010, Rivas et al 2010a, Rodriguez-Rosario and Sudarshan 2011, Haikka et al 2011, Brodutch et al 2012).

Thus having in mind the foundations of the Markovian open systems theory (Rivas and Huelga 2011), the transition $\{S, E\} \to \{S', E'\}$ can, in general, pose insurmountable obstacles to solving the task.

However, there is a class of the open-systems models that are immune to these obstacles–the so-called linear models. This is the subject of the next section.

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[35] Interestingly enough, the basic method in the field, the so-called Nakajima-Zwanzig projection method, is inapplicable for the structural considerations, see Section 6.3.4.

6.3 Quantum Brownian motion

"Brownian motion" is a realistic physical effect for the center of mass of "Brownian particle" (BP). Internal structure of the particle does not contribute to the Brownian motion effect. For this reason it is legitimate to forget about the internal BP degrees of freedom, and, for simplicity (without any loss of generality), to investigate the one-dimensional system, S, which can be modelled as a free particle or as a harmonic oscillator.

The particle's environment is usually modelled as a set of non-interacting linear harmonic oscillators in thermal equilibrium.

6.3.1 The LCTs and the structures of interest

Let us consider a set of three-dimensional particles, which are defined by their respective position and momentum observables, $\vec{r}_i$, $\vec{p}_j$, where $i, j = 1, 2, ..N$ enumerates the particles, and $[x_{i\alpha}, p_{j\beta}] = \delta_{ij}\delta_{\alpha\beta}$, $\alpha, \beta = 1, 2, 3$.

We introduce the total system's center of mass and the relative positions, denoted CM and R, respectively[36]:

$$\vec{R}_{CM} = \sum_i m_i \vec{r}_i / M, \quad \vec{\rho}_{Rl} = \vec{r}_i - \vec{r}_j, \quad l(\equiv \{i, j\}) = 1, 2, ...N - 1. \tag{58}$$

The inverse to eq.(58) reads as:

$$\vec{r}_i = \vec{R}_{CM} + \sum_{l=1}^{N-1} \omega_{li} \vec{\rho}_{Rl}, \tag{59}$$

with the real coefficients ω.

Regarding the system's Hamiltonian, there appears the so-called "mass polarization" term [see Supplement]:

$$M_{Rll'} = \frac{m_{l+1} m_{l'+1} \dot{\vec{\rho}}_{Rl} \cdot \dot{\vec{\rho}}_{Rl'}}{M} = \frac{m_{l+1} m_{l'+1} \vec{p}_{Rl} \cdot \vec{p}_{Rl'}}{m_l m_{l'} M}, \tag{60}$$

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[36] A generalization of eqs. (4), (5).

where appear the time derivatives of the relative positions and their scalar product; $[\vec{\rho}_{Rl}, \vec{p}_{Rl'}] = \imath\hbar\delta_{ll'}$. The set of the "reduced masses":

$$\mu_l = \frac{m_{l+1}(M - m_{l+1})}{M}. \tag{61}$$

The kinetic term for every constituent "particle" preserves the standard form, e.g.:

$$T_{CM} = \frac{\vec{P}^2_{CM}}{2M}, \quad T_{Rl} = \frac{\vec{p}^2_{Rl}}{2\mu_l}. \tag{62}$$

As elaborated in Supplement, external fields for the original particles become interactions for the CM and R systems, while the distance-dependent interactions of the original particles become external fields for the R system. Hence the form of the composite system's Hamiltonian completely changes–except the kinetic terms. Nevertheless, the composite system's Hamiltonian, H, preserves its general form (compare to eq.(5))

$$H_S + H_E + H_{SE} = H = H_{S'} + H_{E'} + H_{S'E'}, \tag{63}$$

where we assume that the open system S is one of the "original particles" while the rest constitutes the environment E, and we identify the systems, $CM \equiv S'$ and $R \equiv E'$. To this end [as emphasized above]–since the original open system S and the new one S' are of the same number of the degrees of freedom–the respective environments, E and E', are of the same number of the degrees of freedom.

In the terms of Chapter 2, the considered transformations are structurally described as follows:

$$\mathcal{S} = \{\vec{r}_S, \vec{r}_{Ei}\} \to \mathcal{S}' = \{\vec{r}_{S'}, \vec{\rho}_{E'i}\}. \tag{64}$$

So our task (Section 6.1) reads as: to investigate the occurrence of decoherence for some bipartitions of certain models described by the general expressions eqs.(58)-(64).

6.3.2 The Caldeira-Leggett model

We are interested in the Caldeira-Leggett model (Caldeira and Leggett 1983) defined by the following Hamiltonian for the "original" structure $S + E$:

$$H = \frac{p_S^2}{2m_S} + V(x_S) + \sum_i \left(\frac{p_{Ei}^2}{2m_{Ei}} + \frac{m_{Ei}\omega_{Ei}^2 x_{Ei}^2}{2} \right) \pm x_S \sum_i \kappa_i x_{Ei} \equiv H_S + H_E + H_{SE} \tag{65}$$

Physically, this is a model of a one-dimensional system S immersed in a thermal bath of mutually non-interacting harmonic oscillators (that are collectively denoted as the environment E). The interaction

$$H_{SE} = \pm x_S \sum_i \kappa_i x_{Ei} \tag{66}$$

is bilinear and with the strength determined by the coefficients κ; both signs, ±, appear in the literature without making any substantial change regarding the open-system's (the S's) dynamics.

The open system's dynamics can be described in terms of the open-system's state dynamics (the Schrödinger picture), $\rho_S(t)$, or in terms of the open system's-variables dynamics (the Heisenberg picture), $x_S(t)$, $p_S(t)$.

Typically[37], the initial state for the composite system is assumed to be tensor product, $\rho_S(t = 0)\rho_E(t = 0)$. Furthermore, the following *ansatz* is typically used (Breuer and Petruccione 2002): the total system's state in every instant in time reads

$$\rho_S(t)\rho_E, \quad \rho_E = \exp(-\beta H_E)/Tr_B(\exp(-\beta H_E)), \forall t. \tag{67}$$

It is also assumed: the environment oscillators are mutually uncoupled (non-interacting), while interaction of S and E is "weak". These simplifications

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[37] For the sake of Markovianity of the particle's dynamics.

come from the general open-systems theory: without these simplifications, the search for the general form of the Markovian master equations becomes practically intractable (Rivas and Huelga 2011).

For the phenomenologically inspired choice of the environment "spectral density", one obtains the following (high temperature) master equation [in the Schrödinger picture] for the quantum Brownian motion (QBM):

$$\frac{d\rho_S(t)}{dt} = -\frac{\imath}{\hbar}[H_S, \rho_S(t)] - \frac{\imath\gamma}{\hbar}[x_S, \{p_S, \rho_S(t)\}] - \frac{2m_S\gamma k_B T}{\hbar^2}[x_S, [x_S, \rho_S(t)]]; \tag{68}$$

the curly brackets denoting the anticommutator, $\{x_S, \rho_S(t)\} = x_S\rho_S(t) + \rho_S(t)x_S$, and γ representing the phenomenological "friction" parameter[38].

The last term in eq.(68) is the decoherence term. The approximate "pointer basis" (i.e. the "preferred") states are Gaussian states[39].

Physically, Brownian particle undergoes the decoherence process and dissipation that become obvious in the Heisenberg-picture for the particle's position and momentum observables.

Let us now consider the transformations of variables distinguished in Section 6.3.1.

Placing the expressions eq.(58), (59) into the Hamiltonian eq.(65) for one-dimensional system, one obtains for the alternate structure $S' + E'$ [while bearing in mind $S' \equiv CM$ and $E' \equiv R$]:

$$H = H_{S'} + H_{E'} + H_{S'E'}, \tag{69}$$

with the following terms:

$$H_{S'} = \frac{P_{S'}^2}{2M} + \frac{M\Omega_{S'}^2 x_{S'}^2}{2}$$

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[38] As a consequence of the choice of the spectral density.

[39] Not of the minimal uncertainty.

$$
\begin{aligned}
H_{E'} &= \sum_i \left(\frac{p_{E'i}^2}{2\mu_i} + \frac{\mu_i \nu_{E'i}^2 \rho_{E'i}^2}{2} + V_{E'} \right) \\
H_{S'E'} &= \pm x_{S'} \sum_i \sigma_i \rho_{E'i}.
\end{aligned} \tag{70}
$$

Formally, eq.(70) is similar to eq.(65). Physically, there is another one-dimensional system S' in interaction with a set of the linear harmonic oscillators. The only formal distinction lies in the appearance of the interaction term $V_{E'}$ for the constituents of new environment E'. Interaction in the new structure, $S' + E'$, is of the same, bilinear form of eq.(66).

Delving into details, we obtain (Dugić and Jeknić-Dugić 2012) precise definitions for the terms in eq.(70) for the two cases: the S system as the free particle, and the S system as a harmonic oscillator[40].

Free particle ($V_S = 0$): $M\Omega_{S'}^2/2 = \sum_i (\pm\kappa_i + m_{Ei}\omega_{Ei}^2/2)$, $\mu_i \nu_{Ei}^2/2 = \pm\omega_{Si} \sum_j \kappa_j \omega_{ij} + \sum_j m_{Ej}\omega_{Ej}^2\omega_{ij}^2/2$, and $\sigma_i = \sum_j (\kappa_j\omega_{ij} + \kappa_j\omega_{Si} + m_{Ej}\omega_{Ej}^2\omega_{ij})$. The internal interaction term $V_{E'} = \sum_{i\neq j} [C_{ij} p_{E'i} p_{E'j}/\mu_i\mu_j + (\Omega_{ij} + \omega_{Si}\Omega_j)\rho_{E'i}\rho_{E'j}]$; the "mass polarization terms" $C_{ij} = m_{E(i+1)} m_{E(j+1)}/M$ and $\Omega_i = \sum_j \kappa_j \omega_{ij}$, while $\Omega_{ij} = \sum_k m_{Ek}\omega_{Ek}^2 \omega_{ik}\omega_{jk}/2$.

Harmonic oscillator ($V_S = m_S \omega_S^2 x_S^2/2$): As distinct from the free particle case, the S system as a harmonic oscillator provides the harmonic term, which should be simply added to the free-particle Hamiltonian. So the Hamiltonian for the harmonic oscillator follows from adding the following term to the free-particle Hamiltonian: $m_S\omega_S^2 x_{S'}^2/2 + \sum_i m_S \omega_S^2 \omega_{iS}^2 \rho_{E'i}^2/2 + \sum_{i\neq j} m_S\omega_S^2 \omega_{iS}\omega_{jS}\rho_{E'i}\rho_{E'j}/2 + x_{S'} \sum_i m_S \omega_S^2 \omega_{iS} \rho_{E'i}$.

The new open system, S', is a harmonic oscillator even if the original S system is a free particle. LCTs inevitably introduce the internal interaction $V_{E'}$, which couples the E'-system oscillators; there are the linear momentum-momentum and the position-position coupling for the constituents of the new environment E'; see Supplement for details.

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[40] By $\omega_{iS} \equiv \omega_{Si}$ we assume the real parameters appearing in eq.(59).

6.3.3 S' is a Brownian particle

The two forms of the composite system's Hamiltonian, eq.(65) and eq.(70), are almost isomorphic. However, this does not *per se* imply that the dynamics of the open systems, S and S', are mutually equal.

As emphasized in Section 6.2, in general, there is a number of obstacles for providing master equation for the new open system S' that is worth repeating. First, if the initial state for the $S+E$ structure is tensor product, $\rho_S(t=0)\rho_E$, then there are initial correlations regarding the alternate structure $S'+E'$ (in general, see Section 3.2, there are quantum correlations with non-zero one-way discord[41]). As a consequence, the S' system's dynamics may be non-Markovian (and also non-completely positive). Second, if the original environment E is initially in thermal equilibrium, this is not the case for the new one, E' [see Lemma 6.1 below]. Third, the "new" oscillators (subsystems of the new environment E') are mutually coupled. For interacting oscillators, the master equation eq.(68) is not necessarily valid–there may be both memory effects for the environment as well as a change in the spectral density.

Nevertheless, as we show below, the open system S' also undergoes Brownian dynamics.

Let us first emphasize irrelevance of the $V_{E'}$ term in eq.(70).

For the new environment E', we introduce the "normal coordinates", $Q_{E'i}$, and the conjugate momentums, $P_{E'i}$, as the new canonical variables:

$$Q_{E'i} = \sum_m \alpha_{mi} x_{E'm}, \quad P_{E'i} = \sum_n \beta_{ni} p_{E'n}, \quad [Q_{E'i}, P_{E'j}] = \imath\hbar\delta_{ij}. \tag{71}$$

The choice of the new variables is constrained by the requirement of non-coupling of the new variables as well as by the commutator in eq.(71). For the potential $V_{E'}$, which is of the bilinear form regarding the position and

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[41] Remind: the two-way discord tends to be larger than one-way discord, Section 3.2.

momentum observables, this is always possible to do. So, the E' system can be considered as a set of mutually noninteracting linear harmonic oscillators, which are described by the normal coordinates, $Q_{E'i}$ in eq.(71), as the oscillators position-observables. Then instead of eq.(70) one obtains:

$$\begin{aligned} H_{S'} &= \frac{P_{S'}^2}{2M} + \frac{M\Omega_{S'}^2 x_{S'}^2}{2} \\ H_{E'} &= \sum_i \left(\frac{P_{E'i}^2}{2} + \frac{\lambda_i^2 Q_{E'i}^2}{2} \right) \\ H_{S'E'} &= \pm x_{S'} \sum_i \sigma_i' Q_{E'i}. \end{aligned} \tag{72}$$

where the new coupling constants $\sigma_i' = \sum_j \alpha_{ij}' \sigma_j$; here we use the inverse to eq.(71), $x_{E'i} = \sum_j \alpha_{ij}' Q_{E'j}$.

Thus we have performed the following global[42] (non-trivial, irreducible[43]) change in the new-environment's structure:

$$\mathcal{S}_{E'} = \{x_{E'i}\} \to \mathcal{S}'_{E'} = \{Q_{E'i}\}, \tag{73}$$

while the environment Hilbert state space now obtains new factorization, $\mathcal{H}_{E'} = \otimes_i \mathcal{H}_{E'i}^{(Q)}$, and the environment a set of mutually noninteracting oscillators, eq.(72). Thereby, in this step, the total system has undergone the following local structure transformation:

$$\mathcal{S} = \{x_{S'}, x_{E'i}\} \to \mathcal{S}' = \{x_{S'}, Q_{E'i}\}, \tag{74}$$

which now makes the two forms of the Hamiltonian, eq.(65) and eq.(72), *fully isomorphic.*

The open system's state, $\rho_{S'}$, is defined by the tracing out operation, $\rho_{S'}(t) = tr_{E'}\rho_{S'+E'}(t)$–the "$tr_{E'}$" operation is taken over the whole Hilbert space of

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[42] If we bear the S system in mind, the transformation is, of course, local.

[43] See Section 2.2.

the E' system. The basis-independence of the tracing out operation can be represented e.g.

$$tr_{E'}A_{E'} = \int \langle \{x_{E'i}\}|A_{E'}|\{x_{E'i}\}\rangle \Pi_i dx_{E'i} = \int \langle \{Q_{E'i}\}|A_{E'}|\{Q_{E'i}\}\rangle \Pi_i dQ_{E'i} \tag{75}$$

for the different structures of E'; $|\{x_{E'i}\}\rangle = \otimes_i|x_i\rangle_{E'}$, $|\{Q_{E'i}\}\rangle = \otimes_i|Q_i\rangle_{E'}$. So, eq.(75) clearly states: the open system's state, $\rho_{S'}(t)$, is *unique*, i.e. is *not* environment-structure dependent. Therefore dynamics of the open system S' [e.g. derivation of the related master equation] is not conditioned by the choice of the E'-system's structure.

Now we return to the consequences of QCR, Section 3.2. As emphasized above, a change of the open system's structure will in general lead to a change in form of the system's quantum state, as well as in the amount of quantum correlations carried by the state. However, there are the following special cases: (a) the composite system is at zero temperature ($T = 0$), and (b) the composite system is at nonzero temperature T. These cases are actually known and investigated, e.g. in (Paz 1996, Bellomo et al 2005, Anglin et al 1997).

Exact solutions to the Schrödinger equation for the Hamiltonian eq.(65), i.e. eq.(72), are not yet known. Nevertheless, for the case (a), it is known that the ground energy state is non-degenerate (i.e. is unique) and entangled for the bipartition, "system+environment" system. Regarding the case (b): at non-zero temperature, the total system's state

$$\rho = \frac{e^{-\beta H}}{Z}, \quad Z = tre^{-\beta H} \tag{76}$$

where H is the total system's Hamiltonian, for the canonical ensemble; β is the "inverse temperature". Of course, the state eq.(76) is non-factorized.

The following point should be strongly emphasized: all the conclusions referring to the cases (a) and (b) equally concern to both structures, $S + E$ and

$S' + E'$. e.g. The Hamiltonian H appearing in eq.(76) is given by eq.(65) for the $S + E$ and by eq.(72) for the $S' + E'$ structure. So for the cases (a) and (b), the two model-structures are formally *fully isomorphic*. The *physical* distinctions between the two structures–correlations in the initial state for the new structure, and non-stationary state of the new environment–are known *not* to change the physical picture (Lutz 2003, Romero and Paz 1996, Bellomo et al 2005, Anglin et al 1997). Hence we can conclude that (Dugić and Jeknić-Dugić 2012):

The "new" open system, S', is a Brownian particle itself.

The case of the initially non-equal temperatures of the open system S and the environment E is not easy to handle[44]. In such case, as emphasized above, due to QCR, the two models are not fully isomorphic[45]. Along with the existing literature, here we do not tempt to offer a general description of this situation. Nevertheless, we offer a scenario that is a *speculative* physical picture, which bears some generality compared to the non-realistic ansatz eq.(67) for the $S + E$ structure.

Having in mind Section 6.2 and eq.(70), we collect the constraints for deriving master equation for the S' system. First, from eq.(70), we can see that interaction $H_{S'E'}$ is of the strength of the order of H_{SE}, i.e. it's weak. From Section 6.2 we learn that the initial state for the $S'+E'$ structure is in general a mixture $\rho_{S'+E'}(t = 0) = \sum_i \lambda_i \rho_{S'i} \otimes \rho_{E'i}$. Thus one cannot adopt Markovian approximation for the S' system (Rivas and Huelga 2011). Having in mind that the S and S' are one-particle systems, the two environments E and E' are also of equal dimensionality (of equal number of oscillators).

Then we start from eq.(3.113) of (Breuer and Petruccione 2002) [in the in-

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[44] See Section 6.3.4.

[45] It is worth noticing: this situation refers physically to the situation, in which the open system is suddenly brought in touch with the thermal bath.

teraction picture]:

$$\frac{d\rho_{S'}(t)}{dt} = -\int_0^t ds tr_{E'}[H^I_{S'E'}(t), [H^I_{S'E'}(s), \rho_{S'+E'}(s)]]. \qquad (77)$$

Without further ado, we resort to the following *ansatz*:

$$\rho(t) = (1 - \epsilon_\circ(t)) \sum_i \sigma^{t>t_\circ}_{S'i} \sigma_{E'\circ} + \sum_i \epsilon_i(t) \sigma^{t>t_\circ}_{S'i} \delta^{t>t_\circ}_{E'i}, \quad tr_{E'} \delta^{t>t_\circ}_{E'i} = 1, \forall i, t, \quad (78)$$

where $|\epsilon(t)| \ll 1, \epsilon(t) = \max\{\epsilon_i(t)\}, \forall t > t_\circ$.

Physically, eq.(78) means: the environment E' undergoes thermal relaxation much faster than the open system S'. From eq.(78): $\rho_{E'} \approx \sigma_{E'\circ}$ after some instant $t > t_\circ$ [the initial instant is assumed $t = 0$]. The open system's state $\rho_{S'}(t) \approx \sum_i \sigma_{S'i}(t), t > t_\circ$.

Further, instead of the total environment E', we consider a small part of the E' system that should appear in eq.(78). Namely, we divide $E' = E'_1 + E'_2$, where the part E'_2 monitors E'_1 and does not interact with the S' system[46]. Then eq.(78) reduces to the standard *ansatz* eq.(67): if the limit $\epsilon \to 0$ is available for the time intervals of γ^{-1}, then eq.(78) reduces to $\rho_{S'}(t)\sigma_{E'_1\circ}$; γ is the E'_1-system's relaxation rate.

Substituting eq.(78) into eq.(77):

$$\frac{d\rho_{S'}(t)}{dt} \approx -\int_0^t ds tr_{E'_1}[H^I_{S'E'_1}(t), [H^I_{S'E'_1}(s), \rho_{S'}(s) \otimes \sigma_{E'_1\circ}]]. \qquad (79)$$

If we assume thermal state for the E'_1 environment, $\sigma_{E'_1\circ} = \rho_{th}$, then eq.(79) strongly suggests applicability of the Markov approximation[47] and hence the

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[46] One can think of this tripartition in analogy with the DISD method of (Dugić 2000).

[47] Remind: the environment state $\sigma_{E'_1\circ}$ is thermal–no state change in eq.(79) for the environment (except in very short time intervals). The exact form of eq.(79) contains non-Markovian corrections that are, according to the ansatz eq.(78), assumed to be small.

master equation (see (Breuer and Petruccione 2002) for details):

$$\frac{d\rho_{S'}(t)}{dt} \approx -\int_0^\infty ds tr_{E'_1}[H^I_{S'E'_1}(t), [H^I_{S'E'_1}(s), \rho_{S'}(t) \otimes \rho_{th}]], \tag{80}$$

which is formally the starting point for deriving the master equation eq.(68)– but this time for the S' system. So, again, we obtain the above-brought conclusion, which is the title of this section.

Eq.(80) is approximate ($|\epsilon(t)| > 0$) and valid for the time instants $t > t_\circ$. Nevertheless, it's applicable for arbitrary initial state of the composite system. Of course, whether or not this plausible derivation may be used in the more general context remains unanswered as Markovian approximation for the rhs in eq.(79) is another plausible ansatz, not a rigorous physical condition yet.

6.3.4 A limitation of the Nakajima-Zwanzig projection method

Derivation of eq.(80) assumes Markov approximation, which, as we already know (Rivas and Huelga 2011), cannot be valid for the $S'+E'$ structure. Nevertheless, plausibility of this simplification stems from the form of the rhs of eq.(79) as well as from the fact that the neglected term is non-Markovian. So we hope for *approximate* Markovianity of the S' system's dynamics (assuming that $\epsilon \ll 1$, and only after some time interval $t_\circ$).

At first sight, we could have used the methods adapted to description of non-Markovian dynamics, notably the so-called time-convolutionless method (Breuer and Petruccione 2002). However, as we show below, this method is *not adapted* to the structural considerations.

The Nakajima-Zwanzig projection method is the central method of modern open quantum systems theory (Breuar and Petruccione 2002, Rivas and Huelga 2011). It's the very basis of modern open systems theory and application that include the time-convolutionless method.

The key idea behind the Nakajima-Zwanzig projection method consists of the introduction of a certain projection operator, $\mathcal{P}$, which acts on the operators of the state space of the total system "system+environment" $(S+E)$. If ρ is the density matrix of the total system, the projection $\mathcal{P}\rho$ (the "relevant part" of the total density matrix) serves to represent a simplified effective description through a reduced state of the total system. The complementary part (the "irrelevant part" of the total density matrix), $\mathcal{Q}\rho = (I - \mathcal{P})\rho$. For the "relevant part", $\mathcal{P}\rho(t)$, one derives closed equations of motion in the form of integro-differential equation. The open system's density matrix $\rho_S(t) = tr_E \mathcal{P}\rho(t)$ contains *all* necessary information about the open system S. Here, we refer to the mostly-used kind of projection:

$$\mathcal{P}\rho(t) = tr_E \rho(t) \otimes \rho_E \equiv \rho_S(t) \otimes \rho_E \tag{81}$$

where $\rho_E \neq tr_S \rho$ for any instant in time. The open system's state

$$\rho_S(t) = tr_E \rho(t) = tr_E \mathcal{P}\rho(t) \Leftrightarrow tr_E \mathcal{Q}\rho(t) = 0, \forall t; \tag{82}$$

the $\mathcal{Q}$ projector satisfies $\mathcal{P} + \mathcal{Q} = I$.

The Nakajima-Zwanzig projection method assumes a concrete, in advance chosen and fixed, system-environment split (a "structure"), $S+E$, which is uniquely defined by the associated tensor product structure of the total system's Hilbert space, $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. The division of the composite system into "system" and "environment" is practically motivated. In principle, the projection method can equally describe arbitrary system-environment split i.e. arbitrary factorization of the total system's Hilbert state.

However, our task points out a limitation of the Nakajima-Zwanzig method. In the more general terms, the task reads as: for a pair of open systems, S and S', pertaining to the different system-environment splits of a composite system, can the Nakajima-Zwanzig and/or the related projection methods provide *simultaneous* dynamical description of the open systems, S and S'?

The answer is provided by the following theorem:

Theorem 6.1. *Quantum correlations relativity precludes simultaneous pro-*

jection-method-based description of a pair of system-environment splits.

Proof: There are only two options for writing the *simultaneous* master equations for the S and S' systems. First, if the projection adapted to the $S+E$ structure can be used for deriving the master equation for the S' system. Then it is required, that $tr_E \mathcal{P}\rho(t) = \rho_S(t)$ *and* $tr_{E'} \mathcal{P}\rho(t) = \rho_{S'}(t)$, i.e. $tr_E \mathcal{Q}\rho(t) = 0$ *and* $tr_{E'} \mathcal{Q}\rho(t) = 0$ for *every* instant in time. Second, if we perform in parallel, i.e. if we use the different projection operators, $\mathcal{P}$ and $\mathcal{P}'$, for the two structures independently of each other. Then it is required, $tr_E \mathcal{P}\rho(t) = \rho_S(t)$ *and* $tr_{E'} \mathcal{P}'\rho(t) = \rho_{S'}(t)$, i.e. $tr_E \mathcal{Q}\rho(t) = 0$ *and* $tr_{E'} \mathcal{Q}'\rho(t) = 0$ for *every* instant in time. We use the following lemmas.

Lemma 6.1. *Quantum correlations relativity in dynamical terms, for the mixed states, reads as:* $\rho_S(t) \otimes \rho_E = \sum_i \lambda_i \rho_{S'}(t) \otimes \rho_{E'}(t)$. *The possible time dependence of the weights* λ *is irrelevant.*

Lemma 6.2. *For the most part of the composite system's dynamics,* $tr_E \mathcal{Q}\rho(t) = 0$ *implies* $tr_{E'} \mathcal{Q}\rho(t) \neq 0$, *and vice versa.*

Lemma 6.3. *The two structure-adapted projectors* $\mathcal{P}$ *and* $\mathcal{P}'$ *do not mutually commute and cannot be simultaneously performed.*

Lemma 6.1 establishes time-dependence of states of *both* subsystems, S' and E'. Bearing eqs.(28)-(29) in mind, we realize that it may happen that there are only classical correlations for the $S'+E'$ structure.

Lemma 6.2 establishes: for the most part of the composite system's dynamics, projection $\mathcal{Q}\rho$ (or $\mathcal{Q}'\rho$) brings some information about the open system S' (or S)–in *contradiction* with the basic *idea* of the Nakajima-Zwanzig projection method.

On the other hand, Lemma 6.3 establishes: for any pair of structures, $S+E$ and $S'+E'$, one *cannot* choose/construct a pair of compatible projectors defined by eq.(81). So Lemma 6.3 precludes simultaneous (for the same time interval) derivation of master equations for the two open systems, S and S'.

From Lemma 6.2 and 6.3, it directly follows the claim of the theorem. Q.E.D.

Thus the Nakajima-Zwanzig projection method faces a limitation. While it can be separately performed for any structure (either $\mathcal{P}$ or $\mathcal{P}'$), it cannot be *simultaneously* used for a pair of structures. Once performed, projection does not in general allow for drawing complete information about an alternative structure of the composite system–projecting is non-invertible (”irreversible”).

Our finding refers to *all projection-based methods*–including the above mentioned time-convolutionless method. In formal terms: Lemma 2 implies that, in an instant of time, $d\mathcal{P}\rho(t)/dt$ allows tracing out over only one structure of the composite system. If that structure is $S + E$, then $tr_{E'} d\mathcal{P}\rho(t)/dt \neq d\rho_{S'}(t)/dt$ [as long as $\rho_{S'}(t) = tr_{E'}\rho(t)$]. On the other hand, Lemma 3 excludes simultaneous projecting, i.e. simultaneous master equations for the two structures. E.g., $d\mathcal{P}\rho(t)/dt = d\rho_S(t)/dt \otimes \rho_E$ is in conflict with $d\mathcal{P}'\rho(t)/dt = d\rho_{S'}(t)/dt \otimes \rho_{E'}$: due to QCR, Section 3.2, only one of them can be correct for arbitrary instant in time.

Despite the fact that quantum correlations relativity can have exceptions for certain states, our findings presented by Theorem 6.1 do not. Even if QCR does not apply to an instant in time (i.e. to a special state of the total system), it is most likely to apply already for the next instant of time in the unitary (continuous in time) dynamics of the total system C. This general argument makes the above lemmas universal, i.e. applicable for every Hilbert state space and every model and structure (the choice of the open systems S and S') of the total system. Hence our findings and conclusions refer to the finite- and infinite-dimensional systems and to all kinds of the transformations of variables.

These findings do not present any inconsistency with the open systems theory or with the foundations of the Nakajima-Zwanzig method. Rather, our findings point out that the Nakajima-Zwanzig projection method has a *limitation*, i.e. is *not suitable* for the above-posed task.

Everything told in this section equally refers to the open systems S and S'

that are macroscopically "almost equal"–e.g. in number of their respective constituent particles. Even if the S' system follows from the (local) transformation of joining a single particle of the E system with the S system, thus obtaining the new S' and E' systems, the projection method cannot be straightforwardly used to derive master equation for the S' system. Hence we conclude: there is not a priori a hope that the small changes in the system-environment split would effect in small changes in dynamics. In other words, we can conclude: the "shortcuts" for describing the alternative-open-systems dynamics may be non-reliable and delicate.

Proof of Lemma 6.1. Without any loss of generality, and in order to eliminate the weights λ from consideration, consider $\rho_S(t)\otimes\rho_E = \rho_{S'}(t)\otimes\rho_{E'}$. Then calculate $trx_{E'}$, where $x_{E'} = \alpha x_S + \beta x_E$. Then $trx_{E'} = \alpha tr_S x_S \rho_S(t) + \beta tr_E x_E \rho_E$, which is time dependent. On the other hand, $trx_{E'} = tr_{E'} x_{E'} \rho_{E'}$, which is time-independent. In order to reconcile the two, we conclude that also $\rho_{E'}$ must be time dependent. Q.E.D.

We borrow the proofs of the lemmas from the original paper (Arsenijević et al 2013b).

Proof of Lemma 6.2. Given $tr_E \mathcal{Q}\rho(t) = 0, \forall t$, we investigate the conditions that should be fulfilled in order for $tr_{E'}\mathcal{Q}\rho(t) = 0, \forall t$. The $\mathcal{Q}$ projector refers to the $S+E$, not to the $S'+E'$ structure. Therefore, in order to calculate $tr_{E'}\mathcal{Q}\rho(t)$, we use ER. We refer to the projection eq.(81) in an instant of time:

$$\mathcal{P}\rho = (tr_E\rho)\otimes\rho_E. \tag{83}$$

A) Pure state $\rho = |\Psi\rangle\langle\Psi|$, while $tr_E\mathcal{Q}|\Psi\rangle\langle\Psi| = 0$.

We consider the pure state presented in its (not necessarily unique) Schmidt form

$$|\Psi\rangle = \sum_i c_i |i\rangle_S |i\rangle_E, \tag{84}$$

where $\rho_S = tr_E|\Psi\rangle\langle\Psi| = \sum_i p_i |i\rangle_S\langle i|$, $p_i = |c_i|^2$ and for arbitrary $\rho_E \neq$

$tr_S|\Psi\rangle\langle\Psi|$. Given $\rho_E = \sum_\alpha \pi_\alpha |\alpha\rangle_E\langle\alpha|$, we decompose $|\Psi\rangle$ as:

$$|\Psi\rangle = \sum_{i,\alpha} c_i C_{i\alpha} |i\rangle_S |\alpha\rangle_E, \tag{85}$$

with the constraints:

$$\sum_i |c_i|^2 = 1 = \sum_\alpha \pi_\alpha, \sum_\alpha |C_{i\alpha}|^2 = 1, \forall i, \tag{86}$$

Then

$$\mathcal{Q}|\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi| - \sum_{i,\alpha} p_i \pi_\alpha |i\rangle_S\langle i| \otimes |\alpha\rangle_E\langle\alpha|. \tag{87}$$

We use ER:

$$|i\rangle_S|\alpha\rangle_E = \sum_{m,n} D^{i\alpha}_{mn} |m\rangle_{S'}|n\rangle_{E'} \tag{88}$$

with the constraints:

$$\sum_{m,n} D^{i\alpha}_{mn} D^{i'\alpha'*}_{mn} = \delta_{ii'}\delta_{\alpha\alpha'}. \tag{89}$$

With the use of eqs.(85) and (88), eq.(87) reads as:

$$\sum_{m,m'n,n'} [\sum_{i,i',\alpha,\alpha'} c_i C_{i\alpha} c^*_{i'} C^*_{i'\alpha'} D^{i\alpha}_{mn} D^{i'\alpha'*}_{m'n'} - \sum_{i,\alpha} p_i \pi_\alpha D^{i\alpha}_{mn} D^{i\alpha\ *}_{m'n'}] |m\rangle_{S'}\langle m'| \otimes |n\rangle_{E'}\langle n'|. \tag{90}$$

After tracing out, $tr_{E'}$:

$$\sum_{m,m'} \{ \sum_{i,\alpha,n} \sum_{i',\alpha'} c_i C_{i\alpha} c^*_{i'} C^*_{i'\alpha'} D^{i\alpha}_{mn} D^{i'\alpha'*}_{m'n} - p_i \pi_\alpha D^{i\alpha}_{mn} D^{i\alpha*}_{m'n} \} |m\rangle_{S'}\langle m'| \tag{91}$$

Hence

$$tr_{E'} \mathcal{Q}|\Psi\rangle\langle\Psi| = 0 \Leftrightarrow \sum_{i,\alpha,n} [\sum_{i',\alpha'} c_i C_{i\alpha} c^*_{i'} C^*_{i'\alpha'} D^{i\alpha}_{mn} D^{i'\alpha'*}_{m'n} - p_i \pi_\alpha D^{i\alpha}_{mn} D^{i\alpha*}_{m'n}] = 0, \forall m, m' \tag{92}$$

Introducing notation, $\Lambda_n^m \equiv \sum_{i,\alpha} c_i C_{i\alpha} D_{mn}^{i\alpha}$, one obtains:

$$tr_{E'}\mathcal{Q}|\Psi\rangle\langle\Psi| = 0 \Leftrightarrow A_{mm'} \equiv \sum_n [\Lambda_n^m \Lambda_n^{m'*} - \sum_{i,\alpha} p_i \pi_\alpha D_{mn}^{i\alpha} D_{m'n}^{i\alpha*}] = 0, \forall m, m'. \tag{93}$$

Notice:

$$\sum_m A_{mm} = 0. \tag{94}$$

which is equivalent to $tr\mathcal{Q}|\Psi\rangle\langle\Psi| = 0$, see eq.(87).

B) Mixed (e.g. non-entangled) state.

$$\rho = \sum_i \lambda_i \rho_{Si} \rho_{Ei}, \quad \rho_{Si} = \sum_m p_{im} |\chi_{im}\rangle_S \langle\chi_{im}|, \rho_{Ei} = \sum_n \pi_{in} |\phi_{in}\rangle_E \langle\phi_{in}|, \tag{95}$$

In eq.(95), having in mind eq.(83), $tr_E \mathcal{Q}\rho = 0$, while $tr_E\rho = \sum_p \kappa_p |\varphi_p\rangle_S \langle\varphi_p|$, and $\rho_E = \sum_q \omega_q |\psi_q\rangle_E \langle\psi_q| \neq tr_S \rho$.

Constraints:

$$\sum_i \lambda_i = 1 = \sum_p \kappa_p = \sum_q \omega_q, \quad \sum_m p_{im} = 1 = \sum_n \pi_{in}, \forall i. \tag{96}$$

Now we make use of ER and, for comparison, we use the same basis $\{|a\rangle_{S'}|b\rangle_{E'}\}$

$$|\chi_{im}\rangle_S |\phi_{in}\rangle_E = \sum_{a,b} C_{ab}^{imn} |a\rangle_{S'} |b\rangle_{E'}, |\varphi_p\rangle_S |\psi_q\rangle_E = \sum_{a,b} D_{ab}^{pq} |a\rangle_{S'} |b\rangle_E. \tag{97}$$

Constraints:

$$\sum_{a,b} C_{ab}^{imn} C_{ab}^{im'n'*} = \delta_{mm'} \delta_{nn'}, \quad \sum_{a,b} D_{ab}^{pq} D_{ab}^{p'q'*} = \delta_{pp'} \delta_{qq'}. \tag{98}$$

So

$$\mathcal{Q}\rho = \rho - (tr_E\rho) \otimes \rho_E = \sum_{a,a',b,b'} \{\sum_{i,m,n} \lambda_i p_{im} \pi_{in} C_{ab}^{imn} C_{a'b'}^{imn*}$$

$$-\sum_{p,q}\kappa_p\omega_q D^{pq}_{ab}D^{pq*}_{a'b'}\} \quad |a\rangle_{S'}\langle a'|\otimes|b\rangle_{E'}\langle b'|. \tag{99}$$

Hence

$$tr_{E'}\mathcal{Q}\rho = 0 \Leftrightarrow \Lambda_{aa'} \equiv \sum_{i,m,n,b}\lambda_i p_{im}\pi_{in}C^{imn}_{ab}C^{imn*}_{a'b} - \sum_{p,q,b}\kappa_p\omega_q D^{pq}_{ab}D^{pq*}_{a'b} = 0, \forall a, a'. \tag{100}$$

Again, for $a = a'$:

$$\sum_a \Lambda_{aa} = 0, \tag{101}$$

as being equivalent with $tr\mathcal{Q}\rho = 0$, see eq.(99).

Both eq.(93) and eq.(100) represent the sets of the simultaneously satisfied equations. We do not claim non-existence of the particular solutions to eq.(93) and/or to eq.(100), e.g. for the finite-dimensional systems. We just emphasize, that the number of states they might refer to, is apparently negligible compared to the number of states for which this is not the case. For instance, already for the fixed a and a', a small change e.g. in κs (while bearing eq.(96) in mind) undermines equality in eq.(100).

Quantum dynamics is continuous in time. Provided $tr_E\mathcal{Q}\rho(t) = 0$ is fulfilled, validity of $tr_{E'}\mathcal{Q}\rho(t) = 0$ might refer *only* to a special set of the time instants. So we conclude: for the most part of the open S'-system's dynamics, $tr_{E'}\mathcal{Q}\rho(t) = 0$ is not fulfilled. By exchanging the roles of the S and the S' systems in our analysis, we obtain the reverse conclusion, which completes the proof. Q.E.D.

Proof of Lemma 6.3. The commutation condition, $[\mathcal{P}, \mathcal{P}']\rho(t) = 0, \forall t$. With the notation $\rho_P(t) \equiv \mathcal{P}\rho(t)$ and $\rho_{P'}(t) \equiv \mathcal{P}'\rho(t)$, the commutativity reads as: $\mathcal{P}\rho_{P'}(t) = \mathcal{P}'\rho_P(t), \forall t$. Then, $\mathcal{P}\rho_{P'}(t) = tr_E\rho_{P'}(t)\otimes\rho_E = \rho_S(t)\otimes\rho_E$, while, according to Lemma 6.1, $\mathcal{P}'\rho_P(t) = tr_{E'}\rho_P(t) = \sigma_{S'}(t)\otimes\sigma_{E'}(t)$. So, the commutativity requires the equality $\sigma_{S'}(t)\otimes\sigma_{E'}(t) = \rho_S(t)\otimes\rho_E, \forall t$. However, quantum dynamics is continuous in time. Like in Proof of Lemma 2, quantum correlations relativity guarantees, that, for the most of the time instants, the equality will not be fulfilled. Q.E.D.

6.4 The LCTs preserve linearity of a composite-system's model

Physically, the structure $\mathcal{S}' = \{x_{CM}, Q_{Ri}\}$–Brownian particle is the total system's center of mass, while the environment is composed of the normal modes for the relative positions for the original structure $S+E$. Nevertheless, the $\mathcal{S}'$ structure is not very special. The procedure presented in Sections 6,3,2 and 6.3.3 is applicable formally for arbitrary LCTs eq.(6). In other words: linear canonical transformations preserve linearity[48] of the original structure $S+E$. The whole structural transformation can be presented as:

$$\mathcal{S}_\circ = \{x_S, x_{Ei}\} \to \mathcal{S} = \{x_{S'}, x_{E'i}\} \to \mathcal{S}' = \{x_{S'}, Q_{E'i}\}, \tag{102}$$

for every LCT eq.(6).

However, there are certain constraints for the LCTs, in order to make the alternate structure physically sensible. For the case presented in Section 6.3, the constraints are: $M\Omega^2_{S'} > 0$ and $\mu_i \nu^2_{E'i} > 0, \forall i$. The analogous constraints appear for all the alternate structures. Thereby the physical relevance of the alternate structure $\mathcal{S}'$ is not unconditional.

The "linear model" refers also to some other physically relevant models. e.g. In (Bellomo et al 2005), a [non-relativistic] charged particle is embedded in the electromagnetic-field modes at zero temperature. Interestingly enough, initial state of the total system is correlated, and is shown that decoherence is related to the time dependent "dressing" of the particle. A similar analysis (of a linear model) is provided by (Stokes et al 2012) with the explicit LCTs performed on the total system "atom+EM-field". An emphasis is placed on the range of validity of the quantum optical master equations for the composite system; for details see Section 7.3.

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[48] "Linearity" means that the Hamiltonian is quadratic, with the bilinear interaction, eq.(66), and uncoupled environment oscillators.

Here we do not elaborate on this any further. The reason is probably apparent: depending on the choice of LCTs, i.e. of the new variables and the related parameters range, the results may vary–i.e. are *case dependent*. Subtlety and complexity of investigating the occurrence of decoherence is fairly expressed by (Anglin et al 1997) [our emphasis]:

"*In this paper we will effectively argue that many perceived universalities in the phenomenology of decoherence are artifacts of studying toy models, and that the single neat border checkpoint should be replaced as an image for decoherence by* the picture of a wide and ambiguous No Man's Land, filled with pits and mines, *which may be crossed on a great variety of more or less tortuous routes. Once one has indeed crossed this region, and travelled some distance away from it, the going becomes easier: we are not casting doubt on the ability of the very strong decoherence acting on macroscopic objects to enforce effective classicality. ... By presenting a number of theoretically tractable examples in which various elements of phenomenological lore can be seen to fail explicitly, we make the point that each experimental scenario will have to be examined theoretically on its own merits, and from first principles.*".

Nevertheless, as emphasized above, there is the following, generally valid, observation: linearity of the total system's model is preserved by linear canonical transformations. Encouraged by Section 6.3, we dare to state the following

Conjecture 1. *For the linear models one can expect in principle the occurrence of decoherence also for some alternate degrees of freedom, which are provided by the linear canonical transformations.*

6.5 More than one "classical world"

Section 6.3 teaches us: if the open system S is a Brownian particle, then also the open system S' is necessarily a Brownian particle. This seemingly naive observation is physically remarkable.

Every Hamiltonian generates the *simultaneously* unfolding dynamics for different structures of a composite system. Of all possible structures, for the standard QBM model, we distinguish and consider only those emphasized in Section 2.2.2: mutually global, non-trivial and irreducible structures. In Section 6.3, we consider a pair of such structures and find the *parallel occurrence of decoherence* for the structures.

The standard "decoherence program" (Giulini et al 1996, Schlosshauer 2004) bases itself on the following assumption: quantum decoherence is in the root of the appearance of "classical world" in quantum theory. Now, as we elaborate below, our result on the parallel occurrence of decoherence suggests: for a composite (closed) system C, Section 6.3, there are at least two, mutually autonomous and irreducible "classical world*s*"–*one classical world for one structure, i.e. for one Brownian particle*[49].

In a set of mutually global and irreducible structures, every [physically reasonable] structure[50] has the following characteristics:

(a) It is completely describable by the universally valid quantum mechanics;

(b) It has its own set of "elementary particles" and the interactions between them, and is (cf. Section 2.2) irreducible and information-theoretically separated from any alternative, global and irreducible structure;

(c) It dynamically evolves in time, simultaneously with but totally independently (autonomously) of any other structure;

(d) It has its own Brownian particle;

(e) Is locally indistinguishable from the others: an observer belonging to one (and to *only one*) structure cannot say which structure he belongs to;

(f) Physically is *not*, *a priori*, less realistic than any other.

Thereby, physically, the model-universe C, Section 6.3, *hosts* more than one *dynamical classical world*. As the worlds are mutually global and irreducible, there is more than one "classical world" for one and the unique (a single)

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[49] Needless to say, not every structure bears classicality. Therefore "classicality" of a physical system is *relative*–it's a matter of the system's structure.

[50] $C = S + E = S' + E' = ...$

"universe" C. Thereby, if the standard decoherence program provides the "appearance of *a* Classical World" (Giulini et al, 1996), our results suggest the "appearance of *the* Classical World*s*".

This observation challenges foundations of the standard decoherence program and requires additional interpretational analysis, which will be presented in Chapter 8.

6.6 A few general notions

The composite system C is closed–a model-universe subject to the Schrödinger law. For the closed systems, which are not observable from the outside, there does not seem to exist a privileged fundamental decomposition into subsystems (structure). Regarding the open composite systems, see the next chapter.

Our considerations are explicit only for the linear models. So, the parallel occurrence of decoherence is in its infancy yet. The natural question whether or not our considerations can be applied to the more realistic models of the many-particle open systems here remains unanswered. To this end, see the quote from (Anglin et al 1997) in Section 6.4.

Of course, instead of decoherence, one can use some other criteria for classicality, i.e. for the "appearance of the classical world". e.g. One can use the absence of non-classical correlations as such a criterion. An example in this regard for an open system is given in Section 7.2. For some results concerning the information theoretic description of the decoherence process, see (Coles 2012).

Chapter 7

Decoherence-Induced Preferred Structure

”Observing” is *local*. Of a composite system, only a small fraction of degrees of freedom is accessible to observation. That is, only a small amount of information about a composite system is acquired in realistic experimental situations.

There is no observer outside the Universe. Observer is a part of the structure he observes. From Section 6.5 we learn: there are certain structures of the Universe that cannot be observed by an observer belonging to another structure. More on this in Chapter 8. Here we are interested in structures of local systems, which are *open*–i.e. in unavoidable interaction with their environments. This means, as distinct from Chapter 6, the transformations of variables leave environmental degrees of freedom *intact*.

Which degrees of freedom are accessible to an observer (Def.5.1), i.e. what constitutes ”system” in a given physical situation? Are there some general rules and/or limitations? What is origin of the classical prejudice, which is described in Section 2.1? Those are the main questions of interest in the remainder of this chapter. For a couple of models, we obtain that the environment selects a ”preferred” structure of the open system.

7.1 Decoherence-based classicality

Decoherence Program (Giulini et al 1996, Schlosshauer 2004) offers a clue regarding the above posed questions: environment decoheres only a fraction of the open system's degrees of freedom. The decoherence-preferred degrees of freedom are considered to be accessible (directly measurable in the sense of Def.5.1) and therefore "objective" for an observer.

For instance, quantum vacuum monitors atomic R system, not atomic CM system (Breuer and Petruccione 2002, Rivas and Huelga 2011). Atomic de-excitation, i.e. the state decay, refers to the atomic R system: detection of a photon reveals the atomic internal-energy decay, which, typically, does not affect the atomic CM system. Bearing in mind Section 5.1, it is now clear: quantum vacuum only partially monitors atomic electron(s) and proton(s)[51]. Interaction between the open system S and its environment E:

$$H_{SE} = A_S \otimes B_E \tag{103}$$

models a measurement of the system's observable, A_S, that is performed by the environment E. If this interaction dominates the composite system's ($S+E$'s) dynamics, then the eigenstates of A_S appear as the preferred (e.g. the approximate "pointer basis") states for the open system S. In general, spectral form of the interaction Hamiltonian gives only a hint–not necessarily a definition–of the pointer basis states (Dugić 1996, 1997).

So, the environment-induced decoherence naturally offers the following *basis* for answering the above posed questions:

Clue. *Decoherence-selected preferred states (and the related preferred observables) determine the preferred structure of the open system.*

For instance, it is easy to design the phenomenologically inspired effective interaction that promotes the CM system as a preferred subsystem:

$$H_{SE} = X_{CM} \otimes B_E; \quad S = CM + R. \tag{104}$$

For Brownian particle, neglecting the particle's R system, the model eq.(104) is presented by eq.(66), i.e. $B_E = \sum_i \kappa_i x_{Ei}$.

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[51] For some details see (Jeknić-Dugić et al 2011).

Similarly, Stipulation 1 of Section 4.2.2 assumes, at least approximate, commutation $[H_{K_N E}, K_N] = 0$, that can be modelled e.g. as[52]:

$$H_{K_N E} = K_N \otimes B_E. \tag{105}$$

However, eqs. (104)-(105) are *constructed*, i.e. *designed* (or stipulated) in order to fit with phenomenology. However, in order to answer the above posed questions, it is desirable to have *derived* (not merely stipulated) the preferred structure of an open system.

In the next sections we will justify the Clue. We consider specific models without posing any stipulation. Thereby we come to the conclusion: *decoherence may provide* a unique preferred structure *of the open system*.

In this context it is natural to reject physical reality for the degrees of freedom representing linear combinations of the decohered degrees of freedom. E.g., cf. Section 2.1 [and Footnote 27], the Earth's and the Venus' CM systems are decohered, but the CM system for the Earth's and the Venus' CM-systems is not–and is therefore an empty point in space, not an object–in full agreement with the classical intuition described in Section 2.1; for more details see Section 8.2.

Of course, classicality of certain [decohered] degrees of freedom does not imply non-observability of the alternative (non-decohered) degrees of freedom. As it is emphasized in Sections 2.4 and 5.1, "local action" is a relative concept, which is usually well defined in a concrete physical situation.

So, we are concerned with the following task:

$\mathcal{T}$. *Are there some realistic models that do not require "construction" or stipulation of the preferred structure of an open composite system*?

In the next sections we give just a few such models referring to the few-degrees-of-freedom open systems. The models employ different criteria for classicality–a definition of the open system's pointer basis (and correlation

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[52] See eq.(3.164) in (Giulini et al 1996).

in the composite system), and the validity range of certain kind of master equations, respectively. We are not aware of any other technically elaborated considerations.

7.2 Asymptotic dynamics of a two-mode system

For a pair of modes, we investigate asymptotic ($t \to \infty$) behavior[53] of the environment-induced preferred states. Following generally accepted decoherence procedures, we find that there is only one structure of the composite system which allows for the preferred states to be regarded to bear classicality.

We consider a pair of uncoupled modes in the "phase space" representation (as a pair of non-interacting linear harmonic oscillators) that are independently subjected to the quantum amplitude damping channels. A pair of noninteracting linear oscillators, 1 and 2, with the respective frequencies and masses, ω_1, ω_2. and m_1, m_2. The "phase space" position variables, x_1 and x_2, and the conjugate momentums, p_1 and p_2, respectively. The total Hilbert state space factorizes $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and the total Hamiltonian $H = H_1 + H_2$, $H_i = p_i^2/2m_i + m_i\omega_i^2 x_i^2/2, i = 1, 2$.

We analytically (exactly) solve the Heisenberg equations of motion in the Kraus representation (Fan and Hu 2009, Jiang et al 2011, Zhou et al 2011, Ferraro et al 2005, Kraus 1983, Breuer and Petruccione 2002, Rivas and Huelga 2011) and analyze the obtained results for the original, as well as for some alternative, degrees of freedom of the open system. The considered structures are *local* in the sense that the environmental degrees of freedom remain intact. We find that the environment non-equally "sees" the different structures. It appears, that there is *only one* structure that is distinguished by classicality and locality of the environment influence.

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[53] For Markovian bipartite open systems, which is our case, cf. eq.(106), (Ferraro et al 2010) pointed out non-occurrence of discord sudden death, i.e. the smooth disappearance of non-classical correlations. This is the reason we, in search for classicality, stick to the asymptotic solutions.

For an oscillator (mode) subjected to a lossy channel (or cavity at zero temperature), the master equation reads (Jiang et al 2011):

$$\frac{d\rho}{dt} = -\kappa \left[2a\rho a^{\dagger} - \{a^{\dagger}a, \rho\} \right] \tag{106}$$

with the bosonic "annihilation" operator a and the damping parameter κ. The master equation eq.(106) is known to be representable in the Kraus form (Ferraro et al 2005, Fan and Hu 2009, Jiang et al 2011, Zhou et al 2011):

$$\rho(t) = \sum_{n=0}^{\infty} K_n(t)\rho K_n^{\dagger}(t) \tag{107}$$

with the completeness relation $\sum_{n=1}^{\infty} K_n^{\dagger}(t)K_n(t) = I, \forall t$. For the amplitude damping process, i.e. for the master equations eq.(106), Kraus operators (Ferraro et al 2005, Fan and Hu 2009, Jiang et al 2011, Zhou et al 2011):

$$K_n(t) = \sqrt{\frac{(1-e^{-2kt})^n}{n!}} e^{-kNt} a^n, \quad N = a^{\dagger}a. \tag{108}$$

In the Heisenberg picture, the state ρ does not evolve in time. Then, in the Kraus representation, dynamics of an oscillator's observable A reads:

$$A(t) = \sum_{n=0}^{\infty} K_n^{\dagger}(t)A(t=0)K_n(t) = \sum_{n=0}^{\infty} \frac{(1-e^{-2kt})^n}{n!} a^{\dagger n} e^{-ktN} A(t=0) e^{-ktN} a^n. \tag{109}$$

The infinite sum in Eq.(109) is often approximated by a few first terms, e.g. in (Liu et al 2004). However, below we give exact solutions to Eq.(109) without calling for or imposing any approximation.

7.2.1 Original degrees of freedom

The structure we are interested in

$$(1 + E_1) + (2 + E_2) \tag{110}$$

can be described by the following form of interaction: $V = \alpha \sum_{k=1}^{2} (A_{S_1 k} \otimes B_{E_1 k} + A_{S_2 k} \otimes B_{E_2 k})$ (Rivas and Huelga 2011). If the open system's dynamics is Markovian [of the Lindblad form], one can totally separate dynamics of the two subsystems, 1 and 2, for the initial tensor-product[54] state ρ_{12}.

For the above interaction V, the master equation for $C = 1 + 2$ is of the form (Rivas et al 2010b, Rivas and Huelga 2011):

$$\frac{d\rho_{12}}{dt} = -\imath \sum_i [H_i + \alpha^2 H_{LS}^{(i)}, \rho_{12}]$$
$$+\alpha^2 \sum_{\omega,i,k,l} \gamma_{kl}^{(i)}(\omega) \left[A_k^{(i)}(\omega)\rho_{12}A_l^{(i)\dagger}(\omega) - \frac{1}{2}\{A_l^{(i)\dagger}(\omega)A_k^{(i)}(\omega), \rho_{12}\} \right]. \quad (111)$$

By tracing out eq.(111), $\rho_i = tr_j \rho_{12}, i \neq j = 1, 2$, with the use of $tr_i[B_j, \rho_{12}] = 0, i = j$ and $tr_i[B_j, \rho_{12}] = [B_j, \rho_j]$ for $i \neq j$, $i, j = 1, 2$, one easily obtains the following master equation:

$$\frac{d\rho_i}{dt} = -\imath [H_i + \alpha^2 H_{LS}^{(i)}, \rho_i]$$
$$+\alpha^2 \sum_{\omega,k,l} \gamma_{kl}^{(i)}(\omega) \left[A_k^{(i)}(\omega)\rho_i A_l^{(i)\dagger}(\omega) - \frac{1}{2}\{A_l^{(i)\dagger}(\omega)A_k^{(i)}(\omega), \rho_i\} \right] \quad (112)$$

for *both*, $i = 1, 2$.

We are interested in the independent, environment-induced amplitude-damping processes for the two oscillators, 1 and 2. For the "amplitude damping channel" for one oscillator, there is only one Lindblad operator, a–the "annihilation" boson operator. So, eq.(112) now obtains the form of eq.(106) for both oscillators (modes) with the respective damping parameters κ_i.

To facilitate our considerations, we switch to the Kraus representation of the master equation eq.(106). We do that in the Heisenberg picture.

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[54] For correlated state ρ_{12}, the S_i system is in initial correlation with the effective environment, $S_j + E, j \neq i = 1, 2$, and thus its dynamics is not Markovian (Rivas and Huelga 2011); see Section 6.2.

Independent amplitude damping channels for the two modes are presented by mutually non-correlated, local, Kraus operators, $K_m^1 \otimes I_2$ and $I_1 \otimes K_n^{(2)}$, i.e. by the separable total operation $K_m^{(1)} \otimes K_n^{(2)}$. This operation gives for a one-mode operator, A_1:

$$\begin{aligned} &\sum_{m,n=0}^{\infty} K_m^{(1)\dagger} \otimes K_n^{(2)\dagger} A_1(t=0) \otimes I_2 K_m^{(1)} \otimes K_n^{(2)} = \\ &\sum_{m=0}^{\infty} K_m^{(1)\dagger} A_1(t=0) K_m^{(1)} \otimes \sum_{n=0}^{\infty} K_n^{(2)\dagger} K_n^{(2)} = A_1(t) \otimes I_2 \end{aligned} \tag{113}$$

Similarly for a $A_1 B_1$ operator:

$$\begin{aligned} &\sum_{m,n=0}^{\infty} K_m^{(1)\dagger} \otimes K_n^{(2)\dagger} A_1(t=0) B_1(t=0) \otimes I_2 K_m^{(1)} \otimes K_n^{(2)} = \\ &\sum_{m=0}^{\infty} K_m^{(1)\dagger} A_1(t=0) B_1(t=0) K_m^{(1)} \otimes \sum_{n=0}^{\infty} K_n^{(2)\dagger} K_n^{(2)} \equiv \\ &(A_1 B_1)(t) \otimes I_2. \end{aligned} \tag{114}$$

Above we used the completeness relation for the 2 system's Kraus operators. Of course, the completeness relation for the two-mode Kraus operators is fulfilled: $\sum_{m,n=0}^{\infty} K_m^{(1)\dagger} \otimes K_n^{(2)\dagger} K_m^{(1)} \otimes K_n^{(2)} = I_1 \otimes I_2 \equiv I_{12}$. For the two-mode operators:

$$\begin{aligned} &\sum_{m,n=0}^{\infty} K_m^{(1)\dagger} \otimes K_n^{(2)\dagger} A_1(t=0) \otimes A_2(t=0) K_m^{(1)} \otimes K_n^{(2)} = \\ &\sum_{m=0}^{\infty} K_m^{(1)\dagger} A_1(t=0) K_m^{(1)} \otimes \sum_{n=0}^{\infty} K_n^{(2)\dagger} A_2(t=0) K_n^{(2)} \equiv \\ &A_1(t) \otimes A_2(t), \end{aligned} \tag{115}$$

which exhibits independence of the actions of the two environments, E_1 and E_2.

We use the following generalization of the Baker-Hausdorff lemma (Mendaš and Popović 2010):

$$e^{-sA}Be^{-sA} = B - s\{A,B\} + \frac{s^2}{2!}\{A,\{A,B\}\} - \frac{s^3}{3!}\{A,\{A,\{A,B\}\}\} + \ldots \tag{116}$$

where the curly brackets denote anti-commutator, $\{A,B\} = AB + BA$. So

$$e^{-ktN}ae^{-ktN} = e^{kt}ae^{-2ktN}, \quad e^{-ktN}a^{\dagger}e^{-ktN} = e^{-kt}a^{\dagger}e^{-2ktN} \tag{117}$$

Substituting eq.(1117) into eq.(109) one directly obtains:

$$a^{\dagger}(t) = e^{-kt}a^{\dagger}\sum_{n=0}^{\infty}\frac{(1-e^{-2kt})^n}{n!}a^{\dagger n}e^{-2ktN}a^n = e^{-kt}a^{\dagger}. \tag{118}$$

Similarly:

$$a(t) = -e^{kt}\sum_{n=0}^{\infty}\frac{(1-e^{-2kt})^n}{(n-1)!}a^{\dagger n-1}e^{-2ktN}a^n + e^{kt}a. \tag{119}$$

With the use of $\sum_{n=0}^{\infty}\frac{(1-e^{-2kt})^n}{(n-1)!}a^{\dagger n-1}e^{-2ktN}a^n = (1-e^{-2kt})a$, we obtain:

$$a(t) = e^{-kt}a. \tag{120}$$

In the completely analogous way one obtains:

$$\begin{aligned}(a^2)(t) &= e^{-2kt}a^2\\ (a^{\dagger 2})(t) &= e^{-2kt}a^{\dagger 2}\\ (a^{\dagger}a)(t) &= e^{-2kt}a^{\dagger}a.\end{aligned} \tag{121}$$

Now with the aid of

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a + a^{\dagger}), \quad p = \imath\left(\frac{m\hbar\omega}{2}\right)^{1/2}(a^{\dagger} - a), \tag{122}$$

we obtain the following solutions to the Heisenberg equations for the position and momentum observables:

$$
\begin{aligned}
&x(t) = e^{-kt}x, \quad p(t) = e^{-kt}p \\
&x^2(t) = e^{-2kt}x^2 + \frac{\hbar}{2m\omega}(1 - e^{-2kt}) \\
&p^2(t) = e^{-2kt}p^2 + \frac{m\hbar\omega}{2}(1 - e^{-2kt}).
\end{aligned}
\tag{123}
$$

From eq.(123), one directly obtains asymptotic solutions:

$$
\lim_{t\to\infty} x(t) = 0 = \lim_{t\to\infty} p(t), \quad \lim_{t\to\infty} x^2(t) = \frac{\hbar}{2m\omega}, \lim_{t\to\infty} p^2(t) = \frac{m\hbar\omega}{2}. \tag{124}
$$

From eq.(124) directly follows product of the standard deviations in the asymptotic limit for *both* oscillators:

$$
\lim_{t\to\infty} \Delta x(t)\Delta p(t) = \frac{\hbar}{2}. \tag{125}
$$

Physically, eq.(125) is clear: asymptotic states, for both oscillators, are the minimum uncertainty states. In the position-representation, those states are the minimum uncertainty Gaussian states–the well-known Sudarshan-Glauber coherent states.

For the Markovian bipartite open systems (which is our case for the structure eq.(110) and for both oscillators, 1 and 2) it is well known, that non-classical correlations smoothly disappear in the asymptotic limit–there is no discord sudden death (Ferraro et al 2010). On the other hand, for Gaussian states (Adesso and Datta 2010), the only bipartite-system states that have zero discord are the tensor product states–no correlations at all. Hence, we directly conclude about the *preferred asymptotic states*, (the approximate pointer basis) for the pair of oscillators, that satisfy eq.(125):

$$
|\alpha\rangle_1|\beta\rangle_2, \tag{126}
$$

where $|\alpha\rangle_1$ and $|\beta\rangle_2$ are the Sudarshan-Glauber coherent states, i.e. the minimum uncertainty Gaussian states for the two oscillators, 1 and 2.

7.2.2 Alternative degrees of freedom

We introduce formally a pair of the degrees of freedom, X_A and ξ_B, with the conjugate momentums, P_A and π_B, $[X_A, P_A] = \imath\hbar$ and $[\xi_B, \pi_B] = \imath\hbar$; of course, $[X_A, \pi_B] = 0 = [\xi_B, P_A]$. Without loss of generality, let us consider the following linear canonical transformations[55]:

$$\begin{aligned} X_A &= \sum_i \alpha_i x_i, \quad P_A = \sum_j \gamma_j p_j, \quad i,j = 1,2 \\ \xi_B &= \sum_m \beta_m x_m, \quad \pi_B = \sum_n \delta_n p_n, \quad m,n = 1,2. \end{aligned} \tag{127}$$

for the pair of oscillators considered in Section 7.2.1.

Then the total system's Hilbert state space factorizes, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, while the Hamiltonian obtains the general form $H = H_A + H_B + H_{AB}$.

According to the above task, $\mathcal{T}$, we are interested in solutions to the Heisenberg equations for the alternative degrees of freedom.

However, we cannot directly use the master equation eq.(106) in order to derive the Kraus operators for the new subsystems, A and B.

The transformations eq.(127) are local, i.e., they leave the environmental degrees of freedom intact. On the other hand, as the oscillators are out of any external (classical) field, bearing in mind experience with the model in Section 6.3, we directly conclude that there is not any interaction between the new subsystems, A and B, i.e. that $H_{AB} = 0$. However, the LCTs eq.(127) change the character of interaction with the environment. This is easily seen from the forms of the Kraus operators for the original oscillators, eq.(108). Placing the inverse to eq.(127) into eq.(108) directly provides the following conclusion: for the new subsystems, A and B, the environment $E = E_1 + E_2$

---

[55] With the constraints: $\alpha_i \gamma_i = 1 = \beta_i \delta_i$, and $\alpha_i \delta_i = 0 = \beta_i \gamma_i$.

acts as a *common* environment, non-locally. This is, one can easily show:

$$K_m^{(1)} \otimes K_n^{(2)} \neq K_m^{(A)} \otimes K_n^{(B)}. \tag{128}$$

Physically, it means that *non-local* action is exerted by the *total* environment E on the pair $A + B$.

This conclusion also [directly] follows from eq.(25) in the context of Entanglement Relativity: according to ER, the preferred states eq.(126) typically obtain entangled form for the new structure, $A + B$. So, while the environment E independently acts on the 1 and 2 systems, its action on the A and B systems is [typically] non-local. Finally, one can deal with eq.(106) by expressing the old Lindblad operators via the new subsystem's operators. On this basis one expects nonseparation of master equations for the new subsystems A and B, i.e. nonvalidity of the master equation eq.(112) for the new subsystems A and B.

In the structure terms, the model of the total system (as distinct from eq.(110)) reads:

$$(A + B) + E. \tag{129}$$

Fortunately enough, the Kraus operators formalism deals with the infinite *sums*, not with the individual Kraus operators. So, we can circumvent all the technical problems by dealing with the infinite sums of the Kraus operators for the original structure, eq.(110), while expressing the new variables through the old ones.

With the use of eqs.(123), (127), we can directly write for the new position and momentum observables:

$$\begin{aligned} X_A(t) &= \sum_i \alpha_i x_i(t), P_A(t) = \sum_i \gamma_i p_i(t) \\ \xi_B(t) &= \sum_i \beta_i x_i(t), \pi_B(t) = \sum_i \delta_i p_i(t). \end{aligned} \tag{130}$$

Similarly, e.g.

$$X_A^2(t) = \sum_{i,j} \alpha_i \alpha_j (x_i x_j)(t), P_A^2(t) = \sum_{i,j} \gamma_i \gamma_j (p_i p_j)(t); \tag{131}$$

of course [cf. eqs.(114), (115)], $(ab)(t) \equiv \sum_{m,n=0}^{\infty} K_m^{(1)\dagger}(t) K_n^{(2)\dagger}(t) \quad ab\ K_m^{(1)}(t)$ $K_n^{(2)}(t)$. Analogous expressions can be directly written for the B system.

For the tensor product initial state $\rho_{12}(0) = \rho_1(0)\rho_2(0)$, with the aid of eq.(123), we obtain:

$$\begin{aligned}
&(\Delta X_A(t))^2 = tr_{12} \left[\sum_{i,j} \alpha_i \alpha_j (x_i x_j)(t) \rho_{12}(0) \right] - \left[tr_{12} \sum_i \alpha_i x_i(t) \rho_{12}(0) \right]^2 = \\
&\sum_i \alpha_i^2 (\Delta x_i(t))^2 + \sum_{i,j \neq i} \alpha_i \alpha_j \left[\langle (x_i x_j)(t) \rangle - \langle x_i(t) \rangle \langle x_j(t) \rangle \right] = \\
&\sum_i \alpha_i^2 (\Delta x_i(t))^2.
\end{aligned} \tag{132}$$

In complete analogy, one can calculate all the other standard deviations finally to obtain in the asymptotic limit:

$$\begin{aligned}
\Delta X_A(\infty) \Delta P_A(\infty) &= \hbar \sqrt{\left(\frac{\alpha_1^2}{2m_1\omega_1} + \frac{\alpha_2^2}{2m_2\omega_2} \right) \left(\frac{\gamma_1^2 m_1 \omega_1}{2} + \frac{\gamma_2^2 m_2 \omega_2}{2} \right)} \\
\Delta \xi_B(t) \Delta \pi_B(t) &= \hbar \sqrt{\left(\frac{\beta_1^2}{2m_1\omega_1} + \frac{\beta_2^2}{2m_2\omega_2} \right) \left(\frac{\delta_1^2 m_1 \omega_1}{2} + \frac{\delta_2^2 m_2 \omega_2}{2} \right)}.
\end{aligned} \tag{133}$$

In general, the rhs of both expressions in eq.(133) are larger than $\hbar/2$.

On the other hand, the common environment ($E = E_1 + E_2$) for the subsystems A and B is expected to induce correlations for the A and B systems, even if the initial state is tensor product. This can be easily justified by the use of the "covariance function", e.g. $C(t) = \langle X_A(t) \xi_B(t) \rangle - \langle X_A(t) \rangle \langle \xi_B(t) \rangle$.

From eqs.(123) and (127) we obtain:

$$C(\infty) = \lim_{t\to\infty} \sum_{i,j} [(x_i x_j)(t) - x_i(t) x_j(t)] =$$

$$\sum_i \alpha_i \beta_i \left(\Delta x_i(\infty)\right)^2 = \alpha_1 \beta_1 \frac{\hbar}{2m_1\omega_1} + \alpha_2 \beta_2 \frac{\hbar}{2m_2\omega_2}, \tag{134}$$

which, typically, is non-zero; in eq.(134), likewise for eq.(123), we used notation $(x_i x_j)(t) = x_i(t) x_j(t), i \neq j$, for the tensor product initial state.

Non-zero covariance function reveals presence of correlations[56] in the $A+B$ structure of the composite system, even in the asymptotic limit.

7.2.3 Preferred structure

For the A representing the center of mass and the B representing the "relative particle" for the pair of equal-mass ($m_1 = m_2$) and resonant ($\omega_1 = \omega_2$) oscillators[57], i.e. for $\alpha_1 = \ 1/2 = \alpha_2, \beta_1 = 1 = -\beta_2, \gamma_1 = 1 = \gamma_2$ and $\delta_1 = 1/2 = -\delta_2$, one obtains equalities on the rhs of eq.(133), $\Delta X_A(\infty)\Delta P_A(\infty) = \hbar/2$ and $\Delta\xi_B(\infty)\Delta\pi_B(\infty) = \hbar/2$, as well as the absence of correlations, $C(\infty) = 0$.

However, typically, the preferred states for the $A+B$ structure are not the minimum uncertainty states and are correlated.

The states eq.(126) are arguably the most classical bipartite system states of all. They are free of any kind of correlations (classical or quantum) and are of the minimum quantum uncertainty. Hence, [in the asymptotic limit], one can imagine the pair 1+2 as a pair of "individual", mutually distinguishable and non-correlated systems. In a sense, this is a definition of "classical systems" (Giulini et al 1996, Zurek 2003, Schlosshauer 2004). On the other hand,

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[56] However, zero covariance function does not guarantee the absence of correlations. The correlations can be classical or quantum–to distinguish between them, one should use discord, Section 3.2.

[57] These are the common assumptions–that simplify calculation, see e.g. (Paz and Roncaglia 2008)–that are absent from our considerations.

none of these is in general valid for the alternate structure $A+B$: even for the initial tensor product state for $A+B$, non-local action of the common environment induces correlations, even in the asymptotic limit. So, one can say that the environment composed of two noninteracting parts, which induce independent (local) amplitude damping processes, makes the 1 + 2 structure special ("preferred").

7.3 Atom in electromagnetic field

The composite system C consists of an atom's internal degrees of freedom (A) in electromagnetic field (EM); $C = A + EM$.[58] The C system is monitored by the environment, which is *supposed* to be photon absorbing and quickly to thermalize (Stokes et al 2012). A similar analysis can be found in (Stokes 2012).

Structural changes in C are performed by certain unitary operations that give rise to the different forms of the C's Hamiltonian, H.

Different forms of the Hamiltonian are expected to give rise to different master equations for different structures of the open system. The authors introduce the following *criterion of classicality*: the preferred structure is the one that provides predictions in accordance with the presence of the photon-absorbing environment. Some other characteristics of the environment, i.e. of physical situation, could lead to different conclusions about the preferred structure of the open system C.

The following forms of the composite system's Hamiltonian are of interest. The original structure, $A+EM$, is defined by the so-called minimal-coupling Hamiltonian:

$$H = H^{(min)} = \frac{1}{2m_A}[\vec{p}_A + e\vec{A}_{EM}(\vec{0})]^2 + V(\vec{r}_A) +$$

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[58] The A represents the atomic internal (R) system for the standard $CM + R$ atomic structure, Chapter 5. Only the subsystem R is in interaction with the electromagnetic field. For this reason, the atomic CM system is omitted from considerations–compare to Section 5.3.

$$\frac{1}{2}\int d^3\vec{x}\left[\frac{1}{\mu_\circ}|\vec{B}_{EM}(\vec{x})|^2 + \frac{1}{\epsilon_\circ}|\vec{\Pi}_{EM}(\vec{x})|^2\right]. \tag{135}$$

In eq.(135), one can easily recognize the EM self-energy (the last term) and the minimal coupling of the atom with the electromagnetic field. The conjugate observables are $\vec{r}_A, \vec{p}_A$, for the atom, and $\vec{A}_{EM}, \vec{\Pi}_{Em}$ for the EM field; $\vec{B} = \vec{\nabla} \times \vec{A}$.

With the use of the specific unitary transformations, the following forms of the Hamiltonian are obtained:

$$\begin{aligned}
&H = H^{(mult)} = \frac{\vec{p}_1^{\,2}}{2m_A} + V(\vec{r}_1) + \\
&\frac{1}{2}\int d^3\vec{x}\left[\frac{1}{\mu_\circ}|\vec{B}_2(\vec{x})|^2 + \frac{1}{\epsilon_\circ}|\vec{\Pi}_2(\vec{x})|^2\right] \quad \text{[multipolar]}, \\
&H = H^{(rw)} = \sum_{\vec{k},\lambda} \hbar g_{\vec{k}\lambda}\sigma_{ex}^{+} a_{F\vec{k}\lambda} + H.c. + \hbar\omega_\circ \sigma_{ex3} + \\
&\sum_{\vec{k}\lambda} \hbar\omega_k a^\dagger_{F\vec{k}\lambda} a_{F\vec{k}\lambda}, \quad [\mathrm{rotating-wave}].
\end{aligned} \tag{136}$$

The transformations behind these forms of the total system's Hamiltonian are specific in that they do not change the degrees of freedom: $\vec{r}_1 = \vec{r}_A$ and $\vec{A}_2 = \vec{A}_{EM}$, hence $\vec{B}_2 = \vec{B}_{EM}$. However, their conjugate momentums change so as $[\vec{p}_A, \vec{p}_1] \neq 0$. The rotating wave form of the total system's Hamiltonian is obtained after approximating the atomic internal system by the exciton two-level model (compare to Section 4.1)–hence the Pauli operators σ and the annihilation and creation operators on the bosonic Fock space in eq.(136). The "rotating wave" structure is thus a variant of the famous spin-boson model.

The structure transformations can be described as:

$$\mathcal{S}_{min} = \{\vec{r}_A, \vec{A}_{EM}, \vec{p}_A, \vec{\Pi}_{EM}\} \to \mathcal{S}_{mult} = \{\vec{r}_A, \vec{A}_{EM}, \vec{p}_1, \vec{\Pi}_2\} \to \mathcal{S}_{rw} = \{\vec{\sigma}_{ex}, N_F\} \tag{137}$$

$N_F \equiv a^\dagger_F a_F$. Definitions of the momentum observables as well as physical interpretation of the structures can be found in the original paper (Stokes et al 2012). These subtle details are not substantial for our considerations.

By applying the second order perturbation approximation, the authors derive master equations[59] for the different structures. Expectably, these master equations are both formally and physically different.

As it is emphasized above, the criterion for classicality relies on the experimental evidence with the photon-absorbing environment. Such environment (that quickly thermalizes after the photon absorption) does not support spontaneous emission for the atom in the ground state–there are not photons in the field that could re-excite the atom. For this specific, yet realistic, physical situation, the authors were able to show that only the "rotating wave" Hamiltonian provides the proper master equation [with notation adapted to eq.(136)] (see their eq.(67)):

$$\frac{d\rho_{ex}}{dt} = -\imath\omega_\circ[\sigma_{ex3}, \rho_{ex}] + \frac{1}{2}A_-(2\sigma_{ex}^-\rho_{ex}\sigma_{ex}^+ - \{\sigma_{ex}^+\sigma_{ex}^-, \rho_{ex}\}). \tag{138}$$

Formally, this is the master equation eq.(80). From eq.(138) is calculated the stationary state photon emission rate, $I_{ss} = 0$, which is *in accordance* with the experimental evidence. The other master equations, that correspond to other structures, give physically unreasonably large photon emission [without any external driving]. Thereby, for the considered physical *situation*, the *preferred structure* is $\mathcal{S}_{rw}$.

The authors emphasize that a change of the criterion for classicality, which would correspond to another physical situation, would, in general, distinguish some other structure of the composite system as "preferred structure".

7.4 Outlook

Interaction determines correlation of "system" and its environment (Dugić 1996, 1997); see Supplement for some technical details. The kind and the

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[59] Not yet emphasizing the complications originating from QCR.

type of correlation determines the preferred structure.

If the total system ("system+environment") is in entangled state:

$$|\Psi\rangle_{SE} = \sum_i c_i |i\rangle_S |i\rangle_E, \tag{139}$$

both the open system's and the environment's state are unique for every structure. Regarding the model of Section 7.2, eq.(110), in accordance with the solutions to eqs.(111)-(112), the total system's state in the asymptotic limit is tensor product [in simplified form] $|\phi\rangle_{1+E_2}|\chi\rangle_{2+E_2} = \sum_\alpha c_\alpha |\alpha\rangle_1 |\epsilon(\alpha)\rangle_{E_1}$ $\sum_\beta d_\beta |\beta\rangle_2 |\epsilon(\beta)\rangle_{E_2}$. However, for the structure, $S + E = (1+2) + (E_1 + E_2)$, the state takes the form of eq.(139):

$$|\Psi\rangle_{SE} \equiv |\Psi\rangle_{12E} = \sum_{\alpha,\beta} C_{\alpha\beta} |\alpha\rangle_1 |\epsilon(\alpha)\rangle_{E_1} |\beta\rangle_2 |\epsilon(\beta)\rangle_{E_2} \equiv \sum_k d_k |k\rangle_{12} |k\rangle_E, \tag{140}$$

where $C_{\alpha\beta} \equiv c_\alpha d_\beta$ and $k \equiv (\alpha, \beta)$, for both S and E.

However, for the alternate $A + B$ structure, eq.(140) acquires the form:

$$|\Psi\rangle_{SE} \equiv |\Psi\rangle_{ABE} = \sum_k d_k |k\rangle_{AB} |k\rangle_E, \tag{141}$$

where, of course, the preferred states for the total system S[60], $|k\rangle_S = |k\rangle_{12} = |k\rangle_{AB}, \forall k$, but, in general, $|k\rangle_{AB}$ is not of the tensor-product form relative to the $A + B$ structure. The environment E acts as a whole, simultaneously on both subsystems A and B–the subsystems A and B have common environment E. From Section 3.1 we know that, for at least some states $|k\rangle_{12}$ in eq.(140), $|k\rangle_{12} = \sum_m c_{km} |m\rangle_A |m\rangle_B$. So collecting eq.(140) and eq.(141) we

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[60] The nonorthogonal Gaussian states constitute an approximate pointer basis–compare to eq.(148).

can write ($1+2=S=A+B$):

$$\sum_k d_k|k\rangle_{12}|k\rangle_E = \sum_k d_k \left(\sum_m c_{km}|m\rangle_A|m\rangle_B\right)|k\rangle_E, \tag{142}$$

which clearly exhibits the *preferred states*, $|k\rangle_S$, *and* the *preferred structure*, $1+2$, of the open system S–$|k\rangle_S = |k\rangle_{12} = |\alpha\rangle_1|\beta\rangle_2$, eq.(126)–which justifies the Clue from Section 7.1.

The model considered in Section 7.3 does not offer such a clear picture on the choice of the preferred structure. For this to be provided, solutions to *all* master equations referring to the different structures are needed. Needless to say, this is a complicated task. Nevertheless, bearing in mind eq.(142), one can expect analogous conclusions.

So we find the results of Sections 7.2 and 7.3 mutually qualitatively consistent and also consistent with the told in Section 7.1. This consistency encourages us to state

Conjecture 2. *The environment (i.e. its interaction with the open system) is responsible for existence of the "preferred" structure of the open system.*

In this context, it becomes clear: there is not any reason to claim or suppose existence of "preferred structure" (or of the preferred states and/or observables) for a closed physical system (i.e. for the Universe)–cf. Chapter 6 and Chapter 8 for details.

The above conjecture is in intimate relation with the recent suggestion in (Harshman 2012a): "*the physically-meaningful observable subalgebras are the ones that minimize entanglement in typical states.*" Rigorously speaking, this is *another criterion of classicality*, which is not considered in this book: *minimum correlations* in open system[61]. This condition is already fulfilled for the model considered in Section 7.2: the state eq.(126) is without any correlations *relative* to the preferred structure $1+2$. Similarly, regarding the *more*

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[61] The opposite, i.e. the requirement for the maximum correlations, is essential for quantum information processing. To this end see (Fel'dman and Zenchuk, 2012).

general considerations of the Markov open systems (Arsenijević et al 2012), the minimum correlations as a criterion of classicality distinguishes the model eq.(110).

In summary, we can conclude: typically, the environment [i.e. its *interaction* with the open system's degrees of freedom–compare e.g. eq.(110) with eq.(129)] distinguishes preferred structure of the open composite system. We conjecture that this is a universal rule of the open systems theory. Regarding the closed systems, of course, this is not the case, as we elaborate in the next chapter.

Chapter 8

Some Interpretation-Related Issues

Classical ”phase space” of a physical system is *unique*. All degrees of freedom (and their conjugate momenta) of the system, that are mutually related by linear transformations, belong to the same phase space. This analogously applies to the quantum mechanical counterpart. As we have emphasized in Section 2.3, state space of a quantum system is unique Hilbert space. Quantum state of a system is unique in every instant of time.

8.1 Global irreducible structures with decoherence

Let us consider the Universe as a closed quantum system. By definition, there is nothing outside the Universe, including ”observer”. To this end, there is no room for any operational definition of the Universe preferred structure. Without any additional condition/criterion, all structures of the Universe are equally physically valid. Every structure, denoted σ_i, is defined by a set of observables, whose locality is adapted to the tensor factorization of the Hilbert state space. All the structures share the same physical space and time, and their dynamics are uniquely determined–there is unique (pure) quantum state of the Universe in every instant in time.

Every structure σ_i is composed of some ”elementary particles” and by structure-specific fundamental interactions (i.e. symmetries) between them. Every instantaneous universal state can be expressed (cf. Section 3.1) in a unique way for every structure separately.

In every σ_i structure, additional LCTs are allowed *locally* to re-define the structure[62]. If a local transformation is indexed by α, then $\sigma_{i\alpha}$ represents the αth local variation of the σ_i structure. This subtle topic will be considered in Section 8.2.

Of all possible structures, σ_i, we are interested in the structures, $\mathcal{S}'_n$, that are, including our structure (denoted $\mathcal{S}_\circ$), mutually global and irreducible; $\{\mathcal{S}'_n\} \subset \{\sigma_i\}$. For such structures, the respective sets of "elementary particles" are mutually irreducible. Dynamics of such structures, although unique on the level of the Universe, are mutually independent, autonomous. Physical interactions, as well as the related symmetry conditions, may be totally different (Anderson 1993, 1994, Harshman 2012b, Manzano et al 2013). Of course, provided the full details for one structure are known, one can mathematically describe all other structures, in full detail. Such structures are (Section 2.2) mutually information-theoretically independent, separated. Symmetry fixed for one structure uniquely determines (induces) the symmetry rules for every other structure.

One can still ask if a local measurement in one structure can represent a measurement of certain variables characteristic for an alternative structure. This subtle question regards both local structures, which will be considered in Section 8.2, as well as the issue of the "quantum reference frame", which will be discussed in Section 8.3.2. One should still keep in mind: "observation" [cf. Chapter 7] is local. So, *an observer can directly "see" only the systems, which belong to the structure he lives in.* Acquiring information about the subsystems of the alternate structures is inevitably indirect and limited, i.e. partial, Lemma 2.1.

Having in mind equal physical status of the considered structures $\mathcal{S}'_n$, it is apparent: *observer cannot operationally conclude which structure he is a part*

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[62] E.g., in our structure, instead of $e+p$, the hydrogen atom can be described as $CM+R$– see Chapter 5.

of. Due to invertibility of the LCTs, our structure is alternative relative to the other structures. Which structure is then primary[63]?

We place a special emphasis on the $\mathcal{S}_i$ structures which are subject to decoherence-induced classicality (for an example see Section 6.3). This additionally shrinks the set of the structures of interest for us: $\{\mathcal{S}_i\} \subset \{\mathcal{S}'_n\}$. So we are interested in the structures that are, *relative to each other as well as to our structure*, global and irreducible, and of all of them, we are interested only in the structures that *support decoherence* for certain local degrees of freedom.

8.2 Local structures and classicality

In Section 8.1 we distinguished the set of mutually global and irreducible structures, $\{\mathcal{S}_i\}$, which carry decoherence for some of their respective degrees of freedom. Let us denote by $\mathcal{S}_\circ$ the one we belong to, and the other by $\mathcal{S}_j, j = 1, 2, ...$

Every such structure is defined by a set of the fundamental degrees of freedom, which can be subject to local transformations of variables. An illustration is given by Example 2 in Section 2.2. Here we use notation of Section 2.2 to emphasize local transformations:

$$\mathcal{S}_1 = \{1e, 2e, 1p, 2p\} \to \mathcal{S}_2 = \{1H, 2e, 2p\} \to \mathcal{S}_4 = \{1CM, 1R, 2CM, 2R\}, \tag{143}$$

for every pair of "neighbor" structures. Analogous transformations can be performed for every structure $\mathcal{S}_j$.

Grouping the particles and imposing certain boundary conditions can lead to formation of a local alternative structure $\mathcal{S}'_\circ$ for our structure. Physically, the new subsystems can be some composite particles, like mesons, atoms, molecules, compounds, large bodies and so on. This local re-structuring can be performed for every structure $\mathcal{S}_j$.

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[63] Our structure may look like the $CM + R$ structure for some alternate structure of the Universe.

How many local structures, $\mathcal{S}_{i\alpha}$, of the $\mathcal{S}_i$ structure (here: $i = 0, 1, 2, 3, ...$), can carry decoherence? According to Sections 7.2 and 7.3, there is only one such a local structure for every $\mathcal{S}_i$. However, this is only a plausible conjecture–cf. Conjecture 2 in Section 7.3. Justifying/unjustifying this conjecture, i.e. defining local "systems" for a structure $\mathcal{S}_i$, is an open issue yet (Arsenijević et al 2012, Harshman 2012a, Zanardi 2001)[64].

This subtlety of "what is 'system'?" (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008) clearly exhibits limitations of the pure theoretical considerations. Rather, *some phenomenological facts are needed.* It is not surprising, as quantum mechanics offers much more than our experience can support[65].

As emphasized in Section 7.1: local structural variations *are meaningless for the already decohered structure.* Decohered degrees of freedom (subsystems of a composite system) are quasi-classical. For the quasi-classical degrees of freedom, the transformations of variables become nonphysical, a mathematical artifact. As it is emphasized throughout this book (cf. e.g. Chapter 5): the center-of-mass positions of the macroscopic bodies are quasi-classical and hence regarded as (locally) physically *realistic.* Due to the very meaning of "realistic"[66], linear combinations of the centers of mass of the macroscopic bodies cannot be realistic. This way, *we justify the classical prejudice* distinguished in Section 2.1: our structure [*phenomenologically*] supports decoherence, and decohered degrees of freedom have classical reality. Of course, this reality is *local*, i.e. of relevance and interest *only* for *our* structure, which we are a part of–what's realistic in one structure does not determine what is realistic in any other structure.

Local structures, including the "classical" ones provided by decoherence, are

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[64] e.g. The atoms presented by the structure $\mathcal{S}_3 = \{1H, 2H\}$, where "$H$" denotes a hydrogen atom, which, as a subsystem of the Universe, can be differently decomposed. See also the molecule structures $\mathcal{S}_1$ and $\mathcal{S}_5$ in Section 4.1.

[65] Recall the efforts to introduce the one-particle models, *in order to avoid quantum entanglement*, for the composite systems in nuclear physics and condensed matter physics.

[66] "Realistic" serves primarily to define what is "not realistic".

reducible. Observing classical structures gives rise to the classical prejudice (Section 2.1) and directly results in classical intuition on finite decomposability of the physical matter. Apotheosis of this position brings about the naive reasoning as described in Section 2.1–classical reasoning precludes the idea of the alternative quantum structures $\mathcal{S}_j$.

Composition of our decoherence-defined structure of the Universe is a consequence of a *dynamical change* of local structures: the systems are constantly exchanging particles, some systems are in formation while some other are splitting (or decaying). This dynamical particles-exchange is an instance of the trivial LCTs (Section 2.2.1). It provides dynamical local changes in our structure and stresses the fact, that the time-independent models, typical for the decoherence theory (cf. Chapters 6 and 7), as well as for the standard open systems theory (Breuer and Petruccion 2002, Rivas and Huelga 2011), are somewhat artificial. In such dynamical system, some *effective* and approximate structures are expected, and the physical description can be complicated. Furthermore, there may appear some "emergent" properties of the macroscopic bodies that are poorly understood in physical sciences, but vastly referred to, in biology, economy, social sciences, psychology etc. (Auyang 1998).

It is worth repeating: everything told for our structure $\mathcal{S}_\circ$ and local observations can be in principle applied to every other structure $\mathcal{S}_i$. While we do not claim existence of "observer" in any of the alternate structures, we use this standard vocabulary to highlight physical equivalence of the Universe structures we are interested in.

8.3 A unifying physical picture

The group-theoretic character of the LCTs can formally link the structures, which are endowed by decoherence. However, this mathematical possibility is physically irrelevant. Actually, according to Section 8.2: performing LCTs on the local (decoherence endowed) structures is physically pointless. So one can say:

The group-theoretic character of LCTs does not imply physical *reducibility of all structures onto one and only one structure of the Universe.*

Nevertheless, there is a subtlety, which might not be obvious. In Section 8.3.1 we connect the microscopic and macroscopic domains for our structure of the Universe. In Section 8.3.2, we discuss the recently elevated issue of "quantum reference frames".

8.3.1 Microscopic vs macroscopic domain

The microscopic physical domain is phenomenologically described in Chapter 5. In theoretical analysis, all kinds of LCTs are in principle allowed–that constitutes the core of the "what is 'system'?" issue (Dugić and Jeknić 2006, Dugić and Jeknić-Dugić 2008).

The "macroscopic domain" is the classical physics domain. Its quantum mechanical origin seems naturally to appear within the universally valid quantum mechanics (Giulini et al 1996, Zurek 2003, Schlosshauer 2004). For the Universe as a whole there may be different structures, whose local variations can be endowed by decoherence for certain (local) degrees of freedom. We can think of these structures in analogy with our own, which, in turn, is a dynamical system with the local particles exchange, i.e. with weakly defined border-line between the systems, and between the systems and their environments. Of course, classicality of the alternative structures is a matter of the "parallel occurrence of decoherence", which is as yet rigorously established only for the quantum Brownian motion model, Section 6.3.

In our structure, which is paradigmatic for our considerations, there is continuous exchange of particles between the systems. The Universe split into subsystems is subtle and, as yet, not well known a topic. This may be a sign for a need for a new methodology, which could encompass all the subtleties regarding the many-particle systems structures.

In the absence of such methodology, below we collect the findings from the previous Chapters as kind of "algorithm" for defining the possible structures of the Universe:

(a) For our structure, we phenomenologically learn about the set of elementary particles and their local compositions such as the atoms, molecules etc. Its dynamics allows local structural variations on the both micro- and macroscopic level (domain). Regarding the macroscopic domain, we recognize decoherence as the *fundamental* and also *universal* quantum mechanical process. This process provides the (quasi)classical dynamics of certain degrees of freedom and defines what's "local" and "realistic" in a given instant in time. This bases our classical intuition, and, as yet, the dominant view of the quantum Universe.

(b) Perform the LCTs of the fundamental (microscopic) degrees of freedom of our structure. Of all thus obtained structures, consider those that are global and irreducible relative to each other as well as to our structure. Of all such structures, choose only those supporting decoherence for some of their local degrees of freedom[67]. Everything told in the (a) above, should be analogously expressed for such alternate structures of the Universe. The structures of the kind are mutually information-theoretically separated, and, due to decoherence in all of them, application of the LCTs on their (quasi)classical structures loses its physical meaning and relevance.

(c) An observer belongs to one and only one such structure. The only degrees of freedom he is able directly to observe are the parts of the structure he belongs to. While existence of intelligent observer is not required for all the structures (Dugić et al 2002), we use this terminology to highlight physically equal status of all the structures as well as to emphasize the possibility to choose the classical reference frame in every of them. Some subtleties regarding the recently raised issue of quantum reference frames will be considered in the next section.

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[67] In principle, existence of such structures is provided in Section 6.3.

8.3.2 The quantum reference frame issue

Quantum decoherence provides quasiclassical behavior of certain open-system's degrees of freedom. "Observer" is usually assumed to be a classical system that can collect (classical) information about the open system.

However, "observation" assumes existence of "reference frame" where "observer" is spatially placed. Hence the familiar classical reference frames. To this end, it is important to stress: if x_S is a system's position observable, its measurement from the O reference frame is defined by the $x_S - X_O$ variable, where X_O is the reference-frame position, which is a *classical* variable–a c-number. In order to highlight this definition, we introduce the standard "hat" mark for the quantum mechanical observables: $\hat{x}_S - X_O\hat{I}$, where the $\hat{I}$ is the identity operator. So it is clear: the variable $\hat{x}_S - X_O\hat{I}$ is *not* obtained via canonical transformation. If there are more than one reference frame, then $\hat{x}_S - X_i\hat{I}$ denotes the system's position seen from the ith (classical) reference frame. Transitions from a classical reference frame to another one are the standard symmetry transformations–e.g. the spatial translation–that do not change structure of the observed system.

However, the *quantum* reference frames refer to the microscopic (quantum) systems, which are not subjected to decoherence. This raises non-trivial questions, e.g., as to how the electron in the hydrogen atom can see the atomic proton, and *vice versa* (for a similar considerations see, e.g., (Angelo et al 2011)). Then, by definition, the proton's position measured by the electron is defined as $\hat{\vec{r}}_p - \hat{\vec{r}}_e$. Notice that the reference-system's position is not a classical c-number but a *dynamical* quantum observable, $\hat{\vec{r}}_e$. For a many-particle system, if the particle 1 is the reference system, then the position observables of all the other particles are defined in the 1 reference system:

$$\hat{\vec{\rho}}_i^{\,1} = \hat{\vec{r}}_i - \hat{\vec{r}}_1. \tag{144}$$

As distinct from the classical reference frames, the quantum reference frames

(QRF) raise a number of interesting observations and open questions. Below, we consider one out of plenty of structures $\mathcal{S}_i$ introduced in Section 8.1–e.g. our structure $\mathcal{S}_\circ$. We consider exclusively the QRFs belonging to the same Universe structure $\mathcal{S}_\circ$[68] of the Universe.

First, it is obvious that the QRF-defined variables, eq.(144), are obtained via the global LCTs, which introduce a specific kind of the "relative positions" observables for the considered structure.

Second, the different QRFs perceive the different structures of the R system. To see this, we emphasize that, in principle, the structure's CM system cannot be observed from a local QRF (Angelo et al 2011)[69]. So there remains the "relative positions"–i.e. the R system is the *only* one that (of course, locally) can be observed.

For a quantum observer in the 1 QRF system, the R's subsystems are described by the relative positions eq.(144). As a consequence, every distance-dependent interaction[70] $V(|\vec{r}_i - \vec{r}_1|)$ is an external ("classical") field, $V(|\vec{\rho}_i^1|)$, for the ith particle. The interactions $V(|\vec{r}_i - \vec{r}_j|), i, j \neq 1$ remain interactions. However, for an observer in the 2 QRF system, the physical picture is different. Then $V(|\vec{r}_i - \vec{r}_2|)$ become the external fields, while the $V(|\vec{r}_i - \vec{r}_j|), i, j \neq 2$ remain interactions in the total system Hamiltonian.

Of course, different interactions produce different correlations between the constituents of the structure's R system. In effect, two quantum observers perceive two *different structures* of the R system. These structures are global to each other, but are local to the $\mathcal{S}_\circ$ structure, which consists also of the CM system. So, according to the quantum correlations relativity, Section 3.2, we conclude about the different correlations at the quantum observers disposals.

Now, quantum correlations relativity points out the following striking obser-

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[68] Everything equally applies to the case that there existed a preferred structure of the Universe.

[69] See also Chapter 6.

[70] We drop the "hat"-mark for the observables.

vation: as "quantum observer" can perceive only the R system, the correlations in the R system he can perceive need not be present in the considered structure $\mathcal{S}_\circ$, eq.(145) below.

Finally, the requirement that "*all* [QRF] *perspectives must agree on the probability of detector clicks*" (Angelo et al 2011) does not seem to resolve the following, now naturally appearing foundational question.

Assume that the structure $\mathcal{S}_\circ$ is defined by the set $\{x_m, p_m\}$ of the fundamental degrees of freedom. The fact that no QRF can see the structure's CM system, but only the "relative positions", which are different for the different reference systems, raises the following question:

is there a fundamental lack of information about the Universe structure for QRFs?

Having in mind Entanglement Relativity, i.e. the possible entanglement between the structure's CM and the QRF-defined "internal" degrees of freedom, we re-phrase the above question:

may it be the case, that the [inevitably local] QRFs cannot provide the fundamental description of any of the Universe structures?

Formally, introduction of the QRFs gives rise to the following structure transformation:

$$\mathcal{S}_\circ = \{x_m, p_m, m = 1, 2, ..., N\} \rightarrow \mathcal{S}_\circ^{(i)} = \{CM_\circ, R_\circ^{(i)}\} \tag{145}$$

for the ith QRF. Regarding the universal state for the considered structure of the Universe, entanglement may be expected for the $\mathcal{S}_\circ^{(i)}$ structure:

$$\sum_p c_{pi} |p\rangle_{CM} \ |p\rangle_{R^{(i)}}, \quad \forall i. \tag{146}$$

Then for the ith "quantum observer", quantum state of the degrees of freedom in his disposal is *mixed*:

$$\rho_{R^{(i)}} = \sum_p |c_{pi}|^2 |p\rangle_{R^{(i)}} \langle p|. \tag{147}$$

That is,

Even the universal validity of the Schrödinger law may be at stake for a quantum observer.

Leaving these questions out of further consideration, we stick to the standard understanding of the classical reference frames and of "classical observer" as presented above and used throughout this book.

8.3.3 The unifying picture

Bearing in mind that all basic concepts–of the composite system's degrees of freedom, locality, correlations, classical reality–are *relative*, i.e. *structure dependent*, we face the following physical picture of the Universe:

The Universe hosts a number of dynamical structures. All these structures are equally described by quantum mechanical formalism. While the local[71] *laws and symmetries may be different, physical reality of the structures cannot be a priori rejected. Of all structures, we consider only those that are global and irreducible relative to each other as well as to our structure, and that support decoherence for some of their local degrees of freedom. An observer, in principle, cannot say which structure he belongs to. An observer is a part of one and only one structure and cannot directly observe subsystems of the alternative structures of the Universe.*

8.4 Some interpretational issues

Prima facie, Section 8.3.3 may seem to re-phrase the Ithaca interpretation of quantum mechanics (Mermin 1998). However, as distinct from the Ithaca interpretation, we consider a limited set, $\{\mathcal{S}_i\}$ (Section 8.1), of the Universe

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[71] The only "global" physical law valid for all structures is the Schrödinger law.

structures. In other words, we go beyond the Ithaca interpretation: not arbitrary structures of the Universe are relevant for our study. Only the structures that are mutually nontrivial, global and irreducible, and endowed by decoherence, are of interest. Thus Lemma 2.1 makes our conclusions irreducible to the Ithaca interpretation–our conclusions are basically in agreement with phenomenology.

Bohmian theory (Durr et al 2012) contradicts our considerations. In Bohmian theory existence of the fundamental, ontological structure of the Universe is postulated. The transformations of variables are mathematical artifacts. This contradiction tackles the issue of completeness of the standard quantum theory. For our position see Section 8.6.

As the Complementarity principle [but properly understood, cf. (Dugić 2012)] remains intact by our considerations, we believe that the standard Copenhagen interpretation, as well as the collapse-based interpretations, are in no conflict with quantum correlations relativity.

However, this does not apply to the Everett Many Worlds Interpretation (MWI) as we are going to reproduce from (Jeknić-Dugić et al 2011).

8.4.1 Non-branching of the Everett worlds

It is a universal requirement in the context of interpretation of quantum mechanics: every physically reasonable, even *gedanken*, situation must be consistent with the interpretation foundations. This, however, is not the case with the Everett MWI *in the context* of the quantum Brownian motion model, Section 6.3.

To see this, we first show, that "branching" of one structure excludes the alternative-structure "branching". Consider a decoherence-induced "history" for the $S + E$ structure of the QBM setup for the different instants of time, $t_\circ < t_1 < t_2$, as required by Everett interpretation:

$$|x_S(t_\circ), p_S(t_\circ)\rangle_S |\epsilon(x_S(t_\circ), p_S(t_\circ))\rangle_E \to |x_S(t_1), p_S(t_1)\rangle_S |\epsilon(x_S(t_1), p_S(t_1))\rangle_E$$

$$\to |x_S(t_2), p_S(t_2)\rangle_S |\epsilon(x_S(t_2), p_S(t_2))\rangle_E. \quad (148)$$

In eq.(148), we introduce the tensor-product states for the subsystems S and E as a consequence of the decoherence-induced "branching"[72]. The "history" eq.(148) describes dynamics of one, out of plenty, of Everett worlds. The states of the S system are Gaussian states [not necessarily of the minimal uncertainty][73]. These states represent the approximate pointer basis, i.e. the preferred set of (non-orthogonal) states for the open system S. The environment states, that appear in eq.(148), bring information about the open system's states.

According to Section 6.3, there exists another structure, $S' + E'$, for which the open system S' undergoes quantum Brownian motion. That is, both open systems (S and S') are quantum Brownian particles.

Now, due to Entanglement Relativity, Section 3.1, it becomes clear and *unavoidable*: at least some of the instantaneous states in eq.(148) will be endowed by entanglement–i.e. are *non-branched*–for the $S' + E'$ structure. So, Everett branching for the $S+E$ structure excludes Everett branching for the $S' + E'$ structure. More precisely: for a time interval for which the $S + E$ structure is branched, the $S' + E'$ structure cannot be branched. Due to the assumption that branching is fast, i.e. of the order of the decoherence time (Schlosshauer 2004, Saunders et al 2010), non-branching for the $S' + E'$ structure refers to the most of the composite system's dynamics.

Physical equivalence of the two structures (see Section 8.2) directly provides the following observation: Everett branching for the $S+E$ structure excludes Everett branching for the $S' + E'$ structure, and *vice versa*. As the only consistent statement now appears:

World branching is not allowed for the QBM structures $S + E$ and $S' + E'$.

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[72] This is essential for the Everett MWI in order to be able [at least approximately] to mimic the "state collapse".

[73] See, e.g. Wallace, chapter 1 in (Saunders et al 2010).

So we conclude (Jeknić-Dugić et al 2012)[74]:

There is at least one physically relevant model of a composite system in decoherence theory which cannot be described by the Everett interpretation.

8.4.2 Emergent structures and decoherence

Decoherence is typically studied starting from a fairly unprincipled choice of system-environment split. In this sense, decoherence is by its nature an approximate process and so the process of branching is likewise approximate. In other words (Wallace, chapter 1 in (Saunders et al 2010)) [our emphasis]: "*...decoherence is an emergent process occurring within an already stated microphysics: unitary quantum mechanics. It is* not *a mechanism to define a part of that microphysics*".

Within this new wisdom, one may suppose that there should be an emergent structure for the QBM model of Section 6.3, i.e. that world-branching refers to some "emergent" Brownian particle, B, *not* directly to the "microscopic", S and S', Brownian particles. In the absence of a general *physical* definition of "emergent properties" (i.e. of the "higher level ontology") of complex systems (Auyang 1998), we are forced to speculate about the possible ways to obtain a branching-eligible structure for the QBM model. To this end, we are able to detect only two possibilities. We find both of them inappropriate for defining an emergent QBM structure.

We distinguish the following bases for emergentism. First, it is dynamical exchange of particles between the "system" and the "environment", which encompasses the standard choice of the "dividing line" in the von Neumann sense (the von Neumann "chain", (von Neumann 1955)). Second, one may suppose, that there is an alternate, third structure providing an emergent Brownian particle, B, for the pair of Brownian particles, S and S'. To see that

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[74] Note that neither ER nor POD separately are sufficient for the conclusion. Even ER+POD is not sufficient. The point is that ER+POD, *when* applied to a pair of mutually global and irreducible structures ($S + E$ and $S' + E'$), makes the case: the Everett interpretation is not applicable to the QBM model.

the first doesn't work for the QBM model is straightforward. Actually, both Brownian particles are one-dimensional and there is not, by definition, any possibility of exchanging particles of the S system with the environment E (or of the S' system with the environment E'); of course, due to irreducibility of the two structures, exchange of the particles between the S system with the environment E' (i.e. of the S' system with E) is not even defined. The variant that an environmental oscillator takes the role of Brownian particle is also not allowed. For both structures, the environmental particles do not mutually interact and therefore there is not a properly defined environment for the variant–not even to mention that this *a priori* excludes the possibility (Section 6.3) that the S system is a "free particle" (not an oscillator).

The second option is a bit more subtle yet. To this end we justify the statements of Sections 2.2.2 and 6.5: (1) obtaining information about one Brownian particle (e.g. S) provides no information about the other one (e.g. the particle S'); (2) there does not exist any observable, X_B (of the subsystem B of the composite system C), which could approximate a pair of observables of the two Brownian particles, S and S'. In effect, there does not exist any structure $B+E_B$ that could be emergent for the structures $S+E$ and $S'+E'$.

Regarding the point (1), we first remind (cf. Section 3.1): the S' system is the original-structure's ($S+E$'s) center-of-mass. So the position-observable of the S' system is subject to Lemma 2.1. Thereby one can say: Brownian particles, S and S', cannot approximate each other, neither there is any information flow between them.

The arguments for the point (1) apply to the point (2). As the only probability density that can provide probability density for arbitrary subsystem is the universal state, $|\Psi\rangle$, there is not any subsystem's (B's) probability density, $\rho(X_B, X'_B)$, that could provide probability density for both the S and the S' systems. e.g. The definition $X_B = f(x_S, x_{S'})$ gives rise to the probability density $\rho(X_B, X'_B) = \rho(x_S, x'_S, X_{S'}, X'_{S'})$, which, as emphasized in the proof of Lemma 2.1, cannot provide the probability densities $\rho(x_S, x'_S)$ or $\rho(x_{S'}, x'_{S'})$

by integrating over $X_{S'}$ and x_S, respectively. So, there is not any observable of the B system whose measurement might approximate simultaneous measurement of any pair of observables for the two Brownian particles, S and S'. Physically, this means that we cannot imagine a third system B, which undergoes Brownian-motion-like dynamics *and* can approximately describe both "microscopic" Brownian particles, S and S'. As we cannot recognize any other basis for emergentism, we are forced to conclude that the above-distinguished inconsistency between the QBM model and the modern Everett interpretation remains intact.

Finally, we emphasize: the standard QBM model, Section 6.3, is a (paradigmatic theoretical) decoherence model pertaining to the realistic macroscopic situation of "Brownian motion". There are not any structural phenomenological facts about Brownian motion known to us that go beyond the standard QBM model–there is no need for any "emergent" Brownian particle.

Bearing this in mind, the possibility that the structures considered in Section 6.3 are not susceptible to the Everett interpretation directly raises the following foundational question: Whether or not decoherence is sufficient for the Everett branching? If it is, then the told above is unavoidable. If not, then some additional requirement for branching, i.e. for completeness of the Everett interpretation, is needed. e.g. One may require some amount of "complexity" of the composite system to be subject to the modern Everett interpretation (Saunders et al 2010). Certainly, then the range of applicability of the modern Everett interpretation shrinks, as distinct from the competitive interpretations. As the "additional requirement" is not a part of the present state of the art in the field, we will not elaborate on this any further, and we finally return to the conclusion of Section 8.4.1.

8.5 There are no "particles"

Physical picture presented in Section 8.1 strongly suggests:

There are no "particles".

"Particles" pertains to some special states of the Universe. The kind and behavior of the elementary particles is structure dependent, and is otherwise determined by the Universe global symmetry as well as by the local laws (interactions) that are characteristic for the structure. Decoherence independently occurs in the different structures, and the *contents* of physical reality is relative, i.e. structure dependent.

Section 8.2, and the parallel occurrence of decoherence, Section 6.3, naturally support the position, that "there are no particles" even for the local structures, i.e. on the lower-ontological level (Zeh 1993, Primas 1994).

This position naturally describes certain experiments without raising any further puzzles. Some points presented below are already raised in Chapter 5.

8.5.1 Delayed choice experiments

In order to exhibit weirdness of the quantum world, Wheeler (Wheeler 1978) emphasized, that classical reasoning can lead to inconsistency with quantum mechanical conclusions. A recent elaboration due to Peres (Peres 2000) abandons the classical prejudice on individuality of "quantum particles". Instead, Peres distinguishes operational reality of quantum entanglement and implicitly points out entanglement relativity.

In this picture, that is experimentally tested (Ma et al 2012), entanglement relativity, Section 3.1, naturally appears. Everything can be expressed in terms of correlations for different partitions of the composite system (entanglement swapping), without even mentioning the constituent "particles" (i.e. the qubits).[75]

Of course, the use of the concept of particles may be physically correct. Our point is, that it is *neither necessary nor the simplest description* of the entanglement-swapping-based delayed-choice experiment.

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[75] In a sense, physical picture is easily described in terms of "correlations without correlata" (Mermin 1998).

8.5.2 Interaction-free quantum measurements

Recently, based on the "interaction-free measurement", see e.g. (Elitzur and Vaidman 1993), a theoretical proposal for "direct counterfactual quantum communication"–that claims that there may be communication without any particles exchange between the parties–has been formulated (Salih et al 2013). While quantum communication without the particle exchange is interesting, this does not provide any spectacular result in "quantum mechanics without particles". Rather, as we briefly point out below, it provides another argument "against particles".

All the phrases and spectacular statements simply disappear if we abandon the classical prejudice, which underlies the phrase "interaction-free" in the original theoretical proposal (Elitzur and Vaidman 1993). In the interference situations, there is not "particle trajectory". Finding a particle in an arm of the interferometer (provided by the click of a detector) does *not* necessarily mean that the particle was there before detection.

The following picture removes the puzzles and the spectacular statements: *Every* detector *is in interaction* with the system of interest (a photon). This gives rise to entanglement of *all* the detectors with the system, *without assumption on the definite spatial position of the system–before, during, or after the measurement*–even if the system's position is measured. By applying e.g. the von Neumann's projection postulate (von Neumann 1955), one easily obtains the standard final state for every detector and for the system after the measurement. A detector's click is a local effect that neither precludes nor implies existence of a "particle" in any arm of the interferometer before [or even after] detection. The puzzling click of one and only one detector is a particular instance of the long-standing problem of quantum measurement–the apparent state collapse–but not more or less than this.

8.5.3 Relativistic quantum processes

Although it is not subject of our considerations, certain relativistic quantum effects provide striking confirmations of relativity of structure as well as of the "there are no particles" position.

Quantum-particles annihilation/creation is really striking. e.g. A pair "electron + positron" transforms into "pair of photons". In such process, one cannot, even in principle, say that the pair "electron + positron" can be decomposed or imagined to consist of a pair of photons, and *vice versa*. The place of quantum vacuum, which is responsible for the effect, is yet to be properly described in the canonical formalism of Chapter 2, (Stokes 2012).

8.6 The universally valid and complete quantum theory

The phrase "there are no 'particles' ", Section 8.5, naturally fits with the hypothesis of the universally valid *and* complete quantum mechanics. In this section we adopt this hypothesis and extend the picture obtained in Section 8.3.3.

8.6.1 Why universally valid and complete quantum theory?

Throughout this book, we respect the hypothesis of the universally valid quantum mechanics by employing universal validity of the Schrödinger law for the closed, isolated, quantum systems. Of course, our findings are susceptible to different interpretations. Then, one can ask the question from the title: which arguments may justify the choice of universally valid and complete quantum mechanics?

The arguments are as follows.

First of all, our approach is *minimalistic*: we do not introduce or add any additional assumption or hypothesis. In this context, it is easiest to get rid of the problematic concepts of "particles", "individuality" and "classical intuition" and to try to *derive* them as the approximate and relative concepts, whose contents are different for the different decompositions (the structures) of the Universe.

Second, modern open systems theory (Breuer and Petruccione 2002, Rivas and Huelga 2011) provides, that practically every physically reasonable dynamics of a system can be described by the unitary (Schrödinger) dynamics on the extended system "system+environment". The inverse, however, as yet, is not the case–unitary dynamics is not derived from the open system's dynamics. Therefore, the unitary quantum mechanics is methodologically more primary than the open system's theory. Furthermore, the unitary quantum theory encompasses the collapse models (Markovian[76], or non-Markovian), and still can describe the models not presenting the state collapse. The inverse, however, is not the case. Therefore we choose the universally valid quantum mechanics.

Third, modern quantum information theory provides the following *conjecture*: quantum state saturates the information contents of a quantum system (Brukner and Zeilinger 1999, Pusey et al 2012). That is, it is conjectured that every possible information about a system can be drawn from the quantum state–there is no room for "hidden variables" of any kind, including those of the modern Bohm's theory (Durr et al 2012)[77]. Therefore we choose complete quantum theory.

So, modern open systems and information theories strongly support the hypothesis of the universally valid and *complete* quantum mechanics. Nevertheless, as we show in Section 8.4, the Everett interpretation is at stake. Hence a new view of the quantum world is needed. For a hint see (Dugić et al 2012).

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[76] See e.g. (Bassi et al 2013).

[77] This means that the Bohmian theories are not "deeper" than the standard quantum mechanical theory.

8.6.2 Completing the picture

Now, the unifying picture of Section 8.3.3 may be extended by the phrase: "*There are particles neither on the most fundamental, i.e. on the ontological, physical level nor on the level of the Universe decompositions (structures). All that we can assume is a fundamental quantum field, whose states can be [non-relativistically] described by different decompositions of the Universe and their local, decoherence-defined structures.*"

While this picture may seem pessimistic, it is not necessarily so. Actually, we do not think that ontological existence of the Universe, seen as a fundamental physical quantum field, should be considered to be non-realistic. Such an option (Vedral 2010) is essentially an *additional condition*, which is absent from the universally valid quantum theory.

Chapter 9

Outlook and Prospects

In Chapter 1 we posed the questions that are worth repeating: Is there unique fundamental structure of a composite quantum system? How do the classical structures (and intuition) appear from the quantum substrate? Can the structural variations be of any practical use that is not known to the classical physics wisdom?

Issued answers are partial–some answers imply another questions, which nevertheless sharpen our view of the quantum world. The only assumption of our considerations is the universal validity of quantum mechanics–for an isolated (closed) quantum system we assume validity of the Schrödinger law. The recently provided technical tools we introduce and use are as follows: (a) Quantum correlations relativity (Section 3.2); (b) Parallel occurrence of decoherence for the quantum Brownian motion model (Section 6.3); (c) Preferred local structures for bipartite decompositions (Section 7.2 and 7.3). Those are the corollaries of the universally valid quantum mechanics.

In Chapters 6 and 8, we found the classical intuition (emphasized in Section 2.1) "mechanistic"–structure is a fundamental and ontological notion that precludes a deeper physical analysis of certain structural variations. However, in the quantum context it seems that there is not any reason to claim existence of the ontologically unique structure of the Universe. Even more, there may be more than one structure that bears the decoherence-induced classicality. In other words: there may be more than one classical world (a structure) hosted by one and only one, unique quantum Universe. For every such quasiclassical world, classical intuition (Section 2.1) is justified as a local rule, which does not preclude reality of the alternative worlds and their local (internal), quasiclassical structures and physical laws. Parallel occurrence of decoherence is conjectured (Conjecture 1, Section 6.4) for all linear models. Whether this conjecture can be justified, and probably extended to the more general models of the many-particle systems, remains an open question of our considerations.

An observer belongs to one and only one such world and can only partly observe the alternative quantum worlds. From a set of the possible local structures of a composite system, the environment chooses *the* preferred structure, Conjecture 2 (Section 7.4). This structure can be directly observable (accessible, Def.5.1) for an observer. In effect, the preferred structure of an open composite system can be considered to be "objective" and "realistic" for the observer. The choice of the preferred local structure of a composite system cannot be provided on the purely theoretical basis–some phenomenological facts are needed. Occurrence of decoherence should be equipped with another theoretical tools, which, as yet we can only speculate about. To this end, we introduce the assumption, that the minimum quantum correlations should be required for "classicality" (Arsenijević et al 2012, Harshman 2012a), which also opens the following speculation. May it be the case that "classicality" is mainly a matter of structure–i.e. that structural studies may provide a basic clue for answering the long-standing problem of the transition from quantum to classical; compare to (Ragy and Adesso 2012)? Needless to say, this new perspective offers a basis for a brand new approach to some old foundational questions in non-relativistic quantum theory.

Quantum interpretation studies provide a unique lecture: "classicality", as we usually see or feel it, may be idealized. Once we better understand "classicality", we might be in a better position to perceive and eventually to solve the long standing problem of quantum measurement. To this end, the quantum structures studies may nontrivially help, as we already know that ”system”, locality and correlations–are *relative*, i.e. the structure-dependent concepts. Unfortunately, [as emphasized above], quantum formalism seems to be much richer than we might ever need. So there does not seem to be any other way but to refer to phenomenology (e.g. to the decoherence and quantum information phenomenology) as a precursor as well as to validate our theories. Experimental evidence, even more, the use, of entanglement relativity, we believe, is a precursor for the new and exciting applications that will emerge from the quantum structure studies.

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Index

Supplement

This Supplement serves to complete and partially extend the contents of the body text.

S.1 Decoherence preferred states and observables

The "orthodox" approach to decoherence deals directly with the unitary operator of time evolution for the composite system "(open)system+environment" $(S+E)$,

$$U = e^{-\imath t H/\hbar}, \tag{149}$$

where the total system's Hamiltonian:

$$H = H_S + H_E + H_{SE}. \tag{150}$$

If the self-Hamiltonians, H_S, H_E, can be neglected (e.g. in the collisional decoherence), then the total-system's (pure) state evolves, approximately, as:

$$e^{-\imath t H_{SE}/\hbar} |\psi\rangle_S |\chi\rangle_E = \sum_i c_i |\phi_i\rangle_S |\chi_i(t)\rangle_E. \tag{151}$$

In eq.(151): $|\phi_i\rangle_S$ is a basis diagonalizing the interaction term, H_{SE}, and the precise form of the $|\chi_i(t\rangle_E)$ depends of the form of H_{SE}.

It can be shown that eq.(151) cannot be valid, in principle, if the interaction is not of the so-called separable kind (Dugić 1996, 1997), which, in turn, can be always diagonalized by an orthonormalized basis in the system's Hilbert state space, $\mathcal{H}_S$. However, whenever such basis exists [and need not be unique], the states $|\phi_i\rangle_S$ diagonalizing H_{SE} represent the "pointer basis" states for the S system–the carriers of the quasi-classical behavior of the open system S.

If the interaction H_{SE} is only approximately of the separable-kind, then there exists a not-necessarily-exactly orthonormalized basis, which approximately diagonalizes H_{SE}. Such a basis represents the approximate pointer basis states–the "preferred" set of states carrying the quasiclassical behavior of S.

For the continuous-variable systems, the minimal-uncertainty gaussian states (the Sudarshan-Glauber coherent states) are typical "preferred" states [see Chapters 6 and 7].

Whenever the self-Hamiltonians cannot be neglected, non-commutativity $[H_S, H_{SE}] \neq 0$ does not allow a choice of the exact pointer basis states. Then reading out the spectral form of the [separable kind] interaction H_{SE} can point out the candidates for the approximate pointer basis. There are the cases not allowing existence of any "preferred" states for the open system (Dugić 1996, 1997).

Formally, the spectral form of the interaction provides information about the pointer basis:

$$\begin{aligned}
&H_{SE} = \sum_{i,j} h_{ij} P_{Si} \otimes \Pi_{Ej} \quad [\text{exact} \quad \text{pointer} \quad \text{basis}] \\
&H_{SE} = \sum_{i,j} h_{ij} P_{Si} \otimes \Pi_{Ej} + H', \|H'\| \ll \|H_{SE}\| \quad [\text{approx} - \text{pointer} - \text{basis}] \\
&[H_S, H_{SE}] \neq 0 \quad [\text{approximate} \quad \text{or} \quad \text{no} \quad \text{pointer} \quad \text{basis}]. \qquad (152)
\end{aligned}$$

S.2 The continuous-variable-system transformations

The center-of-mass and the relative positions

For a pair of one-dimensional particles see eq.(4) in the body text. Generalization to realistic three-dimensional particles is straightforward. Here we consider a many-particles system[78].

There are formally similar, not yet equivalent, variants of the relative positions (R) variables. Here we adopt the following definitions as a direct generalization of eq.(4) in the body text:

$$\vec{R}_{CM} = \frac{\sum_i m_i \vec{r}_i}{\sum_i m_i}, \vec{\rho}_{Rl} = \vec{r}_i - \vec{r}_j, \quad (i,j) \equiv l = 1, 2, 3, ..., N-1. \qquad (153)$$

---

[78] For further details and some proofs see e.g. McWeeney 1978.

Eq.(153) gives rise to the following transformations of the kinetic terms:

$$\sum_i \frac{\vec{p}_i^2}{2m_i} \to \frac{\vec{P}_{CM}^2}{2M} + \sum_i \frac{\vec{p}_{Ri}^2}{2\mu_i} + \sum_{i,j} \frac{m_{i+1}m_{j+1}}{m_i m_j M} \vec{p}_{Ri} \cdot \vec{p}_{Rj} \tag{154}$$

In eq.(154): $M = \sum_i m_i$, the reduced masses, $\mu_i = m_{i+1}(M - m_{i+1})/M$, while $[X_{CMi}, P_{CMj}] = \imath\hbar\delta_{ij}$, and analogously for the R system's variables. Of course, then the total system's Hilbert state space factorizes as $\mathcal{H}_{CM} \otimes \mathcal{H}_R$; $\mathcal{H}_R = \otimes_{i=1}^{N-1}\mathcal{H}_{Ri}$. The third term in eq.(154) is the so-called "mass polarization" term which, for $i \neq j$, becomes internal interaction for the R system. For the $i = j$, the mass polarization term gives rise to the following contribution to the kinetic energy of the ith "relative particle": $\sum_i m_{i+1}^2 p_{Ri}^2 / m_i^2 M$, which will further be neglected.

The inverse to eq.(153) gives rise to:

$$\vec{r}_i = \vec{R}_{CM} + \sum_j \omega_{ij}\vec{\rho}_{Rj} \tag{155}$$

with the real parameters ω. Then the distant-dependent interactions:

$$V(|\vec{r}_i - \vec{r}_j|) = V(|\vec{\rho}_{Rl}|) \tag{156}$$

become the external fields for the R system. However, interestingly enough, the external one-particle field:

$$V(\vec{r}_i) = V(\vec{R}_{CM} + \sum_j \omega_{ij}\vec{\rho}_{Rj}) \tag{157}$$

becomes the interaction between the CM and R systems.

Regarding the *molecules model*, eq.(48), the atomic-nuclei R_N subsystem is divided into two subsystems, the Rot_N (rotation of the atomic nuclei system as a whole described by the Euler angles) and K_N (the conformation system). The kinetic term for rotation $T_{Rot_N} = \vec{L}_N^2/2I_N$, where $\vec{L}_N$ is the molecule angular momentum and I_N is the moment of inertia [in the simplest form]. The kinetic term T_{K_N} is of the standard form eq.(154) for the remaining "relative positions" variables.

Regarding the *QBM model*, eq.(66), the LCTs give rise to the terms proportional to X_{CM}^2 and to $\rho_{Rl}\rho_{Rl'}$, while there is the bi-linear coupling $X_{CM}\sum_i \kappa_i \sum_l \omega_{il}\rho_{Rl}$. So, even for the original free particle model, the new structure provides the harmonic-oscillator Brownian particle S' ($S' \equiv CM$). The above terms $\rho_{Rl}\rho_{Rl'}$ give for $l = l'$ the additional terms ρ_{Rl}^2 thus providing a harmonic term for the new environment. On the other hand, the original harmonic term (for the Brownian particle and/or for the environment), $\vec{r}_i^{\,2} = (\vec{R}_{CM} + \sum_j \omega_{ij}\vec{\rho}_{Rj})^2$, thus providing the harmonic terms for both the new Brownian particle as well as for the new environment, and the bilinear coupling, $X_{CMi}\rho_{Rj}$, which directly gives rise to the coupling in eq.(70).

Regarding the *quantum reference system*, the expression eq.(156) is *not* applicable. The reason is rather simple. For the 1 system as a QRF system: the relative positions $\vec{\rho}_{Rl} = \vec{r}_1 - \vec{r}_l$. But then $V(|\vec{r}_i - \vec{r}_j|) = V(|\sum_l \omega_{il}\vec{\rho}_{Rl} - \sum_{l'} \omega_{jl'}\vec{\rho}_{Rl'}|)$ for $i, j \neq 1$, in contrast to eq.(156).

Building the boson Fock space

For a single harmonic oscillator described by the canonical position and momentum, x and p, with the mass m and frequency ω, one can introduce the "annihilation" and the "creation" operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}(x + \frac{\imath}{m\omega}p), a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{\imath}{m\omega}p), \tag{158}$$

with the commutation relation:

$$[a, a^\dagger] = I. \tag{159}$$

The inverse to eq.(158):

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), p = \imath\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a). \tag{160}$$

The Hermitian operator $N \equiv a^\dagger a$ defines the eigenstates:

$$N|n\rangle = n|n\rangle, n = 0, 1, 2, 3, ... \tag{161}$$

The states $\{|n\rangle\}$ constitute an orthonormalized basis in the so-called Fock space, $\mathcal{H}_F$. The equalities hold:

$$a|n\rangle = \sqrt{n}|n-1\rangle, a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{162}$$

from which:

$$|n\rangle = \frac{a^{\dagger n}}{\sqrt{n!}}|0\rangle, \quad a|0\rangle = 0; \quad \langle 0|0\rangle = 1, \tag{163}$$

In wide use (especially in quantum optics) are the so-called quadratures (Hermitian) operators defined as $X = \sqrt{m\omega/\hbar}x$ and $P = \sqrt{1/m\hbar\omega}p$.

Generalization to the many-particle (multimode) system is straightforward: $(x_i, p_i) \to (a_i, a_i^\dagger)$, so that $[a_i, a_j^\dagger] = \delta_{ij}$. Then the total system's Fock space $\mathcal{H}_F = \otimes_i \mathcal{H}_{Fi}$, where $\mathcal{H}_{Fi}$ is the Fock space for individual oscillators (modes). The eigenbasis of $N = \sum_i N_i$, $\{|n\rangle = \otimes_i |n_i\rangle\}$, $N_i|n_i\rangle = n_i|n_i\rangle$, while $n_i = 0, 1, 2, ..., \forall i$. For the vacuum state, $|0\rangle = \otimes_i |0\rangle_i$, $a_i|0\rangle = 0, \forall i$.

The Bogoliubov-like transformations

For one mode (or one harmonic oscillator) defined on appropriate Fock space $\mathcal{H}_F$, a pair of the "annihilation" and "creation" operators are defined by the commutator relation eq.(159).

The one-mode *boson-translation transformation* is defined by:

$$a \to a(\theta) = a + \theta, \quad \theta \in \mathcal{C}. \tag{164}$$

This is a canonical transformation as

$$[a(\theta), a^\dagger(\theta)] = I, \forall\theta. \tag{165}$$

It can be shown this is an unitary transformation. However, this transformation does not preserve the original Fock space as:

$$a(\theta)|0\rangle = \theta|0\rangle \neq 0. \tag{166}$$

Therefore, the new vacuum state, $|0(\theta)\rangle$, is the vacuum state of another Fock space, $\mathcal{H}'_F$, which is unitary related to the original one.

For a single mode, the *Bogoliubov transformation* is defined as:

$$b = ua + va^\dagger, \quad b^\dagger = u^* a^\dagger + v^* a, \tag{167}$$

where $[a, a^\dagger] = 1$ allows for the new bosonic operators $[b, b^\dagger] = 1$ if $|u|^2 - |v|^2 = 1$. The later condition allows for the following parametrization: $u = e^{\imath\theta_1}\cosh r$ and $v = e^{\imath\theta_2}\sinh r$.

For the fermion system there are analogous transformations with the condition $|u|^2 + |v|^2 = 1$, i.e. with the parametrization: $u = e^{\imath\theta_1}\cos r$ and $v = e^{\imath\theta_2}\sin r$.

The *multimode generalization* is straightforward. e.g. For the boson system, for which $a_i|0\rangle = 0, \forall i$, the operators:

$$a'_i = \sum_j (u_{ij} a_j + v_{ij} a_j^\dagger) \tag{168}$$

satisfy the bosonic commutator relations, $[a'_i, a_j^{'\dagger}] = \delta_{ij}$, if the condition, $\sum_p (u_{ip} u^*_{jp} - v_{ip} v^*_{jp}) = 1$, is fulfilled. For the fermion system, the analogous condition reads as: $\sum_p (u_{ip} u^*_{jp} + v_{ip} v^*_{jp}) = 1$.

S.3 Some spin-system related transformations

Below, we consider nontrivial[79] transformations of variables.

The *Holstein-Primakoff transformation* targets the spin observable $\vec{S}$ (of the spin quantum number s) with the standard basis $|s, m_s\rangle$; $m_s = -s, -s+1, -s+2, , ...s-2, s-1, s$. The leading idea of the transformation is the following correspondence:

$$|s, -s+n\rangle \to (n!)^{-1/2} a^{\dagger n}|0\rangle \tag{169}$$

where appear the bosonic creation operator $a^\dagger$ and the vaccum state $|0\rangle$. Then the transformation is defined by the following prescription:

$$S_z = \hbar(s - a^\dagger a), S_+ = \hbar\sqrt{2s - a^\dagger a}a, S_+ = \hbar a^\dagger\sqrt{2s - a^\dagger a}. \tag{170}$$

Given the standard spin commutator relations, $[S_i, S_j] = \imath\hbar\epsilon_{ijk}S_k$, the bosonic commutator relation is satisfied, $[a, a^\dagger] = I$. Generalization to a system of spins (i.e. to a multimode prescription) is straightforward.

The *Jordan-Wigner* transformation exhibits important prescription between the one-dimensional spin-1/2 chain and a fermion system. If $\vec{S}_i$ distinguishes a set of N one-dimensional-chain of spins, the spin projections $S_{i\alpha}$, $i = 1, 2, ...N, \alpha = x, y, z$, allows introduction of the fermionic annihilation and creation opperators as:

$$a_i = (-2)^{i-1} S_{1z} S_{2z} ... S_{(i-1)z} S_{i-} \Leftrightarrow S_{jz} = a_j^\dagger a_j - 1/2, \tag{171}$$

while $S_- = S_x + \imath S_y$ and $\{a_i, a_j^\dagger\} = \delta_{ij}$.

Fourier transform for fermion system connects mutually the two sets of fermion operators. Consider the fermion operators a_i and $a_i^\dagger$ that are trans-

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[79] By "trivial" transformations, we assume regrouping, fine- or coarse-graining of the constituent particles.

formed as:

$$\beta_m = \sum_i d_{mi} a_i. \tag{172}$$

For the N-fermions system, if chosen

$$d_{mi} = \sqrt{\frac{2}{N+1}} \sin kj, \quad k = \frac{n\pi}{N+1}, \quad n = 1, 2, ..., N, \tag{173}$$

then the anticommutator relations are satisfied:

$$\{\beta_m, \beta_n^\dagger\} = \delta_{mn}. \tag{174}$$