Perspective

Quantumness of correlations in nanomaterials—experimental evidence and unconventional effects

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Abstract: Quantum correlations phenomena, such as entanglement, quantum discord and quantum coherence, are ubiquitous effects caused by interactions between physical systems—such as electrons and ions in a piece of metal, or H atoms/molecules adsorbed in nanoporous materials. Here, we address time-asymmetric quantumness of correlations (QoC), with particular emphasis on their energetic consequences for dynamics and non-equilibrium thermodynamics in condensed matter and/or many-body systems. Some known theoretical models—for example, the quantum Zeno effect and GKSL-type Markovian equations-of-motion, all of them being time-asymmetric—are shortly considered, with emphasis on the general character of one of their common and most intriguing result. Namely, that in clear contradistinction to conventional expectations, degradation (or destruction, decoherence, consumption, smearing out, coarse-graining) of quantum correlations can be a source of work (instead of heat production). The experimental relevance of the theoretical considerations is shown with the aid of a recent scattering experiment exploring the impulsively driven (by neutron collisions) translational dynamics of H_2 molecules in carbon nanotubes and other nanostructured materials— a topic of immediate relevance for material sciences and related technologies.

1. Introduction

Nowadays the importance of quantum correlation phenomena (e.g., the well known entanglement [1,2] and the recently discovered quantum discord [3,4]) in many scientific and technological fields [5] is well recognized. An impressive related application was recently presented in the field of quantum information technology (QIT) by Google's quantum processor Sycamore, which is programmable and

has 53 solid-state superconducting qubits [6]. With reference to the common ensemble interpretation of standard quantum mechanics, let us stress here that the wavefuction underlying the reported calculation of Sycamore describes (or captures) one single quantum system (i.e., the mentioned quantum processor) and not an ensemble of processors.

However, the best way to go beyond the standard Copenhagen interpretation of quantum mechanics and get more physical insight into the meaning of the theoretical term "wavefunction" is—to our opinion—to consider the well known Elitzur-Vaidman effect [7], also known as "bomb-tester" or "interaction-free measurement" (IFM), which in the meantime has also been experimentally confirmed.

This thought experiment demonstrates the following remarkable effect: Using a single photon (neutron, atom, etc.) entering a Mach-Zehnder interferometer (MZI), one can detect an object (a bomb) placed in one of the two paths of the MZI, without any interaction between the photon and the bomb; in other words, the photon did not "touch" the bomb. In other terms, one achieves a successful interaction-free bomb detection without exchange of any known physical quantity—energy, momentum, angular momentum, force, etc., between the bomb and the probe system (photon) entering the MZI. Obviously this is impossible, or even inconceivable, within the frame of classical physics. Moreover, the aforementioned bomb detection, represents a classical record, which should not be gained "at no costs" at all. Hence the only possible conclusion is that these "costs" are provided by the probe's wavefunction and the associated quantum state reduction caused by the bomb's presence— although the probe particle does not "touch" the bomb.

Consequently, the novel Elitzur-Vaidman effect strongly demonstrates that the wavefunction is a real physical entity of a single quantum system (e.g., a photon)—and not just an auxiliary quantity that enables us to perform numerical calculations of expectation values (like the mean value of energy).

As concerns quantum information theory and its applications, for example, quantum computing and quantum communication (confer [5]), the above conclusion is in line with Landauer's and Bennett's insight that "information is physical" [8, 9]. It may be noted that quantum phase relations, and the associated quantum correlations, play also a dominant role in the broad fields of quantum thermodynamics and quantum information theory; for example, the review articles [10, 11] and also Refs. [12–15]. This is not unexpected, since thermodynamics and information theory possess several links, for example, the formal similarity of the formulas of the (classical) Shannon and the (quantum) von Neumann entropies indicates.

It should be emphasized that in the following we consider non-relativistic quantum dynamics only. That is, relativistic quantum theory, as well as classical mechanics and equilibrium quantum thermodynamics, are outside the scope of this paper. Rather, here we consider effects in single quantum systems driven by external forces (e.g., impulsive collisions with neutrons).

In the present paper, the focus is on the "energetic costs" of time-asymmetric quantumness of correlations (QoC) and their experimental accessibility. It turns out that the destruction of quantum phase relations induced by the environment, sometimes loosely called "pure" decoherence, may have a perplexing, peculiar consequence. Notably, in the frame of some broadly known theoretical models, decoherence (and consumption of quantum correlations) turns out to be intrinsically connected with an increase of mean energy of the system—or in other terms, with negative energetic costs.

This is certainly unexpected, since erasure of quantum phases and/or correlations is widely acknowledged as a cause of dissipation and/or loss of information, rather than as a a source of energy production [5, 16].

To prevent a possible misunderstanding and/or confusion, already here it should be pointed out that this paper presents no new mathematical (analytical) derivations of provable formulas or results. To the benefit of the non-specialized readers, the presented parts of the theoretical topics and models are of introductory character and intentionally kept as short (and as simple) as possible. So the following question may be posed: What is the intention, purpose and/or potential significance, of this paper?

Here, we tentatively address this question with the aid of the following two points:

(a) Only small parts of each of the aforementioned four topics (1–4), as presented below, are needed for our main goal, which is to show that all these topics have a "common"consequence— the aforementioned negative energetic costs of decoherence and/or erasure of QoC. Note that this theoretical result may be already well known in the field of quantum thermodynamics, but it appears to be rather unknown in the "broader" fields of experimental physics and material sciences.

(b) The paper and its main message should be accessible to readers being non-specialized in (non-equilibrium) quantum thermodynamics, for example, to investigators specialized in experimental physics and material sciences. A goal is also to provide certain evidence that the considered theoretical results may also be of broader relevance, even for technological and industrial investigations.

The paper is organized as follows:

In Section 1.1 we give a short overview of a few findings of the paper; this may hint at the general picture of QoC underlying the present paper.

Four theoretical topics concerning QoC are considered below, which are:
(1) van Kampen's case against linear response theory (LRT) and the repeated randomization assumption (RRA);
(2) the quantum Zeno effect (QZE);
(3) the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) equation (often shortly mentioned as the "Lindblad equation"); and
(4) the Schulman-Gaveau theoretical model.

The conceptual connection between these topics represents a central point of the paper. Further, for illustration of the applicability the QoC theory, we shortly consider a recent striking experiment dealing with impulsive scattering of neutrons with single H_2 molecules adsorbed within carbon nanotubes. Finally, some potential experimental and technological/industrial applications are indicated.

1.1. Short overview of some results and related conclusions

Aiming to attract the attention of non-specialized readers and facilitate the understanding, some of the main findings and/or conclusions are already summarized here. We feel that this might act intuitively as a guidance to the contents of the following sections.

(A) In contradiction to conventional theoretical (classical and quantum) expectations, destruction (or decoherence, consumption, smearing out, coarse-graining) of quantum correlations and related quantum phase relations can become a source of energy production—instead of heat production.

(B) The schematic presentation in Figure 1, which illustrates the well known quantum Zeno effect, captures the main reason of this effect, namely the time dependence of QoC between a quantum system and its environment. Thus the latter plays an active role in this effect. See Section 3.

(C) That environmentally induced decoherence in a particle-environment system may accelerate, instead to slow down, the moving particle appears certainly paradoxical. However, this is a "strange" consequence of the celebrated Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) equation which plays

a pivotal role in an overwhelming number on studies of decoherence and related phenomena. See Section 4.

(D) Consider two quantum oscillators, *A* and *B*, which are moving and collide from time to time. After a collision, the correct (entangled) state of them is $\rho_{A,B}(t)$. Then one "cancels" the quantum correlations between them and produces the non-entangled state: $\rho(t)_{A,B} \rightarrow \rho_A(t) \otimes \rho_B(t)$ — which is assumed to be the initial state before the next collision. It has been demonstrated by a quantum simulation that this process may lead to a paradoxical effect, that is, an increase of the vibrational energies of both oscillators; as Schulman and Gaveau put it: " ... loosing quantum correlations should not heat the gas. You do not burn your finger because of a partial trace over a density matrix" . See Section. 5.

(E) The above (and several more, similar) consequences of QoC dynamics are theoretically proven but they lack confirmation by means of some real experiment (that is, applying an existing experimental technique). However, we shortly consider such a recent experiment, which concerns translational mobility of single H_2 molecules in carbon nanotubes. The measurements show that a neutron collision with a H_2 initiates a translational motion of the latter, which appears to be strangely "facilitated"— the molecule appears to be much more mobile than every conventional theory can explain thus far, indicating that it receives a fictitious "push" in addition to that provided by the colliding neutron. See Section 6.

2. Van Kampen's case against linear response theory (LRT)—Repeated randomization assumption

Consider the effect of electric resistivity in a piece of metal, as measured in an experiment. A classical-theoretical view of this effect is that the electrons experience some kind of friction that hinders their motion caused by an external voltage. However, the Schrödinger equation of quantum mechanics does not contain any term representing friction. Moreover, friction, and the associated heat production, are dissipative processes, which break the fundamental time symmetry of the underlying basic physical law. Namely the Schrödinger equation describes unitary time evolutions which are reversible. Hence, since the beginnings of statistical thermodynamics, the associated question arose: Is a theoretical derivation of resistivity (and of irreversible phenomena, in general) possible, based exclusively on the fundamental dynamical law of quantum mechanics?

Kubo [17] claimed to have answered this question in the affirmative, and here is the basic idea of his theory. Kubo's derivations start with the many-body Hamiltonian (Eq 1)

$$H(t) = H_0 - A f(t) \tag{1}$$

Here H_0 is the Hamiltonian of the isolated many-body system, and *A* is the system's operator which couples with an external field $f(t)$. This field is *classical* (a *c*-number). For example, in the commonly used example of the electric conductivity (say, in metals,), $f(t)$ is the external electric field, by Eq 2:

$$A = \Sigma e(r_i - r_{i,eq}) \tag{2}$$

e being the charge of the particles (e.g. electrons) at positions r_i, whereas $r_{i,eq}$ are the particles' positions in equilibrium prior to the switching on the field $f(t)$. LRT claims to derive "from first principles" of quantum mechanics a formula for the conductivity, also known as the standard Kubo-Green formula.

(The analogous derivation in the frame of classical many-body dynamics is not considered here, as already pointed out in the Introduction.)

The quantum dynamics of the system's density operator $\rho(t)$ is governed by the von Neumann equation of motion, which represents here the aforementioned basic law (Eq 3),

$$i\hbar \frac{\partial}{\partial t}\rho = [H(t), \rho] \tag{3}$$

To demonstrate the crucial point revealed by van Kampen [18], one may consider a formal equivalent of the von Neuman equation which is given by the Volterra integral equation (Eq 4) [19]

$$
\begin{aligned}
\rho(t) &= \rho_0(t) + \Delta\rho(t)_{exact} \\
&= \rho_0(t) + (i/\hbar) \int_{-\infty}^{t} ds \exp\{-\frac{i}{\hbar}H_0(t-s)\} f(s)[A, \rho(s)] \exp\{\frac{i}{\hbar}H_0(t-s)\}
\end{aligned} \tag{4}
$$

where $\rho_0(t)$ describes the non-interacting (or free) system, and the subscript "exact" is aimed to stress the fact that the correction term $\Delta\rho$ to the density operatoras given by these equations, is still exact. The initial condition is taken as Eq 5:

$$f(-\infty) = 0 \quad \text{and} \quad \rho_0(-\infty) = \rho_{eq} \tag{5}$$

Here ρ_{eq} is the conventional equilibrium canonical density operator of the system; using common notations, it holds $\rho_{eq} = Z^{-1} \exp(H_0/k_B T)$, where k_B is the Boltzmann constant and T the absolute temperature.

At this stage, Kubo [17] introduced the well known linear approximation, or linearization, of $\Delta\rho(t)$ by the replacement Eq 6:

$$Linearization: \quad \int_{-\infty}^{t} ds...\rho(s)... \quad \rightarrow \quad \int_{-\infty}^{t} ds...\rho_0(s)... \tag{6}$$

in the above integral expression. This is the crucial point criticized by van Kampen.

Additionally, the Kubo derivation contains the common assumption that the "undisturbed" system is described by the canonical density operator see Eq 7:

$$\text{for all} \quad s \leq t : \quad \rho_0(s) = \rho_{eq} \tag{7}$$

of thermal equilibrium—which however is not an issue of criticism.

As revealed by van Kampen, this Eq 6 represents an unphysical assumption, in general. To see this, consider an operator B of the system, which is experimentally measured and yields the value as see in Eq 8:

$$\langle \Delta B \rangle = Tr(B\Delta\rho(t)) \tag{8}$$

for the deviation (caused by the external force $f(t)$) from the "undisturbed" value $Tr(B\rho_0(t))$. Introducing the aforementioned linear approximation in the expression of the exact $\Delta\rho(t)$, one gets Eq 9:

$$\langle \Delta B \rangle_{lin} = \frac{i}{\hbar} Tr \int_{-\infty}^{t} ds B_H(t-s)[A, \rho_{eq}]f(s)$$

$$= \frac{1}{i\hbar} Tr \int_{-\infty}^{t} ds [A, B_H(t-s)] \rho_{eq} f(s) \tag{9}$$

where the Heisenberg representation Eq 10:

$$B_H(t) \equiv e^{\frac{i}{\hbar} H_0 t} B \, e^{-\frac{i}{\hbar} H_0 t} \tag{10}$$

of the Schrödinger operator B is introduced, and the cyclic permutation of operators in the trace operation (Tr) is applied; see references [17, 19, 20] for full details of calculations. The expression $\langle B \rangle_{lin}$ is the main result of LRT, which is widely known (and widely applied) in various physical and chemical fields of science and technology.

As van Kampen pointed out for the first time [18], the Eq 6 confuses the macroscopic linearity (as expressed by the macroscopic response $\langle \Delta B \rangle_{lin}$) with the microscopic linearity expressed with the density operator perturbation $\Delta \rho(t)_{exact}$ due to the external force. The measurable quantity $\langle \Delta B \rangle_{lin}$ is due to the randomization of the quantum phases of the many-body state, as represented by ρ, which are wildly changing in the course of time, leading to a cancellation, or averaging, of the complex details of the matrix elements of ρ. So, the Eq 6 is tantamount to a repeated randomization assumption (RRA) [21], concerning the chaotic dynamics of quantum phases and their "averaging" (or coarse-graining, chaotic phase mixing, etc.).

In other terms, the above linearization simulates randomization of the quantum phases, and thereby simulates decoherence and associated dissipation. Moreover, as van Vliet explained in detail [19, 20], nowhere is the dynamics commensurate with dissipation introduced in Kubo's theory. Namely, no time relevant scales (transition or collision duration times, relaxation times between collisions, etc.) are used in the treatment. As a consequence, if the Kubo derivation is physically correct, in principle the Eq 6 must work over all macroscopic time, for example, over 1 s. A numerical estimate in [18] demonstrated that this is an impossibility, since then this would limit the electric field to infinitesimally small values, for example, $E \sim 10^{-18}$ eV/cm! See also van Kmpen's further explanations making use of the so-called Galton board [18].

Of course, the important question therefore is posed: In what sense is LRT physically correct? This however is beyond the scope of the present paper, and the interested reader may consult the extensive literature; see [19, 20, 22] and references cited therein. For example, the relevance of chaos for LRT was pointed out in Reference [22].

Summarizing, we may say that Kubo's LRT tacitly makes use of the RRA, which is not an element of standard quantum dynamics (i.e., the Schrödinger and/or von Neumann equation, which have unitary time evolutions), but an additional theoretical assumption (i.e., the RRA), which is a *non-unitary* process. In more drastic terms: without a means to treat cancellation and/or randomization of quantum phases, irreversible processes cannot be interpreted properly by the Kubo formalism.

For a general approach and the detailed discussion of statistical mechanics of irreversible processes, see also Ref. [21] by van Kampen, in which the indispensable role of randomization assumptions is stressed explicitly and in detail. The reader being interested in a self-contained presentation and consistent amendment of LRT may be referred to the Refs. [19, 20] by van Vliet.

3. Quantum Zeno effect, inhibited decay of an excited state, and intensity deficit

The quantum Zeno effect (QZE), theoretically invented by Misra and Sudarshan [23], is a well known quantum mechanical phenomenon; see [24–27] and references therein. The QZE deals with repeated short measurements of a quantum system, and it shows that the dynamics slows down and, in some limiting cases, it is even possible to completely "freeze" the dynamics into a single state.

Conventionally, the presentation of the QZE considers the inhibited decay of an excited and unstable quantum state due to specific external measurement disturbances. However, the theoretical derivations are of more general character and are in principle applicable to any quantum transition between two states properly "measured" or disturbed. We consider now a short and simple outline of the derivation of this effect.
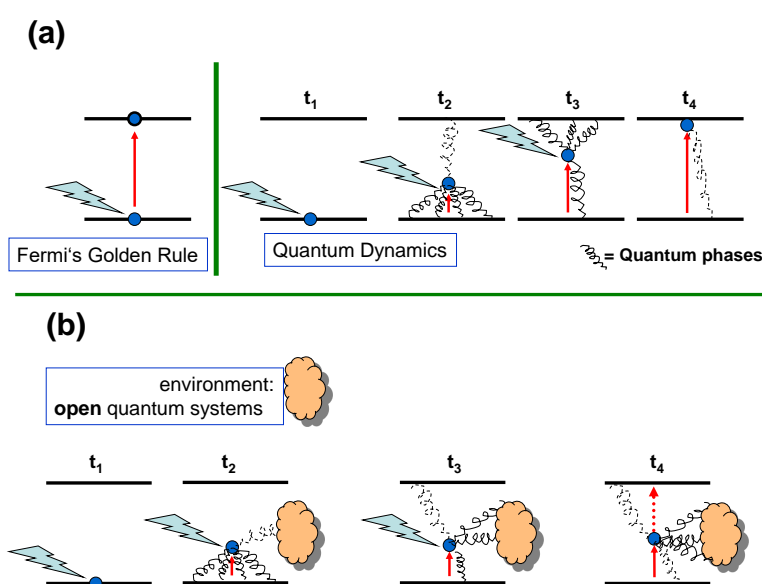

Figure 1. Cartoon about the quantum Zeno effect, in the case of excitation (instead of decay). Left (a): The common Fermi golden rule of the transition, here illustrated as an instantaneous jump (and a vertical red arrow) from initial Ψ_i to final Ψ_f state of a free atom interacting with an external quantum system (e.g., exciting photon, colliding neutron or electron, etc.), here shown as a flash acting on the atom. Right (a): A more time-resolved description of the process: The detailed quantum dynamics of the transition creates quantum phase relations and/or entanglement (shown as springs), involving Ψ_i and Ψ_f in the course of the finite excitation time. (b): The atom is here an open quantum system, in other, there exists some physically relevant "environment". The atom-environment interactions partially destroy (or cancel, or smear out) the development of quantum phase relations (and/or quantum correlations) involving Ψ_i and Ψ_f. So the excitation process becomes slower. Note that this slowdown, that is the reduced transition rate caused by the environment, is tantamount to an associated intensity deficit of the absorption and/or scattering process of the external disturbing field by the atom.

Let $|\phi\rangle$ be the state of a quantum system at the initial time $t = 0$ and H the relevant Hamiltonian of

the system. The time evolution of the state vector, $|\phi(t)\rangle$, is $\exp(-iHt/\hbar)|\phi\rangle$. The associated survival probability $S(t)$ for the system's initial state is then given by the Eqs 11–14:

$$S(t) = |\langle\phi|\exp(-iHt/\hbar)|\phi\rangle|^2 \tag{11}$$

If now one considers small times t, at which the system is observed or measured, a power series expansion is possible:

$$\exp(-iHt/\hbar) \approx 1 - iHt/\hbar - \frac{1}{2}H^2t^2/\hbar^2 + ... \tag{12}$$

Hence $S(t)$ becomes

$$S(t) = |\langle\phi|\exp(-iHt/\hbar)|\phi\rangle|^2 \approx 1 - (\Delta H)^2 t^2/\hbar^2 \tag{13}$$

where

$$(\Delta H)^2 \equiv \langle\phi|H^2|\phi\rangle - \langle\phi|H|\phi\rangle^2 \tag{14}$$

Thus we have $S(t) \to 1$ for sufficiently small times $t \to 0$.

The physical picture of this process is as follows, see Figure 1. The time evolution leads from $|\phi\rangle$ to a linear superposition of certain available quantum states. For example, an excited atomic state may evolve into a superposition of itself and several unexcited states, with the emission of a photon.) A measurement to determine whether the atom remains in the initial state can be formally described as a projection of the superposition onto the initial state $|\phi\rangle$. (This is the common projective or von Neumann-type measurement.) Therefore, in this projective process, quantum phase relations between the involved states are destroyed and decoherence (and/or dephasing) takes place. Thus one may conclude that, if such projective measurements (which should be instantaneous and ideal) are done repeatedly at times $0, \Delta t, 2\Delta t, 3\Delta t, ... n\Delta t, ...$, then the initial quantum state $|\phi\rangle$ is hindered and evolves slower, and in the limit $\Delta t \to 0$ the time evolution is completely "frozen" and the system remains in its initial excited state.

As a generalization, it holds that the QZE is also obtained in the case of continuous measurement of the initial state, and even in the case of not instantaneous and not ideal measurements; see for instance, the review article by Koshino and Shimizu [27].

There exists a large literature on the QZE, in which various scenarios of the mentioned projective measurements are proposed and/or analyzed. In several experimental contexts of particular interest are continuous measurements which may also lead to the Zeno effect [25, 26]. In this case, the time evolution of the process is continuously "observed", or continuously "measured". (In view of the physical applications we have in mind, see e.g., following subjection) this process may be effectuated by particles of the system's environment.) This continuous process can be incorporated in the Hamiltonian, and thus one dispenses with instantaneous quantum jumps, see [25]—as Figure 1b of the schematic depiction in Figure 1 indicates.

Some additional remarks are now in order. The following novel result by Kofman and Kurizki [26] concerning the so-called anti-Zeno effect may shed additional light on the role of quantum phases and correlations. The authors demonstrate that the modification of the decay process is determined by the energy spread incurred by the measurements (as a result of the time–energy uncertainty relation), and the distribution of states to which the decaying (i.e., final) state is coupled. Surprisingly, whereas the common inhibitory quantum Zeno effect may be feasible in a limited class of systems, the opposite effect—accelerated decay—was theoretically predicted to be much more ubiquitous.

Note also that, in the context of QZE, one often speaks of dephasing, or measurement induced dephasing (instead of decoherence).

3.1. QZE and the effect of intensity deficit of neutron scattering from H-atoms

Here we shortly present a direct consequence of the QZE that may have considerably unexpected experimental applications in various well-established fields, like neutron scattering from gaseous or condensed systems.

For illustration, let us consider a neutron impinging on a proton of H_2 (say, of a liquid hydrogen sample). The neutron-proton collisional dynamics (in other terms, the scattering) is mainly incoherent; see Section 6 below. Over the physically relevant finite scattering time, the kicked H is continuously "measured" by the "environment", that is, in this case, the two electrons and the second proton which strongly interact with the struck proton of the H_2 molecule. (The weak intermolecular interactions can be safely ignored here.) This leads to the aforementioned destruction of quantum phases (or decoherence, dephasing) due to the QZE and to the associated hindered transition to the final scattering state(s). Obviously, this process is tantamount with a reduced neutron-proton scattering intensity, which is experimentally accessible.

Note that this effect, as well as the general QZE, is due to a non-unitary dynamics, and hence it is unknown in the standard theory of neutron scattering [28, 29] which is based on the unitary quantum dynamics of standard theory.

It may be noted that this intensity-deficit effect has been observed experimentally in various neutron (and electron) scattering experiments from condensed and gaseous hydrogenous samples(confer [30–32] and references therein).

4. GKSL equation, decoherence and spontaneous energy increase

To describe the dynamics of open quantum systems and decoherence, various generalizations of the Schrödinger equation have been proposed; see the textbook [16]. Among these theoretical approaches, the Born-Markov master equation plays an enormously important role. Master equations of the so-called GKSL form (often simply abbreviated as Lindblad form) refer to a particular (albeit quite general) class of Markovian master equations, which ensure positivity of the reduced density operator $\rho(t)$ describing the system, that is, $\langle \rho(t) \rangle \geq 0$, for any pure state $|\psi\rangle$ of the system and for all t. The most general mathematical form of such equations was derived by Gorini, Kossakowski and Sudarshan [33] and Lindblad [34].

Consider the simplest Lindblad-type ansatz for the master equation for the statistical operator ρ of an open quantum system, which includes only a single Lindblad operator L; in a real system we would have a multitude of such dynamical variables. We set Eqs 15,16:

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] - \Lambda [L, [L, \rho]] \tag{15}$$

where H is the Hamiltonian and $\Lambda > 0$ is a positive constant. The first term on the right-hand side (rhs) gives the common unitary time evolution of the state ρ, and the double commutator term introduces decoherence in the equation of motion. Note that this equation describes "pure" decoherence, in the sense that it does not contain any term describing friction (or relaxation of states' populations); the latter are included in Caldeira-Leggett-type equations; see [16].

A well-known specialization of Eq 15 is the case of an one-particle system that interacts with an environment, in which case L is taken to be the position operator, r. This corresponds to the Joos-Zeh master equation [35].

The double commutator term (in the position representation) of Eq 15 takes the form [16]

$$-\Lambda(r - r')^2\langle r|\rho|r'\rangle \tag{16}$$

which, since $\Lambda > 0$, leads to an exponential decay of the nondiagonal elements of ρ, that is Eq 17:

$$\langle r|\rho(t)|r'\rangle = \langle r|\rho(0)|r'\rangle \exp(-\Lambda(r - r')^2 t) \tag{17}$$

where $t \geq 0$, $t = 0$ being the initial time [16].

This result represents decoherence. It says that the *non-diagonal* elements of the density operator tend to zero, and thus a pure state at $t = 0$, which is a coherent superposition of two components $|r\rangle$ and $|r'\rangle$, develops towards a mixed state and the superposition disappears over time. In condensed (or many-body strongly interacting) systems, which are those we are considering here, this is an ultra-fast phenomenon, so that the diagonal elements of $\rho(0)$ remain essentially unchanged (The latter decay much slower towards their thermal-equilibrium values, which of course are not zero). For example, see the textbook [16].

(Parenthetically, these remarks also mean that processes like e.g., polarization decay of spin ensembles, are not addressed in this paper; cf. the Introduction.)

Equation 15 preserves the normalization $Tr(\rho) = 1$ [34], which of course is satisfactory. However, Ballentine [36] made the following surprising observation: the expectation value of the energy, $\langle H \rangle = Tr(H\rho)$, is in general not conserved but increases with time, because in Eq 18:

$$\frac{d\langle H \rangle}{dt} = \frac{d}{dt} Tr(H\rho) = Tr\left(H\frac{\partial\rho}{\partial t}\right) = -\Lambda\, Tr([H, L][L, \rho]) \tag{18}$$

Here, one uses the trace operation property $Tr(A[B, C]) = Tr([A, B]C)$. Hence, if the Hamiltonian and the Lindblad operator L do not commute, $\langle H \rangle$ is in general not conserved.

To demonstrate of the significance of this result, let us consider the case of a free particle in one dimension with Hamiltonian $H = p^2/2m$. As mentioned above, the decoherence in position due to interactions with the "environment" is achieved by taking L to be the particle's position operator r [35]. Then, since $[p, r] = \hbar/i$ and Eqs 19,20:

$$[p^2, r] = p^2 r - rp^2 = (p^2 r - prp) + (prp - rp^2) = p[p, r] + [p, r]p = \frac{2\hbar}{i}p \tag{19}$$

it follows

$$
\begin{aligned}
\frac{d\langle H \rangle}{dt} &= -\Lambda\, Tr([p^2/2m, r][r, \rho]) \\
&= -\frac{\Lambda}{2m}\frac{2\hbar}{i}Tr(p[r, \rho]) = -\frac{\Lambda}{2m}\frac{2\hbar}{i}Tr([p, r]\rho) \\
&= +\frac{\Lambda\hbar^2}{m} > 0
\end{aligned}
\tag{20}
$$

This surprising result holds also in three dimensions, and also in more complicated cases, in which scalar and/or vector potentials are included. It also remains valid for more general cases, for example, even in cases with the decoherence factor Λ becoming a function of the distance $|r - r'|$; for details see Refs. [36–38].

Undoubtedly, this result may seem quite paradoxical as it contradicts every conventional expectation about what the experimentally observable consequences of decoherence should be. Namely, Eq 20 appears to represent a serious weakness of the theory, because it implies that the mean kinetic energy of a single particle should always increase despite its interactions with the environment (which is expected to cause friction and thus reduce its kinetic energy). Or, in other terms, the environment causing decoherence seems to act as an inexhaustible source of kinetic energy of the atom. Moreover, this continuous gain of kinetic energy is clearly incompatible with the system's attainment of equilibrium [36, 38]. For a thorough discussion of these paradoxical findings, see [36, 37] and the very detailed analysis by Stenholm [38].

Moreover, a significant amendment to the Lindblad-type equations towards the resolution of the considered paradox was proposed by Diósi [39], who showed that an additional term of position diffusion appears into the formalism which has no analogue in the classical Fokker-Planck equation; see Eq 23 of Ref. [39]. For further theoretical aspects and facets of GKSL-type equations, see [40, 41]. However, these and various further related works do not invalidate the main conclusions of Stenholm [38] concerning the "strange" result of Eq 20.

4.1. Decoherence and intensity deficit in impulsive neutron scattering

Parenthetically, another surprising consequence of the Lindblad equation may be shortly noted here. A "first principles" description of scattering from open quantum systems subject to a Lindblad-type dynamics was provided by C.-Dreismann and Stenholm [42]. It was shown that the irreversible time evolution due to the decoherence effect causes a reduction of the system's transition rate excited by the neutron scattering. Obviously, this is tantamount to a shortfall of scattering intensity [42], in other, an "intensity deficit" with respect to conventional expectations. Furthermore, since this theoretical result cannot have a classical analogue, it appears to represent a witness of quantumness of correlations (e.g., entanglement, quantum discord, etc.).

Note that this intensity-deficit effect coincides with the aforementioned neutron Compton scattering effect; see the previous subsection 3.1.

5. Quantum correlations due to two-body collisions, their erasure, and induced energy increase—Schulman-Gaveau model

Here we consider some surprising energetic consequences of decoherence at small times for coupled systems, as shown by a theoretical investigation of Schulman and Gaveau [43, 44]. Their analysis appears to lead essentially to an analogous result—an unconventional energy increase—as the simple Lindblad equation in the previous section. A short description of the general model is as follows.

One considers two quantum oscillators, A and B, with "free" Hamiltonians H_A and H_B (These could belong to some many-body system, e.g., a liquid or gas) . A and B are assumed to move and collide from time to time. Let V_{AB} be the associated interaction Hamiltonian describing the collisional

dynamics, and in Eq 21,

$$H = H_A + H_B + V_{AB} \tag{21}$$

be the corresponding total Hamiltonian. (The translational Hamiltonians between the collision, are not included explicitly in the model.) Before a collision, say at time $t = 0$, the two systems are assumed to be not entangled and hence the complete density matrix $\rho(0)$ should factorize $\rho(0) = \rho_A(0) \otimes \rho_B(0)$. In general, subsequent to their collision the two oscillators are entangled and the exact density operator like Eq 22,

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \tag{22}$$

($U(t)$: time evolution operator) is not a product state of individual density operators $\rho_A(t) = \mathrm{Tr}_B\rho(t)$ and $\rho_B(t) = \mathrm{Tr}_A\rho(t)$.

However, it is widely believed that once the particles are separated the quantum correlations can be dropped (provided one does not perform an experiment of Einstein-Podolsky-Rosen type), simply because measurements of physical quantities of each of the two (spatially separated) particles cannot depend on their correlations. Thus the replacement (Eq 23),

$$\rho(t) \rightarrow \rho_A(t) \otimes \rho_B(t) \tag{23}$$

which is equivalent to the erasure of quantum correlations between the two particles, is usually expected to not affect the energies of the systems.

A striking theoretical result by Schulman and Gaveau [43], however, contradicts this intuitive expectation. Putting Eq 24,

$$\Delta\rho(t) = \rho_A(t) \otimes \rho_B(t) - \rho(t) \tag{24}$$

and for several *specific forms* of the interaction Hamiltonian V_{AB}, they derived the following unexpected result: For sufficiently *short* collisional times the relation holds Eq 25:

$$\Delta E \equiv Tr(\Delta\rho(t)H) = Tr(\Delta\rho(t)V_{AB}) > 0 \tag{25}$$

See Ref. [44] for a detailed derivation of this inequality. Accompanying computer simulation results confirmed this analytical result.

In more physical terms, the replacement of the correct (entangled) $\rho(t)$ with the non-entangled state $\rho_A(t) \otimes \rho_B(t)$ necessarily increases the systems' energies [43,44]. This appears highly paradoxical since, as Schulman and Gaveau put it: " ... loosing quantum correlations should not heat the gas. You do not burn your finger because of a partial trace over a density matrix" [43].

Moreover, this result was shown to be valid for a large class of two-body interaction potentials, although it does not hold universally [44]. This is an interesting feature, and therefore the following details should be mentioned (Eq 26). The spin-boson model Hamiltonian (putting $\hbar = 1$)

$$H_{SB} = H_A + H_B + V_{SB} = \omega_a a^\dagger a + \omega_b b^\dagger b + g(a^\dagger + a)(b^\dagger + b) \tag{26}$$

was shown to exhibit the considered "heating" effect, in clear contrast to the related popular Jaynes-Cummings model Eq 27

$$H_{JC} = H_A + H_B + V_{JC} = \omega_a a^\dagger a + \omega_b b^\dagger b + g(a^\dagger b + b^\dagger a) \tag{27}$$

in which the effect fully disappears [43].

In view of the counter-intuitive result Eq 25, one may object that it is unphysical because it seems to violate energy conservation (since the vibrational energies of both oscillators increase). However this is not the case, as the detailed discussions of Ref. [43] explained. Namely, it was emphasized that, in the situation contemplated, the coupling Hamiltonian must be considered time dependent, because the physical approach and separation of the particles leads to a time-dependent coupling coefficient, that is Eq 28,

$$g \equiv g(t) \tag{28}$$

In other words, the two oscillators represent an open quantum system, and thus, energy conservation need not apply. Moreover, it was discussed in physical terms that this "additional" energy $\Delta E > 0$ is supplied by the *translational* degrees of freedom of A and B [43] (which do not appear explicitly in the Hamiltonian Eq 21) and thus may be considered to represent an effective "environment" which provides this additional energy.

Moreover, of particular physical interest is the following detail, which underlines the quantum nature of the effect under consideration. The crucial difference between the two Hamiltonians H_{SB} and HV_{JC} is the cancellation of the two terms see Eq 29:

$$a^\dagger b^\dagger \quad \text{and} \quad ab \tag{29}$$

of H_{SB}, in order to get H_{JC}. These terms are of true quantum nature, since they describe short-lived quantum fluctuations which have no classical analogue. (They describe simultaneous creation, resp. destruction, of two quanta of energy, seemingly violating energy conservation.) In contrast, the popular Jaynes-Cummings Hamiltonian H_{JC} does not contain such "counter-intuitive" terms. Hence, the Schulman-Gaveau result, Eq 25, is caused by these quantum terms of the Hamiltonian, and the associated collision-induced quantum correlations of the oscillators.

The qualitative analogy between the findings of the Schulman-Gaveau and Lindblad-type theoretical models may be observed.

6. A real experiment—Incoherent inelastic neutron scattering (INS) off H₂ in carbon nanotubes

We consider here an interesting experiment and its striking result, which has found no conventional interpretation thus far. It was carried out by Olsen et al. [45] from single H_2 molecules adsorbed in multi-walled carbon nanotubes (pore diameters $\approx$ 8–20 Å). The molecules undergo rotational and translational motion excited by the collision with the neutron.

The used time-of-flight neutron spectrometer was ARCS, (SNS, Oak Ridge National Laboratory, USA) [46]. This is a new-generation 2-dimensional spectrometer and its detectors (about 100,000) measure a broad area of the momentum-energy ($\hbar K$–E) plane. (K: wave vector transfer; E: energy transfer.)

The experiments were done at $T = 23$ K, with the incident neutron energy $E_0 = 90$ MeV. Hence, the maximally possible E-transfer cannot excite (the much higher lying) molecular vibration, but only rotation and translation, of H_2 which interacts only weakly with the substrate Eq 30:

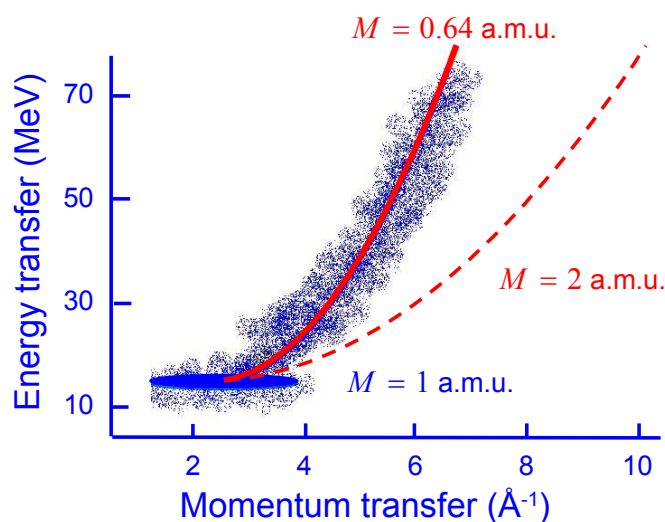$$E = E_{rot} + E_{trans} \tag{30}$$

Figure 2. INS results from H_2 in carbon nanotubes (schematic), adapted from Figure 1 of Ref. [45]. Neutron initial energy: $E_0 = 90$ MeV; temperature: $T = 23$ K. The broad intensity ribbon is due to the translation motion of the recoiling H_2 molecules along the nanotube, also called "roto-recoil" (white-blue ribbon). This starts at the first rotational excitation of H_2, which is centered at $E_{rot} \approx 14.7$ MeV and $K_{rot} \approx 2.7$ Å^{-1} (blue ellipsoid). The momentum-energy (K–E) position of the rotational excitation fully agrees with conventional theory. In clear contrast, the detailed data analysis of the authors of [45] provides a fit (red parabola; full thick line) to the roto-recoil data, which exhibits a striking reduction of the effective mass of recoiling H_2 molecule: The data are consistent with the effective mass of translating H_2 of only 0.64 a.m.u. Comparison with the conventional expectations is given by the red thin (dashed) line, which represents the recoil parabola with effective mass 2.0 a.m.u. For full details of data analysis and further experimental data, see [45]. (Reprinted with permission from [47].)

The experimental two-dim. INS intensity map $S(K, E)$ is schematically shown in Figure 2, which is adapted from the original paper [45]. One may notice the following features. First, the intensive peak with energy around $E_{rot} \approx 14.7$ MeV is due to the well known rotational excitation $J = 0 \rightarrow 1$ of a free H_2 molecule; for ecample, the reference [47] for a discussion. The K-transfer of this intensity peak is $K_{rot} \approx 2.7$ Å^{-1}. It follows that the peak position in the K–E plane fully agrees with the conventionally expected numerical value of the H-mass. That is, the data fulfills the conventional theoretical relation (Eqs 31,32):

$$E_{rot} = \frac{\hbar^2 K^2}{2M_H} \tag{31}$$

($\hbar K$: momentum transfer on the kicked H.) This is the so-called recoil parabola of a particle (here H) with M_H being the mass of the free H atom,

$$\text{rotation:} \quad M_H = 1.0079 \text{ a.m.u.} \tag{32}$$

(a.m.u.: atomic mass units.) In other terms, the impinging neutron exciting a rotation scatters from a

particle with mass M_H. This is fully in line with conventional theory of INS, see the textbook [48], that each neutron scatters from a single H-atom which behaves as being quasi-free during the ultra-short scattering time.

For further illustration of this conventional result, let us mention here a related neutron scattering finding from liquid helium [49]; see Figure 3. The shown scattering results are fully consistent with conventional theory.
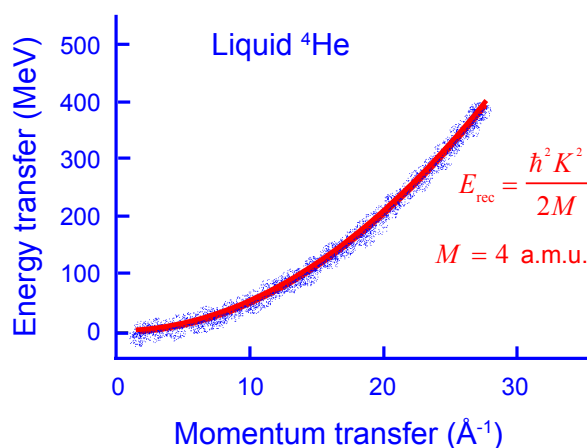

Figure 3. Schematic representation (blue points) of the dynamic structure factor $S(K, E)$ of liquid helium, adapted from Ref. [49]. The experiment was performed with the 2-dimensional TOF-spectrometer ARCS. Red line: The calculated recoil parabola for scattering from ^{4}He atoms with atomic mass 4 a.m.u. (Reprinted with permission from [47].)

In clear contrast to these findings, a detailed analysis of the measured roto-recoil data in frame of conventional theory, yields a significant $\hbar K$-transfer deficit, and an associated strongly reduced effective mass of the whole recoiling H_2 molecule (red parabola, full line, see Figure 2)

$$\text{translation (recoil):} \quad M_{H_2}^{eff} \approx 0.64 \pm 0.07 \ \text{a.m.u.} \tag{33}$$

This represents a dramatic deviation from conventional theoretical expectations (Eq 33).

This observation clearly contradicts the conventionally expected value $M(H_2) = 2.01$ a.m.u. for a freely recoiling (translating) H_2 molecule (right parabola, red dashed line). An extensive numerical analysis of the data is presented in [45], as well as a discussion of the expected conventional results being violated by the INS experiment. The strongly reduced effective mass is far beyond any conceivable experimental error. Thus far this effect has found no conventional theoretical interpretation.

Additionally, the following physical detail may be mentioned. As discussed in our preview works [47, 50, 51] in detail, and according to conventional theory, every H_2-substrate binding and/or interaction must correspond to an increased effective mass of the scattering system (here H atom), since it hinders the free H_2 motion. In contrast, dynamics of QoC (and quantum thermodynamics) revealed the counter-intuitive possibility of a decreased effective mass of the scatterer (here H atom).

This theoretical feature is presented and discussed in more detail in Ref. [51]. In short, the erasure of existing quantum correlations between H_2 and substrate caused by the collision, provides an additional

energy contribution to the energy transfer delivered by the neutron in the collision. This appears to facilitate the H_2-translational motion.
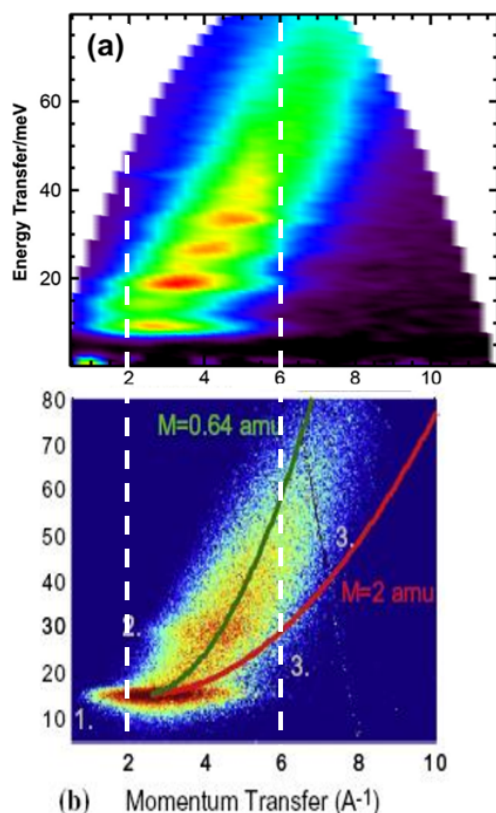

Figure 4. Comparison of the two experimental results: Experimental $S(K, E)$ maps of the two original papers, appropriately stretched/scaled to facilitate comparison. (a): H_2 in HKUST-1 [53]; (b): H_2 in carbon nanotubes [45]. The shown two vertical dashed lines (white) are guides to the eye. The two broad continuous ribbons due to the translational modes are virtually identically positioned in the momentum-energy plane $\hbar K$–E, both exhibiting the quantum effect under consideration. (Reprinted with permission from [51].)

It may be assuring that the considered INS effect has been confirmed with an independent experiment, in other, in a different H_2 containing nano-structured solid, investigated in another laboratory. Namely, the INS measurements were done with the 2-dim. spectrometer MARI (ISIS facility, UK) [52] by an independent group of scientists. The hydrogen containing material was the Cu(II) metal-organic material known as HKUST-1 (see [53] for its chemical formula and structure) which has emerged as a model system for hydrogen adsorption studies. For our present purposes, it is sufficient to note that HKUST-1 constitutes a three-dimensionally connected network that has a trimodal pore structure, having pores with diameters in the range 5–12 Å.

Figure 4, upper panel, provides the INS intensity map $S(K, E)$ of this experiment, in comparison with the corresponding data (lower panel) of the aforementioned experiment with ARCS [45].

Visual comparison of the data of the two experiments reveals that the two broad continuous bands due to the translational modes are virtually identically positioned in the K–E plane. This is quite

astonishing given the fact that the two experiments were done with two different nano-structured materials and using two different 2-dimensional spectrometers.

For more experimental details, a complete presentation of the INS experimental technique, and associated references, see the recent Refs. [47] and [51].

6.1. Ballentine's result and INS from H₂ in carbon nanotubes

A very simple qualitative interpretation of the striking INS finding Eq 33 may be given by making use of the theoretical result of Ballentine, Eq 20, as follows.

The translational energy of H_2 gained by the INS process has two sources: (a) the energy transfer from the neutron, and (b) the contribution $\Lambda\hbar^2/M_{H_2} > 0$ due to decoherence, Eq 20, which accompanies and even facilitates the H_2 translation. Hence the conventional recoil parabola $\hbar^2 K^2/2M_{H_2}$ describing the H_2 translation caused by the collision has to be amended to Eq 34:

$$\frac{\hbar^2 K^2}{2M_{H_2}} + \frac{\Lambda\hbar^2}{M_{H_2}} = \frac{\hbar^2 K^2}{2M_{H_2}^{eff}} \tag{34}$$

Since Ballentine's contribution is positive, this equation can only be fulfilled with Eq 35,

$$M_{H_2}^{eff} < M_{H_2} = 2 \ \text{a.m.u.} \tag{35}$$

From the requirement Eq 34 and the aforementioned INS-determined value $M_{H_2}^{eff} \approx 0.64$ a.m.u. The interested reader may determine the numerical value of the decoherence parameter Λ in the Lindblad Eq 15 referring to the specific experiment [45].

6.2. Weak Values theory and INS from H₂ in carbon nanotubes

Moreover, it should be noticed that this striking INS effect can also find a "mechanistic" interpretation (i.e., in the frame of quantum dynamics of collisions, using Hamiltonians instead of correlations) within the novel quantum theoretical frame of Weak Values (WV) and Two-State Vector Formalism (TSVF) by Y. Aharonov and collaborators; confer the recent review article [54] and extended references therein.

7. Synopsis of new results and research consequences

As alread pointed out in the Introduction, this paper contains no new theoretical derivations and/or theoretical results. The major goal of the paper is to provide the reader with an alternative view and understanding of the physical meaning of the loss of QoC in quantum systems and its implications. Hence it seems appropriate to clarify the paper's original new contributions and to recapitulate explicitly the associated research consequences. These issues are addressed here.

(I) The weakness of standard LRT revealed by van Kampen, see also Section 2, is often understood intuitively in the following sense: The thermal equilibrium state, $\rho_{eq} = Z^{-1} \exp(H_0/k_B T)$ —which is of basic importance in general thermodynamics— defines the initial state before the sufficiently weak perturbation $A \cdot f(t)$ is switched on; additionally, the existing thermal bath couples sufficiently strongly with the system to keep it in thermal equilibrium. So, if van Kampen's argument would be physically

correct (and not a mathematical artifice), then the fundamental character of the concept of thermal equilibrium would be affected.

However, this understanding is not quite correct, because the linearization Eq 6 does not coincide with the continuous persistence of thermal equilibrium as expressed in Eq 7. Namely, the undisturbed density operator $\rho_0(t)$ could be any possible t-dependent state, for example, a steady state far-from-equilibrium—and van Kampen's argument still holds true.

So, we conclude that van Kampen's main point is much more generally valid, and it might be rephrased as follows: Linearization of the exact density operator $\rho(t)$ is a completely different concept than linearization of the expectation value $\langle B \rangle_{lin}$ of an observable B. In other words, $\langle \Delta B \rangle_{lin}$ can be small, but the associated $\Delta\rho(t)_{lin}$ can be huge — and as van Kampen has emphasized: it is!

(II) The QZE, although broadly known among theoreticians, it has found thus far very limited applicability in real experiments, using well established techniques. Hence the experimental neutron scattering context and the finding of scattering intensity deficit, as shortly interpreted in Subsection 3.1, provide a thus far unknown consequence of the QZE in the experimental field of scattering physics.

(III) The "perplexing" theoretical result given by Eq 20 of Section 4 is usually considered as a curiosity of the GKSL theoretical frame, without any realistic physical application. The possibility, or speculative idea, to interpret the anomalous INS-effect of Section 6, shortly described in Subsection 6.1, represents a new research consequence of the work reported in the present paper.

(IV) In Section 5 was discussed the incapability of the popular Jaynes-Cummings Hamiltonian, Eq 27, to capture the Schulman-Gaveau result, due to the two missing terms $a^\dagger b^\dagger$ and ab in the Hmiltonian, which are associated with quantum fluctuations. This was also mentioned in the cited original papers. However, the intrinsic interrelation with the non-conventional energy increase effect addressed in the context of the GKSL equation is firstly addressed explicitly in this paper.

This simple detail is however far from being trivial, as for example, a possible further investigation of the experimental INS effect of Section 6—based on Hamiltonians rather than on QoC—might show. Namely, the operators a and b may refer to the H_2 and to the C-nanotube, respectively, and then the Hamiltonian terms $a^\dagger b^\dagger$ and ab may cause the increase of translational energy of the struck H_2—as experimentally measured—in analogy to the Schulman-Gaveau effect on colliding oscillators. Note that an associated energy increase (e.g., in the form of heat) of the C-nanotube cannot be measured in the INS experiment. Such a theoretical analysis would be of considerable value for experimental and industrial research on materials for hydrogen storage and transfer.

(V) The possibility to theoretically interpret the anomalous INS-effect of Section 6, as provided in Subsection 6.1, represents a new research consequence of the work reported in the present paper.

Summarizing, the paper provides a brief, general overview of different effective quantum-theoretical models and phenomena where the suppression of phase correlations (decoherence) plays a fundamental role. More importantly, based on them, the main claim hold here is that there is nothing indicating that such a degradation of quantumness necessarily means a "heat" production, but that it can be understood, instead, as a source of work.

8. Additional remarks and discussion

Several aspects and/or points related to the topics of the preceding sections are considered in the following.

(A) From the above discussions and considerations it should be obvious that the well known quantum correlation effects between identical particles (like e.g., electrons in molecules) play no role in this paper—we always consider correlations between distinguishable systems (like e.g., H_2 and carbon nanotube in Section 6).

(B) In all topics presented above, destruction and/or erasure of QoC (entanglement, quantum discord, etc.) have a real, and rather simple, cause: The considered material systems (atoms, molecules, solids) are not closed, but open systems, having an environment (e.g. adjacent particles, acting external fields, etc.). Even a part of an isolated system (e.g., molecule) can be considered as the "relevant system", and the rest of the molecule can act as an "environment". Therefore, the mentioned destruction (erasure, washing out) of quantum correlations is trivial due to the following fact: The interactions of the relevant system with its environment create entanglement (or quantum discord) with environmental particles, thus creating correlations with external degrees-of-freedom, which furthermore lead to the aforementioned erasure of quantum phase relations (and correlations) within the relevant system.

In simple physical terms, the quantum phase relations of the relevant system do not fully disappear without leaving any trace, but they "leak out to the environment"—or, they become degradated by becoming mixed with environmental contributions. Consequently, everywhere in this paper the term decoherence is tantamount with "environmentally induced decoherence". Note that exactly this process is the main obstacle hindering the progress in all quantum technological fields; see also [5].

(C) Wavefunctions (or quantum states), their quantum phases and interrelations between them, play a crucial (if not even dominant) role in all topics addressed above. Thus it is natural to mention here the popular density functional theory (DFT), in which the the wavefunction is "replaced" with a so-called density functional. This simplifies immensely the quantum-chemical numerical calculations and thus makes it possible to handle molecular systems with a huge number of atoms—something that present-day computers cannot achieve if the calculations have to based on the Schrödinger equation. Against a rather common belief, however, DFT is only an approximation and not an "ab initio" method. In this context, we may mention here the following remark by Nordén who writes in an Editorial with the title "Which are the 'Hilbert Problems' of Biophysics?" the following comments: "According to a theorem by Kohn and Hohenberg, an electron density functional always exists that can electrostatically uniquely define a molecular ground state without need for consideration of Schrödinger wavefunctions. However, despite this existence proof, nobody has yet been able to produce such a density functional, and so-called DFT methods do not rest on true Density Functionals." [55].

Clearly, operations of a quantum processor like those in [6], or those in any quantum communication protocol, cannot be described (neither conceived) in the frame of DFT.

(D) QoC phenomena, like entanglement, discord and decoherence, play no role in conventional neutron scattering theory [28, 29, 48]. This is due to the fact that conventional scattering theory applies the general formalism of first-order perturbation theory (to which belongs also the well known Fermi Golden Rule), which is based on the unitary time evolution of standard quantum mechanics. In contrast, decoherence, erasure or mixing of quantum phases etc., are governed by non-unitary dynamics—to which belong the QZE, van Kampen's RRA, GKSL-type Markovian dynamics, Schulman-Gaveau effect, and intensity deficit effect in neutron scattering, considered in the preceding sections.

(E) As indicated in the Introduction, the aim of this paper is not to provide complete (or exhaustive) presentations of the theoretical models discussed. For example, in the section on the QZE there is

no remark about the so-called Zeno-time which would be needed in any exhaustive discussion of a complete treatment of QZE (see the cited references). Or, in the section on LRT, the attempts made in order to amend Kubo's theory are not addressed. Thus we refrained from using terms and results from the "heavy" (and very extensive) field of quantum thermodynamics(consult for reference [10–15, 51]) Rather, the main aim is to emphasize the common point made by the various theories addressed, while assuming a minimum of prior knowledge of them, thus hoping that the main message of the paper may reach a broader and non-specialized readership.

9. Conclusion

The general character of the preceding analysis indicates that similar striking effects (like those obtained with INS, Section 6) can be observed in a larger class of materials, as well as by applying other scattering methods (e.g., X-ray scattering on multilayered materials, or quasi-elastic electron scattering.). Consequently, the above theoretical QoC considerations may be useful for further experimental and also technological and industrial applications.

With regard to the latter, here we may mention:
(1) The field of the emerging "hydrogen technology", also referred to as "green energy";
(2) The development of better fast proton conductors [56] for usage in fuel cells;
(3) Effects of hydrogen trapping in metals, for example, dynamics of embrittlement in high-strength Al alloys [57], and
(4) The exploration and development of novel solid materials to be used as ultra-fast ionic conductors in various technical devices, as for example, the very recently discovered crystalline material $La_{0.70}Sr_{0.25}Zn_{0.05}OI_{0.70}$ which exhibits an enormous large conductivity of the iodide anion (I^-), despite the ion's considerably large size [58].

Concluding, we believe that the above remarks strongly support the view that the various kinds of quantumness of correlations represent fundamental quantum properties of matter, the exploration of which may provide additional insights into the physics and chemistry of the considered topics. Moreover, they seem to be of technological and/or industrial interest too.

Last but not least, we would like to highlight the potential importance of QoC for novel developments in technology and materials science, especially for future quantum technologies of the emerging "second quantum revolution". Here we may expect that the various kinds of QoC (e.g., entanglement, quantum discord, quantum coherence, quantum superpositions, weak values) may be used as novel tools, which should open up new avenues of research. Namely, energetic and structural (and more generally, static) features of materials are already successfully treated with quantum chemical calculations, but QoC aspects of them are rather unknown. The latter may provide novel insights into the *dynamics* of materials. Recall that a real application—say for example, a novel proton conductor material for fuel cells; or a nano-structured storage material for improved Li^+-ion batteries—is characterized mainly by the dynamics of mobility of the protons (or Li^+ ions, respectively) in the material, rather than in the static structural properties of it. As already all the theoretical (dynamical) models presented in the preceding sections showed, QoC effects may provide novel insights, which static quantum interactions (as captured by quantum Hamiltonians and the time-independent Schrödinger equation) alone cannot explain. These remarks and considerations are already well appreciated in the emerging fields of quantum information technologies (QIT), in which some of

the aforementioned kinds of QoC play a dominant role; but in material sciences they are still not recognized as being of fundamental importance.

Acknowledgments

Conflicts of interest

The author declares no conflicts of interest in this paper.

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