Decoherence and the Puzzle of Quantum Brownian Motion in a Gas

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1 Introduction

The long time of ignorance after Zeh's publications [1, 2] in 1970–71 on environmental decoherence got broken by Wigner. He summarized his own revelation and Zeh's discovery [3] as follows: *This writer's earlier belief that the physical apparatus' role can always be described by quantum mechanics [...] implied that the "collapse of the wave function" takes place only when the observation is made by a living being—a being clearly outside of the scope of our quantum mechanics. The arguments which convinced me that quantum mechanics' validity has narrower limitation, that it is not applicable to the description of the detailed behavior of macroscopic bodies, is due to D. Zeh. (1970) [...]. The point is that a macroscopic body's inner structure, i.e. its wave function, is influenced by its environment in a rather shot time even if it is in intergalactic space. Hence it cannot be an isolated system [...].* Wigner raised the question: *Can an equation for the time-change of the state of the apparently not-isolated system be proposed?*

Nowadays, after decades, the answer is part of the theory of open quantum systems. But in 1983, it was a novelty that Wigner showed a master equation for the massive object's density matrix, modeling the decoherence of its rotational motion:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] - \sum_{\ell m} \varepsilon_\ell \left[\hat{L}_{\ell m}, [\hat{L}_{\ell m}, \hat{\rho}]\right] , \tag{1}$$

where $\hat{H}$ is the Hamiltonian of the macroscopic object and $\hat{L}_{\ell m}$ are the multipole operators of its angular momentum; strengths of their decoherence are given by the parameters ε_ℓ.

In 1985, Joos and Zeh (JZ) found [4] that decoherence of the center-of-mass position $\hat{\mathbf{x}}$ would be more typical and, what is important, its derivation is simple.

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2 Equation of Positional Decoherence

Consider a macroscopic object, e.g. a dust particle, of mass M under the influence of incoming plane waves of particles, e.g. molecules, of mass $m \ll M$ that are scattered independently by the macroscopic object. JZ took the following unitary transition per single collisions, valid if $M \to \infty$:

$$|\mathbf{p}_i\rangle \otimes |\mathbf{k}_i\rangle \Rightarrow |\mathbf{p}_i\rangle \otimes |\mathbf{k}_i\rangle + \frac{i}{2\pi k_i}\int d\mathbf{k}_f\, f(\mathbf{k}_f, \mathbf{k}_i)\delta(k_f - k_i)\left|\mathbf{p}_f\right\rangle \otimes \left|\mathbf{k}_f\right\rangle, \quad (2)$$

$\mathbf{p}_{i/f}, \mathbf{k}_{i/f}$ are the initial/final momenta of the object and the particle, respectively, where $\mathbf{p}_f = \mathbf{p}_i + \mathbf{k}_i - \mathbf{k}_f$ ensures momentum conservation, and f is the standard scattering amplitude. The authors pointed out that repeated scatterings of the incoming particles contribute to gradual localization of the object, i.e., the off-diagonal terms of the positional density matrix $\rho(\mathbf{x}', \mathbf{x})$ become damped. If the distribution $\rho^{\mathcal{E}}(\mathbf{k}_i)$ of the incoming environmental particles is isotropic then the collisions contribute to the following master equation:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] - \Lambda[\hat{\mathbf{x}}, [\hat{\mathbf{x}}, \rho]]; \quad (3)$$

valid if the coherent extension of the object's position is much smaller than the wavelength of the particles:

$$|\mathbf{x}' - \mathbf{x}| \ll \hbar/k. \quad (4)$$

JZ determined the parameter Λ of localization rate:

$$\Lambda = \frac{1}{\hbar^2} \times \text{incoming flux of particles} \times k^2\sigma_{\text{eff}}. \quad (5)$$

They calculated the effective cross section σ_{eff} from the differential cross section $|f|^2$.

The JZ master equation (3) is paradigmatic in decoherence theory. It describes the gradual damping of the off-diagonal elements of the positional density matrix $\rho(\mathbf{x}', \mathbf{x})$ which is called positional decoherence on one hand and yields localization of the coherent extension of the object on the other. In 1990 Gallis and Fleming [5] revisited the considerations of JZ and refined their derivation of positional decoherence and its rate Λ. It is not clear when, lately, was the localization rate Λ related to the classical diffusion coefficient for the first time. But the research moved to that direction.

3 Quantum Brownian Motion in a Gas

The JZ master equation (3) has an alternative interpretation, independent of and older than the concept of decoherence. It corresponds to momentum diffusion of the Brownian object, with the coefficient D_p of momentum diffusion:

$$\Lambda = \frac{D_p}{\hbar^2} \; . \tag{6}$$

As a beneficial consequence, to obtain and understand the dynamics of decoherence, also to complete the JZ master equation (3) by a term of friction, we could have used the standard quantum theory of Brownian motion in a gas. Just this standard theory did not exist at the time. And it has since remained problematic despite efforts of a community of researchers including myself. We all were motivated by our foundational interest in the quantum behavior of macroscopic objects under the influence of their uncontrollable environments. The efforts [6–10] started in 1995 and culminated in the Vacchini-Hornberger review [10]. These autors say ... *the seminal paper on decoherence by Joos and Zeh [...], seeking to explain the absence of quantum delocalization in a dust particle by the scattering of photons and air molecules, derived and studied what the authors called a Boltzmann-type master equation. Two decades later, the long quest for the characterization of the phenomenon of collisional decoherence has now reached a mature theoretical description, permitting its quantitative experimental confirmation*. Let me outline the story, in my—selective and certainly subjective— interpretation.

In 1995 [6], without mentioning my foundational motivations, I asked the question: what is the quantum Brownian dynamics of the dust in a dilute gas at thermal equilibrum? First I solved the classical problem by the linear variant of the classical Boltzmann-equation where the molecule-molecule collision term is just replaced by the dust-molecule collision term. Unlike the classical case, the derivation of the quantum linear Boltzmann equation (QLBE) was not straightforward. Quantum mechanically, a single collision corresponds to the following unitary transition, generalizing (2) for finite M:

$$|\mathbf{p}_i\rangle \otimes |\mathbf{k}_i\rangle \Rightarrow |\mathbf{p}_i\rangle \otimes |\mathbf{k}_i\rangle + \frac{i}{2\pi k_i^*} \int d\mathbf{k}_f^* f(\mathbf{k}_f^*, \mathbf{k}_i^*)\delta(k_f^* - k_i^*) \left|\mathbf{p}_f\right\rangle \otimes \left|\mathbf{k}_f\right\rangle \; , \tag{7}$$

where $\mathbf{k}_{i/f}^*$ are the initial/final momenta of the particle, respectively, in the center-of-mass frame. As before, $\mathbf{p}_f = \mathbf{p}_i + \mathbf{k}_i - \mathbf{k}_f$ ensures momentum conservation, total energy conservation is ensured by the delta-function. When imposing the distribution $\rho^{\mathcal{E}}(\mathbf{k}_i)$ of the gas molecule momenta, I had to introduce a heuristic *maneouvre of square-root* (MSqR); otherwise the correct mathematical structure [11, 12] of the desired quantum master equation wouldn't have been achieved. The MSqR was equivalent to a deliberate adding off-diagonal elements to the standard diagonal density matrix $\rho^{\mathcal{E}}(\mathbf{k}, \mathbf{k}') \propto \rho^{\mathcal{E}}(\mathbf{k})\delta(\mathbf{k} - \mathbf{k}')$ of the ideal gas molecules. The choice was

$$\rho^{\mathcal{E}}(\mathbf{k},\mathbf{k}') = \sqrt{\rho^{\mathcal{E}}(\mathbf{k})}\sqrt{\rho^{\mathcal{E}}(\mathbf{k}')}\,. \tag{8}$$

This MSqR and some other simple assumptions led to the first QLBE of Brownian motion in a gas. In the diffusion limit it yields the quantum Fokker-Planck equation (QFPE):

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] - \frac{D_p}{\hbar^2}[\hat{\mathbf{x}},[\hat{\mathbf{x}},\hat{\rho}]] - i\frac{\eta}{2\hbar}[\hat{\mathbf{x}},\{\hat{\mathbf{p}},\hat{\rho}\}] - \frac{D_x}{\hbar^2}[\hat{\mathbf{p}},[\hat{\mathbf{p}},\hat{\rho}]]\,. \tag{9}$$

The coefficients of momentum diffusion $D_p = \eta M k_{\mathrm{B}} T$ and friction η correspond to those in the classical Fokker-Planck equation:

$$\frac{d\rho}{dt} = \{H,\rho\}_{\mathrm{Poisson}} + D_p\left(\frac{\partial}{\partial\mathbf{p}}\right)^2\rho + \eta\frac{\partial}{\partial\mathbf{p}}\mathbf{p}\rho\,. \tag{10}$$

However, the quantum version (9) contains a strange term of *position diffusion* which would be nonsense classically. Position diffusion of the Brownian object is a pure quantum effect, the celebrated GKLS theorem [11, 12] puts the following lower bound on the coefficient of position diffusion:

$$\frac{D_x}{\hbar^2} \geq \frac{\eta^2}{4D_p} = \frac{\eta}{4Mk_{\mathrm{B}}T}\,, \tag{11}$$

which was satisfied in [6] by construction. Hornberger [8], applying the MSqR, found an ambiguity—nicely elucidated later in [10]—and derived an alternative QLBE. His was more natural than mine, in particular because his QLBE had the minimum possible value of D_x [cf. (11)], i.e., the minimum rate of the strange position diffusion.

The context of quantum Brownian motion theory and the related results — achieved by physicists mostly working on quantum foundations otherwise—were summarized in 2009 [10] by Vacchini and Hornberger. The QLBE of Hornberger [8] seemed to be the true and ultimate quantum version of the classical linear Boltzmann equation. But soon, an elementary argument of decoherence popped up and questioned it together with all previous versions, including mine.

4 Complete Momentum Decoherence (CMD)

To understand the overlooked dramatic phenomenon indicated by the title above, we only need the momentum and energy conservation of collision in one dimension first:

$$p_i + k_i = p_f + k_f\,, \tag{12}$$

$$\frac{p_i^2}{2M} + \frac{k_i^2}{2m} = \frac{p_f^2}{2M} + \frac{k_f^2}{2m}\,. \tag{13}$$

We express the final momentum of the mass M in the following form:

$$p_f = \mu_+ k_i + \mu_- k_f \ , \tag{14}$$

where $\mu_\pm = (M/m \pm 1)/2$. Observe that the initial momentum p_i of the mass M canceled! Its final momentum depends on the initial k_i and final k_f of the scattered mass m! This fact yields a crisis quantum mechanically. Observe that the reduced post-collision state of the mass M remains the same if we measure the post-collision momentum k_f of the other mass. Assume we do so and measure k_f. Then the above expression of p_f means that we measure the final momentum p_f of the mass M as well and, as a consequence, momentum superpositions for the mass M can exist no more after a single collision! *Any single collision causes complete momentum decoherence* of the mass M.

This trivial fact of CMD surfaced in 2009 [13] and in 2010 [14] in the general case of the three-dimensional collision (7) where the expression (14) survives for the components of $\mathbf{p}_f, \mathbf{k}_i, \mathbf{k}_f$ parallel to the momentum transfer $\mathbf{k}_f - \mathbf{k}_i$ only:

$$p_f^{\parallel} = \mu_+ k_i^{\parallel} + \mu_- k_f^{\parallel} \ . \tag{15}$$

CMD in all three components of $\mathbf{p}_f$ requests just three collisions in a row. CMD is obviously unphysical. It would, in particular, suggest a divergent coefficient $D_x = \infty$ of position diffusion in the QFPE (9).

The obligate question follows: how did the derivations of QLBEs from 1995 over fifteen years got finite D_x against the trivial CMD which imposes $D_x = \infty$. How did they regularize the divergent position diffusion?

5 Collision and Methods Revisited

We go back to the type of elementary considerations of JZ, this time taking the exact collision kinematics like (7) into the account, instead of the approximate (2). To detect CMD and the role of the MSqR in its regularization, it is sufficient to simplify the derivations from three to one dimension. First, let us find the counterpart of (7) in one dimension. Assume, again for simplicity, the repulsive hard-wall potential between the dust and a molecule so that we can ignore that they tunnel through each other. Then the unitary transition (7) in a collision reduces to:

$$|p\rangle \otimes |k\rangle \Rightarrow \left|p + 2k^*\right\rangle \otimes \left|k - 2k^*\right\rangle \ . \tag{16}$$

[For brevity, we stop indicating that all momenta are the initial ones.] Remember the center-of-mass initial momentum $k^* = (Mk - mp)/(M + m)$. If the initial state of the dust is a superposition of momentum eigenstates, the transition of an off-diagonal element of the density matrix reads:

$$|p\rangle\langle p'| \otimes |k\rangle\langle k| \Rightarrow |p+2k^*\rangle\langle p'+2k^*| \otimes |k-2k^*\rangle\langle k-2k^{*\prime}| \ , \tag{17}$$

where $k^{*\prime} = (Mk - mp')(M+m)$. Take the partial trace of both sides, yielding

$$|p\rangle\langle p'| \Rightarrow 0 \ , \tag{18}$$

because the two post-collision states of the molecule, scattered on $|p\rangle$ and $|p'\rangle$, respectively, became orthogonal:

$$\langle k_i - 2k^{*\prime} | k - 2k_i^*\rangle = 0 \ . \tag{19}$$

This proves CMD analytically and confirms the previous measurement theoretical argument: *Any single collision causes CMD* of the dust. This cannot happen in the reality since it would completely delocalize the wave function. It is now obvious that the mentioned two post-collision states of the molecule should overlap!

Our derivations [6, 8–10] of QLBE's created this overlap formally via the MSqR (8), without any awareness or reference to the above physical background. We assumed an environmental ideal gas, i.e., a mixture of plane waves of thermal distribution $\rho^{\mathcal{E}}(k) \propto \exp(-k^2/mk_{\rm B}T)$ of temperature T. But at a certain later stage towards the QLBE, we took the MSqR (8) and postulated the following density matrix:

$$\rho^{\mathcal{E}}(k,k') = \sqrt{\rho^{\mathcal{E}}(k)}\sqrt{\rho^{\mathcal{E}}(k')} \ , \tag{20}$$

which represents a single normalized central real Gaussian wave function $\psi_k^{\mathcal{E}} \propto \exp(-k^2/2mk_{\rm B}T)$, i.e., a central real Gaussian wave packet standing at the origin:

$$\psi^{\mathcal{E}}(x) \propto \exp\left(-\frac{mk_{\rm B}Tx^2}{2\hbar^2}\right) \ . \tag{21}$$

This single pure state served as an effective *substitute* of the single molecule mixed state in the ideal gas. The translation invariance was lost obviously. Nonetheless it became restored since all plane wave components $|k\rangle$ were assumed to collide with the dust:

$$\int dk\psi_k^{\mathcal{E}}\, |p\rangle \otimes |k\rangle \Rightarrow \int dk\psi_k^{\mathcal{E}}\, |p+2k^*\rangle \otimes |k-2k^*\rangle \ . \tag{22}$$

It is of course hard to interpret this assumption but it was implicit in all derivations and, most importantly, restored the translation invariance of the resulting QLBE.

Due to the MSqR (20) the two post-collision states of the molecule are, unlike in (19), no more orthogonal; they overlap, and the effect of CMD disappears, gives its role to finite momentum decoherence . Detailed calculations, omitted here, yield the QFPE (9) with the standard momentum diffusion $D_p = \eta Mk_{\rm B}T$ and the finite coefficient of position diffusion (momentum decoherence) D_x saturating the constraint (11). In all historic QLBEs [6, 8–10] it is the MSqR that removes the divergence of D_x.

Are these D_x's physical? In view of the meaning of the MSqR that a standing wave packet substitutes the ideal gas single-molecule density matrix, a finite D_x may well be an artifact of the MSqR, as suggested by [13, 14].

6 Farwell MSqR

What other, more physical mechanism could explain the finite physical momentum decoherence (position diffusion) if it is tractable at all via the independent collisions. Should one improve on the single molecule density matrix of the ideal gas by taking molecule-molecule interactions into account? Unfortunately, one should not. The diagonal form $\rho(\mathbf{p}, \mathbf{p}') \propto \delta(\mathbf{p} - \mathbf{p}')$ remains because the due translation invariance of the gas equilibrium state. To mitigate CMD, playing with the quantum state $\rho^{\mathcal{E}}(\mathbf{k}, \mathbf{k}') \propto \rho^{\mathcal{E}}(\mathbf{k})\delta(\mathbf{k} - \mathbf{k}')$ of the particles is useless. We play with the collision.

When MSqR turned out to be a kind of unphysical elimination of CMD, the following consideration arose. CMD assumes idealized quantum scatterings that means, e.g., infinite intercollision time $\tau = \infty$. If one takes the finite τ valid even in dilute gas then energy conservation (13) in single collision becomes unsharp and CMD becomes relaxed. This was certainly a more justified mechanism to mitigate CMD than the MSqR had been, I thought in [13], and got a finite coefficient D_x of momentum decoherence (position diffusion):

$$D_x = \frac{1}{3}\left(\frac{\tau^2}{M}\right) D_p. \tag{23}$$

Hornberger and Vacchini [15] claimed that the CMD issue was nonexistent in their QLBE [8–10] which contains the ultimate physics of quantum Brownian motion—I disagreed [16]—as long as binary independent collisions are considered between the dust and the molecules. Also Kamleitner and Cresser [14] blamed the idealization of the scattering process for CMD and introduced a nonzero collision (interaction) time instead of the idealized zero. Apparently, no consensus has since been reached as to the value of D_x neither to the very existence of momentum decoherence (position diffusion).

This issue is not yet too burning since the effect is not testable currently. The experimental significance of a non-zero D_x was anticipated long time ago [17], a possible test was mentioned tangentially [18], a fundamental experiment [19] used and confirmed the QLBE prediction for momentum diffusion only.

7 Epilogue

Many times, questioning the conservative and confirmed wisdom respecting quantum mechanics turns out to be unproductive. Zeh's criticism was different and changed our abstraction and practice about coherence in quantum theory. I only wished to illustrate how Zeh's work, apart from its impact on foundations, opened the Pandora's box of a standard unsolved problem independent of foundations. What is our theory of a quantum Brownian particle in a gas? Theory ran into a puzzle that—I'm afraid—has remained unsolved so far.

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