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# Complete positivity and entangled degrees of freedom

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#### Abstract

We study how some recently proposed noncontextuality tests based on quantum interferometry are affected if the test particles propagate as open systems in the presence of a Gaussian stochastic background. We show that physical consistency requires the resulting Markovian dissipative time evolution to be completely positive.

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## 1. Introduction

Recently, experiments based on neutron [1] and photon [2] interferometry have been proposed to test the hypothesis of noncontextuality in quantum mechanics; the idea is to check whether a Bell-like inequality of the Clauser–Horne–Shimony–Holt form [3] is violated or not. Such an inequality is derived from the assumption that the measured values of physical observables are completely specified by the state of the system prior to measurement and that the actual measurement outcomes do not depend on the context, namely on whether other commuting observables are simultaneously measured.

Unlike Bell-locality tests based on entangled physical systems, the above experiments involve two degrees of freedom of the same physical system; one degree of freedom is translational, related to the two possible paths followed by neutrons or photons inside the interferometer, and the other is the spin (helicity) of neutrons (photons).

Standard Bell-locality tests are not concerned with the time evolution of the particles involved. Only when there is lack of unitarity and loss of probability, as in experiments based on decaying neutral K-mesons [4–6], does the time evolution become important.

More in general, the dynamics is to be taken into account when the test particles behave as open systems S propagating through an environment  $\mathcal{E}$  to which they are coupled. In such cases, one usually traces away the degrees of freedom of  $\mathcal{E}$  ending up, under certain assumptions, with a one-parameter semigroup of linear maps  $\Gamma_t$  on the states of S represented by density matrices  $\rho$ .

The maps  $\Gamma_t$  constitute a so-called reduced dynamics for the open quantum system S and embody the dissipative and mixing effects due to the environment  $\mathcal{E}$ . They are not unitary,

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satisfy the forward in time composition law  $\Gamma_{t+s} = \Gamma_t \circ \Gamma_s$  for  $s, t \ge 0$ , and transform pure states into statistical mixtures. When they enjoy the property known as complete positivity they form a so-called 'quantum dynamical semigroup' [7–10].

Physical consistency requires that the positivity of states of S, i.e. the positivity of the eigenvalues of the corresponding density matrices, be preserved for all times by any meaningful reduced dynamics  $\Gamma_t$ . Indeed, the statistical interpretation of quantum mechanics identifies these eigenvalues with probabilities.

The property of complete positivity guarantees not only that the maps  $\Gamma_t$  preserve the positivity of the states of S, but also that the maps  $I_N \otimes \Gamma_t$  preserve the positivity of all states of the composite system  $S_N + S$ , for any N-level system, with  $I_N$  being the identity operation on  $S_N$  [11,12]. Complete positivity of  $\Gamma_t$  is stronger than positivity and is intimately connected with quantum entanglement; indeed, positivity alone is not sufficient to ensure that  $I_N \otimes \Gamma_t$  preserve the positivity of entangled states of  $S_N + S$ .

Noticeably, the standard quantum mechanical time evolution generated by Hamiltonian operators is unitary, reversible and completely positive. In contrast, the physical literature abounds with dissipative, irreversible, reduced dynamics of quantum open systems that are neither positive, nor completely positive (see, for example, [13–15]).

In particular, in view of the abstract, experimentally uncontrollable coupling of the system of interest S with any N-level system  $S_N$ , the argument that  $\Gamma_t$  should necessarily be completely positive may look like a mathematical convenience and a technical artefact, rather than a physical necessity [16]. In fact, the elimination of the environment degrees of freedom yields an equation of motion with memory terms that have to be eliminated via suitable Markov approximations. It depends on how they are performed whether the resulting semigroups are physically consistent or not [17].

Recently, the issue of complete positivity has been reconsidered in the context of neutral meson dynamics, where a typical experimental situation is that of an entangled, singlet-like, state  $\rho$  of two K or B neutral mesons propagating according to the factorized time evolution  $\Gamma_t \otimes \Gamma_t$  [18–21]. If the dynamical maps  $\Gamma_t$  are assumed to be not of the standard Weisskopf–Wigner form, but modified by a noisy background of gravitational origin, it is shown that  $\Gamma_t$  has to be completely positive. Were it not so, physical inconsistencies, as the production of negative probabilities, would affect  $\Gamma_t \otimes \Gamma_t[\rho]$ . Moreover, these inconsistencies cannot be dismissed as experimentally invisible because they might give rise to detectable effects [20].

In this paper, we consider physical cases where the environment  $\mathcal{E}$  is given by a classical, fluctuating external field [13, 22] and S is a single open quantum system with two degrees of freedom. In such a context, the coupling is not between S and an abstract 2-level system, but between two degrees of freedom of S itself. Then, the physical meaning of complete positivity comes to the fore when we study a time evolution of the form  $I_N \otimes \Gamma_t$ .

Namely, we study what happens if the interferometric apparatuses proposed for noncontextuality tests are placed in weak Gaussian stochastic magnetic fields, or stochastic optical media, coupled to the spin or helicity of neutrons or photons, respectively, that will then propagate as open quantum systems.

In particular, in the case of neutrons, we consider in detail three possible choices of fluctuating magnetic backgrounds. These give rise to reduced dynamics  $I_2 \otimes \Gamma_t$  with  $\Gamma_t$  affecting the neutron spin degree of freedom covering all possible cases, namely to  $\Gamma_t$  completely positive, positivity-preserving, but not completely positive and, finally, to  $\Gamma_t$  not even positivity-preserving. The three possibilities depend on the properties of the stochastic magnetic field. It thus appears that, by reproducing stochastic magnetic backgrounds with the qualities of the three cases we refer to, one would be able to experimentally study the characteristics of the various reduced dynamics.

Furthermore, we study how the Clauser–Horne–Shimony–Holt inequality is modified by the stochastic magnetic field and show that complete positivity of the time evolution  $I_N \otimes \Gamma_t$  is necessary for a consistent physical description; otherwise unacceptable negative eigenvalues appear in the time-evolving physical states describing entangled degrees of freedom.

## 2. Entanglement and noncontextuality tests

In the following we refer to noncontextuality tests using neutron interferometry [1], and photons involving similar arguments [2]. In the experimental set-up proposed in [1], an incoming beam of neutrons with spin along the positive z-direction passes through a beam splitter with transmission and reflection coefficients p and q with  $|p|^2 + |q|^2 = 1$ . The beam is divided into two components that follow two spatially separated paths u and d.

Both the spin and the translational degrees of freedom are described by two-dimensional Hilbert spaces: the former with basis vectors  $|\uparrow_z\rangle$  and  $|\downarrow_z\rangle$ , the latter with basis vectors  $|\psi_u\rangle$  and  $|\psi_d\rangle$  corresponding to the two possible macroscopic paths. Making the beam u component undergo a spin-flip  $|\uparrow_z\rangle \mapsto |\downarrow_z\rangle$ , an initial beam state is prepared

$$|\Psi\rangle = p|\psi_u\rangle \otimes |\downarrow_z\rangle + q|\psi_d\rangle \otimes |\uparrow_z\rangle, \tag{2.1}$$

which then propagates inside the interferometer. A vector state as above corresponds to the one-dimensional projector  $\rho_{\Psi} := |\Psi\rangle\langle\Psi|$ 

$$\rho_{\Psi} = |p|^2 P_1 \otimes Q_2 + |q|^2 P_2 \otimes Q_1 + pq^* P_3 \otimes Q_4 + p^* q P_4 \otimes Q_3, \tag{2.2}$$

with

$$P_{1} := |\psi_{u}\rangle\langle\psi_{u}|, \qquad P_{2} := |\psi_{d}\rangle\langle\psi_{d}|, \qquad P_{3} := |\psi_{u}\rangle\langle\psi_{d}|, \qquad P_{4} := |\psi_{d}\rangle\langle\psi_{u}|, \quad (2.3a)$$

$$Q_{1} := |\uparrow_{z}\rangle\langle\uparrow_{z}|, \qquad Q_{2} := |\downarrow_{z}\rangle\langle\downarrow_{z}|, \qquad Q_{3} := |\uparrow_{z}\rangle\langle\downarrow_{z}|, \qquad Q_{4} := |\downarrow_{z}\rangle\langle\uparrow_{z}|. \quad (2.3b)$$

More in general, neutron beam states are not pure as  $\rho_{\Psi}$ , rather statistical mixtures described by density matrices

$$\rho_{(2)} := \sum_{i,j=1}^{4} \rho_{ij} P_i \otimes Q_j, \tag{2.4}$$

that is by  $4 \times 4$  Hermitian, normalized, positive matrices, whose positive eigenvalues sum up to one (Tr  $\rho_{(2)} = 1$ ). Positivity is crucial for the statistical interpretation of quantum mechanics where the eigenvalues of density matrices play the role of probabilities.

Neutrons spend a typical time t within the interferometer during which they may be subjected to external influences resulting in a dynamical change  $\rho_{(2)} \longmapsto \rho_{(2)}(t)$  of their state. At the exit of the interferometer, a second beam splitter recombines the translational components and shifts the u component by an angle  $\varphi$ 

$$\begin{pmatrix} |\psi_{u}\rangle \\ |\psi_{d}\rangle \end{pmatrix} \longmapsto \begin{pmatrix} |\psi_{u}(\vartheta,\varphi)\rangle \\ |\psi_{d}(\vartheta,\varphi)\rangle \end{pmatrix} = \begin{pmatrix} e^{-i\varphi}\sin\vartheta & \cos\vartheta \\ e^{-i\varphi}\cos\vartheta & -\sin\vartheta \end{pmatrix} \begin{pmatrix} |\psi_{u}\rangle \\ |\psi_{d}\rangle \end{pmatrix}, \quad (2.5)$$

with reflection and transmission probabilities  $\cos^2 \vartheta$  and  $\sin^2 \vartheta$ . Consequently, the neutron beam state emerging from the interferometer is

$$\rho \longmapsto (U(\vartheta, \varphi) \otimes \mathbf{1}_2) \rho_{(2)}(t) (U^*(\vartheta, \varphi) \otimes \mathbf{1}_2), \tag{2.6}$$

where  $U(\vartheta, \varphi)$  is the unitary matrix in (2.5),  $U^*(\vartheta, \varphi)$  is its adjoint and  $\mathbf{1}_2$  is the  $2 \times 2$  identity matrix. The two components of the exiting beam are then intercepted by two counters  $C_{u,d}$  plus spin analysers  $S_{n,-n}$  that record how many neutrons reach them with spins polarized

along suitable directions  $\pm n = \pm (n_1, n_2, n_3)$  in space. The frequencies of counts give the expectations

$$\mathcal{O}_t^{j,n}(\vartheta,\varphi) := \operatorname{Tr}(\rho_{(2)}(t)P_j(\vartheta,\varphi) \otimes Q_n), \tag{2.7}$$

where  $P_j(\vartheta, \varphi) := U^*(\vartheta, \varphi)P_jU(\vartheta, \varphi)$ ,  $P_j$ , j=1,2, are as in (2.3a) and represent observables that are chosen by setting the angles  $\vartheta$  and  $\varphi$  characteristic of the beam splitter. Furthermore,  $Q_n := |\uparrow_n\rangle\langle\uparrow_n|$  projects on to a state with spin along the direction n.

Since translational and spin observables commute, the observables

$$A(\vartheta,\varphi) := P_1(\vartheta,\varphi) - P_2(\vartheta,\varphi), \qquad B(n) := Q_n - Q_{-n}$$
 (2.8)

also commute and have eigenvalues  $\pm 1$ . Choosing angles  $\vartheta_{1,2}$ ,  $\varphi_{1,2}$  and polarization directions  $n_{1,2}$ , one constructs commuting observables  $A_i$ ,  $B_j$ , i, j = 1, 2, called dichotomic [1].

In the hypothesis of noncontextuality, the possible outcomes  $\pm 1$  of a measurement of  $A_i$  and  $B_j$ , respectively, are predetermined by the state  $\rho_{(2)}(t)$  independently of whether  $B_j$  and  $A_i$  respectively, are simultaneously measured with  $A_i$  and  $B_j$ , respectively. From such assumptions, a Clauser–Horne–Shimony–Holt inequality can be derived for the mean values

$$C_{t}(\vartheta, \varphi; \boldsymbol{n}) := \operatorname{Tr}(\rho_{(2)}(t)A(\vartheta, \varphi) \otimes B(\boldsymbol{n}))$$

$$= \mathcal{O}_{t}^{1,n}(\vartheta, \varphi) + \mathcal{O}_{t}^{2,-n}(\vartheta, \varphi) - \mathcal{O}_{t}^{1,-n}(\vartheta, \varphi) - \mathcal{O}_{t}^{2,n}(\vartheta, \varphi), \quad (2.9)$$

with four possible configurations of the control parameters  $\vartheta$ ,  $\varphi$  and n

$$|C_t(\vartheta_1, \varphi_1; n_1) + C_t(\vartheta_1, \varphi_1; n_2) + C_t(\vartheta_2, \varphi_2; n_1) - C_t(\vartheta_2, \varphi_2; n_2)| \leq 2.$$
(2.10)

From equation (2.9), it turns out that the quantities  $C_t(\vartheta, \varphi; n)$  can be measured by frequencies at counters plus spin analysers  $(C_u, S_n)$  and  $(C_d, S_{-n})$  with the beam splitter at the exit of the interferometer set at angles  $\vartheta$  and  $\varphi$ .

If inequality (2.10) is violated, the hypothesis of noncontextuality upon which it was derived cannot hold. Whether this is so or not can be checked in highly efficient experiments where the entanglement between translational and magnetic degrees of freedom is exploited [1] (for a similar argument involving photons see [2]).

Interestingly, by setting appropriately the angles  $\vartheta$  and  $\varphi$  of the beam splitter and the polarization direction n of the spin analysers, the entries of the state  $\rho_{(2)}(t) = \sum_{i,j} \rho_{ij}(t) P_i \otimes Q_j$  can also be measured. From the entries, one has access to the eigenvalues of the beam state after travelling through the interferometer and thus to the effects of the time evolution inside it. Indeed, from equations (2.3), (2.4) and (2.6) it readily follows that

$$\rho_{11}(t) = \mathcal{O}_t^{1,z}(0,0), \qquad \rho_{12}(t) = \mathcal{O}_t^{1,-z}(0,0), 
\rho_{21}(t) = \mathcal{O}_t^{2,z}(0,0), \qquad \rho_{22}(t) = \mathcal{O}_t^{2,-z}(0,0).$$
(2.11)

Furthermore, since operators  $P_i \otimes Q_j$  with i, j = 3, 4 are not self-adjoint, their expectations can only be measured indirectly, through the mean values of the projectors

$$P_{\pm} := P_{1,2}\left(\frac{\pi}{4}, 0\right), \qquad P_{\pm i} := P_{1,2}\left(\frac{\pi}{4}, -\frac{\pi}{2}\right),$$
 (2.12a)

$$Q_{\pm x} := \frac{|\uparrow_z\rangle \pm |\downarrow_z\rangle}{\sqrt{2}} \frac{\langle \uparrow_z| \pm \langle \downarrow_z|}{\sqrt{2}}, \qquad Q_{\pm y} := \frac{|\uparrow_z\rangle \pm i|\downarrow_z\rangle}{\sqrt{2}} \frac{\langle \uparrow_z| \mp i\langle\downarrow_z|}{\sqrt{2}}. \tag{2.12b}$$

Then, from

$$P_3 = \frac{P_+ - P_- + iP_{+i} - iP_{-i}}{2} = P_4^*, \qquad Q_3 = \frac{Q_x - Q_{-x} + iQ_y - iQ_{-y}}{2} = Q_4^*, \quad (2.13)$$

one obtains expressions for all other entries  $\rho_{i_k^j}(t) := \text{Tr}(\rho_{(2)}(t)P_i^* \otimes Q_{j,k}^*)$ . We quote one of them which will be needed in the sequel (the others are reported in appendix A)

$$\rho_{43}(t) = \frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},0)}{4} + i\frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},0)}{4} \\
- \frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},0)}{4} - i\frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},0)}{4} \\
+ i\frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} - \frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \\
- i\frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} + \frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4}. \quad (2.14)$$

## 3. Open system dynamics inside the interferometer

Neutron interferometry has proved to be an extremely powerful tool to investigate gravitational, inertial and phase-shifting effects occurring inside the interferometer [23–29]. In the following we show that neutron interferometry might also be used to investigate the notion of completely positive open system dynamics. In order to do this, we consider the case in which neutrons, while propagating inside the interferometric apparatus, are subjected to weak time-dependent, stochastic magnetic fields coupled to their spin degree of freedom.

We assume the time-dependent Liouville–Von Neumann evolution equation for the  $2 \times 2$  density matrix  $\Sigma$  describing the spin degree of freedom to be of the form

$$\partial_t \Sigma(t) = (L_0 + L_t)[\Sigma(t)], 
L_0[\Sigma(t)] := -i \left[ \frac{\omega_0}{2} \sigma_3, \Sigma(t) \right], \qquad L_t[\Sigma(t)] := -i [V(t) \cdot \vec{\sigma}, \Sigma(t)],$$
(3.1)

where  $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  is the vector of Pauli matrices,  $V(t) = (V_1(t), V_2(t), V_3(t))$  is proportional to the Gaussian stochastic magnetic field and  $H_0 := \frac{\omega_0}{2}\sigma_3$  is due to the coupling to a static magnetic field along the z-direction. Furthermore, we assume V(t) to have zero mean,  $\langle V(t) \rangle = 0$ , and stationary, real, positive-definite covariance matrix  $\mathcal{W}(t) = [W_{ij}(t)]$  with entries

$$W_{ii}(t-s) = \langle V_i(t)V_i(s) \rangle = W_{ii}^*(t-s) = W_{ii}(s-t). \tag{3.2}$$

Because of the stochastic field  $\vec{V}(t)$ , the solution  $\Sigma(t)$  of equation (3.1) is also stochastic; an effective spin density matrix  $\rho(t) := \langle \Sigma(t) \rangle$  is obtained by averaging over the noise. At time t = 0 we may suppose spin and noise to decouple so that the initial state is  $\rho := \langle \Sigma(0) \rangle = \Sigma(0)$ . In order to derive an effective time evolution for  $\rho(t)$ , we follow the so-called convolutionless approach developed in [13].

We average over the noise in the interaction representation, where we set

$$\tilde{\Sigma}(t) := \exp(-tL_0)[\Sigma(t)] = e^{-itH_0}\Sigma(t)e^{itH_0}, \tag{3.3a}$$

$$\tilde{\rho}(t) := \langle \tilde{\Sigma}(t) \rangle$$
 and  $\tilde{L}_t := e^{-tL_0} L_t e^{tL_0}$ . (3.3b)

The result is

$$\tilde{\rho}(t) = \sum_{k=0}^{\infty} M_{2k}(t)[\rho], \tag{3.4}$$

where

$$M_k(t)[\rho] := \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{k-1}} ds_k \langle \tilde{L}(s_1) \tilde{L}(s_2) \cdots \tilde{L}(s_k) \rangle [\rho].$$
 (3.5)

Only even terms contribute to equation (3.4) because the stochastic field is assumed to be Gaussian.

Denoting by  $M_t$  the formal sum in equation (3.4), a resummation gives

$$\partial_{t}\tilde{\rho}(t) = \dot{M}_{t}M_{t}^{-1}[\tilde{\rho}(t)]$$

$$= (\underbrace{\dot{M}_{2}(t)}_{\text{second order}} + \underbrace{\dot{M}_{4}(t) - \dot{M}_{2}(t)M_{2}(t)}_{\text{fourth order}} + \underbrace{\cdots}_{\text{higher orders}})[\tilde{\rho}(t)]. \quad (3.6)$$

Since the action of the magnetic field on the travelling neutrons is, by hypothesis, weak, one can focus on the dominant first term in the expansion, neglecting higher-order contributions [8–10]. By means of equation (3.2), the second-order contribution can be worked out explicitly

$$\dot{M}_{2}(t)[\tilde{\rho}(t)] = -\sum_{a,b=1}^{3} \int_{0}^{t} ds \, W_{ab}(s)[\sigma_{a}(t), [\sigma_{b}(t-s), \tilde{\rho}(t)]]. \tag{3.7}$$

Returning to the Schrödinger representation and using the statistical independence of the Hamiltonian  $H_0$  from the stochastic field, it follows that  $\rho(t) := \exp(tL_0)[\tilde{\rho}(t)]$  solves

$$\partial_t \rho(t) = -i[H_0, \rho(t)] - \sum_{i=1}^3 C_{ij}(t) [\sigma_i, [\sigma_j, \rho(t)]],$$
 (3.8a)

$$C_{ij}(t) := \sum_{\ell=1}^{3} \int_{0}^{t} ds \ W_{i\ell}(s) U_{\ell j}(-s), \tag{3.8b}$$

where

$$\mathcal{U}(t) := \begin{pmatrix} \cos \omega_0 t & -\sin \omega_0 t & 0\\ \sin \omega_0 t & \cos \omega_0 t & 0\\ 0 & 0 & 1 \end{pmatrix}$$
(3.9)

is the unitary matrix  $\mathcal{U}(t) = [U_{ij}(t)]$  such that  $e^{-tL_0}[\sigma_i] = \sum_{j=1}^3 U_{ij}(t)\sigma_j$ . From equations (3.2) and (3.9) it follows that  $\mathcal{C}(t) := [C_{ij}(t)]$  is a real matrix and can thus

be decomposed into symmetric and antisymmetric components. Correspondingly, the second term on the right-hand side of equation (3.8a) splits into a commutator with a Hamiltonian and a purely dissipative contribution

$$\sum_{i,j=1}^{3} C_{ij}(t) [\sigma_i, [\sigma_j, \rho(t)]] = i \left[ \sum_{i,j,k=1}^{3} C_{ij}^A(t) \epsilon_{ijk} \sigma_k, \rho(t) \right]$$
(3.10a)

$$+ \sum_{i,j=1}^{3} 2C_{ij}^{S}(t)(\frac{1}{2}\{\sigma_{i}\sigma_{j}, \rho(t)\} - \sigma_{j}\rho(t)\sigma_{i}), \qquad (3.10b)$$

where  $C_{ij}^{A,S}(t) = (C_{ij}(t) \mp C_{ji}(t))/2$ . When the coupling between system and stochastic field is weak, the memory effects in equation (3.8a) should not be physically relevant; therefore, the use of a Markov approximation is in general justified<sup>1</sup>. In practice this is done by extending to  $+\infty$  the upper limit of the integral in equation (3.8b). The resulting equation of motion has no explicit time dependence

<sup>&</sup>lt;sup>1</sup> More precisely, one can show that a linear, local in time, subdynamics is the result of a limiting procedure in which the coupling constant g between system and external environment, and the ratio  $\tau/T$  between the typical timescale of the system and the decay time of the correlations in the environment, become small [8–10]. The quantities g and  $\tau/T$  regulate both the expansion (3.6) and the Markovian approximation of (3.8b).

$$\partial_t \rho(t) = -i[H, \rho(t)] + L_D[\rho(t)], \tag{3.11a}$$

$$H = H_0 + H_D, \qquad H_D := \sum_{i,j,k=1}^{3} C_{ij}^A \epsilon_{ijk} \sigma_k,$$
 (3.11b)

$$L_D[\rho(t)] := \sum_{i,j=1}^{3} L_{ij}^D - (\frac{1}{2} \{ \sigma_i \sigma_j, \rho(t) \} + \sigma_j \rho(t) \sigma_i), \tag{3.11c}$$

where  $C_{ij}^A$  and  $L_{ij}^D$  are the entries of the real matrices

$$C_A := \int_0^{+\infty} ds \frac{W(s)U(-s) - U(s)W(-s)}{2}, \tag{3.12a}$$

$$\mathcal{L}_D := \int_0^{+\infty} \mathrm{d}s (\mathcal{W}(s)\mathcal{U}(-s) + \mathcal{U}(s)\mathcal{W}(-s)). \tag{3.12b}$$

The Hamiltonian contribution is skew-symmetric, while the purely dissipative one,  $L_D[\cdot]$ , is symmetric; the latter makes the time evolution irreversible, but preserves probability because  $\operatorname{Tr}(L_D[\rho(t)]) = 0$ . The solutions of equation (3.11*a*) thus constitute a semigroup of linear maps  $\Gamma_t : \rho \longmapsto \rho(t) := \Gamma_t[\rho]$  such that  $\Gamma_{t+s} = \Gamma_t \circ \Gamma_s$ ,  $s, t \geqslant 0$  and  $\operatorname{Tr}(\Gamma_t[\rho]) = \operatorname{Tr} \rho$ . It remains to be checked whether they preserve the positivity of spin density matrices, that is whether  $\Gamma_t$  are, in short, positive maps on the spin states, which is the first request for physical consistency.

There is, however, a further constraint that has to be respected for physical consistency. Indeed, if the neutron interferometer is placed in a stochastic classical magnetic field of the kind described above, the translational degree of freedom is not affected and the effective state  $\rho_{(2)}(t)$  at the exit from the interferometer will be  $\rho_{(2)}(t) = (I_2 \otimes \Gamma_t)[\rho_{(2)}]$ , where  $I_2$  denotes the identity operation on the first factors in equation (2.4). It turns out that the positivity of the maps  $\Gamma_t$  does not guarantee the positivity and thus the physical consistency of the maps  $I_2 \otimes \Gamma_t$ ; for this, the stronger notion of complete positivity has to be imposed on the maps  $\Gamma_t$ .

We later investigate these notions in more technical detail. For the moment we observe that, by generating fluctuating magnetic backgrounds with certain decaying properties of their covariance matrix (3.2), one may have experimental access to some physical situations of theoretical interest that we present below.

## 3.1. White noise

The stochastic magnetic field has white-noise correlations

$$W_{ij}(t-s) = \langle V_i(t)V_j(s)\rangle = W_{ij}\delta(t-s), \tag{3.13}$$

where  $W := [W_{ij}]$  is time-independent, symmetric and positive-definite. Then,  $C_A = 0$  and  $\mathcal{L}_D = W$ . Furthermore, writing  $W = A^2$  with  $A = [a_{ij}]$  real and symmetric, the dissipative term in equation (3.11*a*) reads

$$L_D[\rho] = \sum_{k} A_k \rho A_k - \frac{1}{2} \left\{ \sum_{k} A_k^2, \rho \right\}, \tag{3.14}$$

with self-adjoint  $A_k := \sum_{i=1}^3 a_{ki} \sigma_i$ . This is a particular instance of Lindblad's theorem [30,31] which states that a family of linear transformations  $\Gamma_t : \rho \mapsto \rho(t)$  on the *D*-dimensional density matrices is a quantum dynamical semigroup of probability-preserving, completely positive maps if and only if it is generated by the equation of motion

$$\partial_t \rho(t) = -i[H, \rho(t)] - \frac{1}{2} \left\{ \sum_{\ell} A_{\ell}^* A_{\ell}, \rho(t) \right\} + \sum_{\ell} A_{\ell} \rho(t) A_{\ell}^*, \tag{3.15}$$

where  $A_{\ell}$  are *D*-dimensional matrices with adjoint  $A_{\ell}^*$  such that the series are (norm-) convergent. On the other hand, if  $L_D$  in equation (3.11*a*) is as in equation (3.15), then the corresponding  $\mathcal{L}_D$  is positive definite. Furthermore, note that, because of equation (3.13), all higher-order terms in the expansion (3.6) identically vanish, so that the evolution equation (3.15) is in this case exact [22].

## 3.2. Diagonal covariance matrix

The stochastic field has no off-diagonal correlations, while

$$\langle V_1(t)V_1(s)\rangle = \langle V_2(t)V_2(s)\rangle = g^2 B_1^2 e^{-\lambda|t-s|}, \qquad \langle V_3(t)V_3(s)\rangle = g^2 B_3^2 e^{-\mu|t-s|}, \qquad (3.16)$$

where  $B_i$  are constant magnetic field intensities and g is proportional to the neutron magnetic moment. Then

$$C_A = \frac{g^2 \omega_0 B_1^2}{\lambda^2 + \omega_0^2} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{L}_D = 2g^2 \begin{pmatrix} \frac{\lambda B_1^2}{\lambda^2 + \omega_0^2} & 0 & 0 \\ 0 & \frac{\lambda B_1^2}{\lambda^2 + \omega_0^2} & 0 \\ 0 & 0 & \frac{B_3^2}{\mu} \end{pmatrix}.$$
(3.17)

Setting

$$\Delta\omega := \frac{4g^2 B_1^2 \omega_0}{\lambda^2 + \omega_0^2}, \qquad \gamma := \frac{4g^2 B_1^2 \lambda}{\lambda^2 + \omega_0^2}, \qquad a := \frac{B_3^2}{\mu} + \frac{2g^2 B_1^2 \omega_0}{\lambda^2 + \omega_0^2}, \quad (3.18)$$

the matrix in equation (3.12b) becomes

$$\mathcal{L}_D = \frac{1}{2} \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \gamma & 0 \\ 0 & 0 & 2a - \gamma \end{pmatrix}. \tag{3.19}$$

The reason for such a parametrization will become clear in the next section.

Given  $\mathcal{L}_D$ , the entries of the spin matrix

$$\rho(t) = \begin{pmatrix} \rho_1(t) & \rho_3(t) \\ \rho_4(t) & \rho_2(t) \end{pmatrix}$$

are readily shown to satisfy the Bloch-Redfield equations [32]

$$\dot{\rho}_1 = -\gamma \rho_1 + \gamma \rho_2, \qquad \dot{\rho}_3 = -i(\omega_0 + \Delta \omega)\rho_3 - 2a\rho_3$$
 (3.20)

and  $\dot{\rho}_2 = -\dot{\rho}_1$ ,  $\dot{\rho}_4 = (\dot{\rho}_3)^*$ . The coefficients  $2\gamma$  and 2a are the inverse of the relaxation times  $T_1$  and  $T_2$  of the diagonal and off-diagonal elements of  $\rho(t)$ , respectively. From the positivity condition  $2a - \gamma \geqslant 0$ , it follows that  $1/T_2 \geqslant 1/2T_1$ . In [13, 14] it is shown that this typical order relation can be reversed by setting  $B_3 = 0$  and keeping fourth-order terms in equation (3.6). In such a case, however,  $1/T_2 < 1/2T_1$  implies that  $a - \gamma/2 < 0$  and that  $\mathcal{L}_D$  in equation (3.19) is no longer positive-definite.

By Lindblad's theorem, the argument of case 3.1 implies that the corresponding dynamical maps  $\Gamma_t$  generated through equation (3.11*a*) cannot be completely positive. We see in the next section that at least they preserve positivity.

# 3.3. Single component field correlation

The stochastic magnetic field is along the x-direction,  $\vec{V}(t) = (V_1(t), 0, 0)$ , with

$$\langle V_1(t)V_1(s)\rangle = g^2 B^2 e^{-\lambda |t-s|}.$$
 (3.21)

Then.

$$C_A = \frac{g^2 \omega_0 B^2}{2(\lambda^2 + \omega_0^2)} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{L}_D = \frac{g^2 B^2}{\lambda^2 + \omega_0^2} \begin{pmatrix} 2\lambda & \omega_0 & 0 \\ \omega_0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$
(3.22)

Unless  $\omega_0 = 0$  the matrix  $\mathcal{L}_D$  is not positive-definite. By analogy with the parametrization of the previous example, we set

$$\Delta\omega := \frac{2g^2B^2\omega_0}{\lambda^2 + \omega_0^2}, \qquad \gamma := \frac{2g^2B^2\lambda}{\lambda^2 + \omega_0^2}, \qquad b := -\frac{\Delta\omega}{2}. \tag{3.23}$$

Then, the corresponding Bloch–Redfield equations for the entries of  $\rho(t)$  read

$$\dot{\rho}_1 = -\gamma \rho_1 + \gamma \rho_2, \qquad \dot{\rho}_3 = -i(\omega_0 + \Delta \omega)\rho_3 - \gamma \rho_3 + \gamma \rho_4 + 2ib\rho_4, \quad (3.24)$$

and  $\dot{\rho}_2 = -\dot{\rho}_1$ ,  $\dot{\rho}_4 = (\dot{\rho}_3)^*$ .

# 4. Complete positivity versus simple positivity

As already remarked, physical consistency demands that  $\Gamma_t$  preserve the positivity of initial density matrices  $\rho$  describing the neutron spin degree of freedom.

In order to check whether this is so in the preceding cases, it is convenient to decompose the spin density matrices  $\rho$  by means of the Pauli matrices  $\sigma_j$ , j=1,2,3 plus the two-dimensional identity matrix  $\sigma_0$ , namely  $\rho=\sum_{\mu=0}^3 \rho^\mu \sigma_\mu$ . In such a way, density matrices can be represented as four-dimensional ket-vectors  $|\rho\rangle=(\rho^0,\rho^1,\rho^2,\rho^3)$ , where

$$\rho^0 = \frac{\rho_1 + \rho_2}{2}, \qquad \rho^1 = \frac{\rho_3 + \rho_4}{2}, \qquad \rho^2 = \frac{\rho_4 - \rho_3}{2i}, \qquad \rho^3 = \frac{\rho_1 - \rho_2}{2}. \tag{4.1}$$

Since they operate linearly, the commutator and the purely dissipative term  $L_D[\cdot]$  in equation (3.11a) act on the vectors  $|\rho\rangle$  as a skew-symmetric matrix

$$\mathcal{H} = -2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & h^3 & -h^2 \\ 0 & -h^3 & 0 & h^1 \\ 0 & h^2 & -h^1 & 0 \end{pmatrix}, \qquad h^i \in \mathbf{R}, \tag{4.2}$$

and as a real, symmetric matrix

$$\mathcal{D} = -2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & b & \alpha & \beta \\ 0 & c & \beta & \gamma \end{pmatrix}. \tag{4.3}$$

The connection with  $\mathcal{L}_D$  in equation (3.12b) is readily derived to be

$$\mathcal{L}_D = \frac{1}{2} \begin{pmatrix} \alpha + \gamma - a & -2b & -2c \\ -2b & a + \gamma - \alpha & -2\beta \\ -2c & -2\beta & a + \alpha - \gamma \end{pmatrix}, \tag{4.4}$$

which explains the parametrization used in the previous section.

In this representation, the time-evolution equation (3.11a) reads

$$\partial_t |\rho(t)\rangle = (\mathcal{H} + \mathcal{D})|\rho(t)\rangle.$$
 (4.5)

In order to find necessary and sufficient conditions for  $\Gamma_t$  to be positivity-preserving, we now proceed in a few steps.

Firstly, since  $\dot{\rho}^0 = 0$ , the trace is conserved, thus  $\rho^0(t) = 1/2$ . Therefore, the positivity of  $\Gamma_t[\rho]$  is ensured if  $\det[\rho(t)] = 1/4 - \sum_{j=1}^3 (\rho^j)^2 \ge 0$ .

Secondly, the time derivative of the determinant at t=0 must be positive whenever  $\sum_{j=1}^{3} (\rho^{j})^{2} = 1/4$  (so that  $\det[\rho] = 0$ ), otherwise one eigenvalue would become negative for t>0. Using equations (4.3) and (4.5), we thus obtain the necessary condition

$$\frac{\mathrm{d}\det[\rho(0)]}{\mathrm{d}t} = -2\sum_{i,i=1}^{3} \mathcal{D}_{ij}\rho^{i}\rho^{j} \geqslant 0. \tag{4.6}$$

By varying  $\rho^j$ , while keeping  $\sum_i (\rho^j)^2 = 1/4$ , it follows that

$$\mathcal{D}^{(3)} := -2 \begin{pmatrix} a & b & c \\ b & \alpha & \beta \\ c & \beta & \gamma \end{pmatrix} \tag{4.7}$$

must be negative-definite which in turn implies

$$a \ge 0, \qquad a\alpha \ge b^2, \qquad \det \mathcal{D}^{(3)} \ge 0.$$
 (4.8)

Thirdly, conditions (4.8) are also sufficient for  $\Gamma_t$  to preserve positivity. In fact, since  $-\mathcal{D} \geqslant 0$ , we can write  $-\mathcal{D} = \mathcal{B}^2$  with  $\mathcal{B}$  symmetric. Then, the term in the right-hand side of the equality in equation (4.6) is given by  $\|\mathcal{B}|\rho\rangle\|^2$ . Let us suppose  $\det[\rho(t')] < 0$ , at time t' > 0; it follows that  $\det[\rho(t^*)] = 0$  at some time  $t^*$  such that  $0 \leqslant t^* < t'$ . Thus,  $\mathcal{B}|\rho(t^*)\rangle = 0$ , otherwise  $\det[\rho(t)] > 0$  for  $t \geqslant t^*$ . But this implies  $|\rho(t)\rangle = |\rho(t^*)\rangle$  for all  $t \geqslant t^*$  under the time evolution

$$|\rho\rangle \longmapsto |\rho(t)\rangle = e^{t\mathcal{D}}|\rho\rangle = \sum_{\ell=0}^{\infty} \frac{t^{\ell}}{\ell!} \mathcal{B}^{2\ell}|\rho\rangle.$$
 (4.9)

Therefore, as well as the standard dynamics generated by a Hamiltonian operator, the dynamics (4.9) is positivity-preserving. Via the Lie–Trotter product formula, it then follows that the time evolution generated by  $\mathcal{H}+\mathcal{D}$ 

$$\mathcal{G}_t := \exp(t(\mathcal{H} + \mathcal{D})) = \lim_{n \to \infty} (e^{t/n\mathcal{H}} e^{t/n\mathcal{D}})^n, \tag{4.10}$$

also preserves positivity.

However, even if  $\Gamma_t$  preserves positivity of the states describing the neutron spin degree of freedom, this does not guarantee that  $I_2 \otimes \Gamma_t$  preserves the positivity of states in which the spin is entangled with another degree of freedom. For neutrons in the interferometric apparatus of the previous section, such a request is crucial since the maps  $I_2 \otimes \Gamma_t$  tell us how time states  $\rho_{(2)}$  evolve describing both the magnetic and translational degrees of freedom. A theorem of Choi [12] states that  $I_2 \otimes \Gamma_t$  is positivity-preserving if and only if  $\Gamma_t$  is completely positive.

Among the neutron states  $\rho_{(2)}$  propagating through the interferometer, those without correlations between translational and spin degrees of freedom are of the form  $\rho_{\text{space}} \otimes \rho_{\text{spin}}$  or are linear mixtures of them. If  $\Gamma_t$  are positivity-preserving, these tensor-product states remain positive in the course of time; indeed

$$0 \leqslant \rho_{\text{space}} \otimes \rho_{\text{spin}} \longmapsto I_2 \otimes \Gamma_t[\rho_{\text{space}} \otimes \rho_{\text{spin}}] = \rho_{\text{space}} \otimes \Gamma_t[\rho_{\text{spin}}] \geqslant 0.$$
 (4.11)

However, this is not so for entangled states.

Let us take  $p=-q=1/\sqrt{2}$  in equation (2.2), so that the initial beam state is antisymmetric in the two degrees of freedom. If we ask  $I_2 \otimes \Gamma_t$  to preserve the positivity of  $\rho_{\Psi}$ , it must hold that

$$\Delta_{\Phi}(t) := \langle \Phi | (I_2 \otimes \Gamma_t)[\rho_{\Psi}] | \Phi \rangle \geqslant 0 \tag{4.12}$$

for all  $\Phi$ . If  $\Phi$  is orthogonal to  $\Psi$ , the fact that  $\Delta_{\Phi}(0) = 0$  implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta(t)\bigg|_{t=0} = \langle \Phi|(I_2 \otimes L_D)[\rho_{\Psi}]|\Phi\rangle \geqslant 0. \tag{4.13}$$

By varying  $\Phi$  in the three-dimensional subspace orthogonal to  $\Psi$  we obtain the inequalities

$$2R \equiv \alpha + \gamma - a \geqslant 0, \qquad RS \geqslant b^{2}$$

$$2S \equiv a + \gamma - \alpha \geqslant 0, \qquad RT \geqslant c^{2}$$

$$2T \equiv a + \alpha - \gamma \geqslant 0, \qquad ST \geqslant \beta^{2}$$

$$RST \geqslant 2bc\beta + R\beta^{2} + Sc^{2} + Tb^{2}.$$

$$(4.14)$$

These inequalities are stronger than those in equation (4.8) and must necessarily be satisfied if we want to avoid the maps  $I_2 \otimes \Gamma_t$  becoming physically inconsistent by generating negative probabilities out of initially entangled beam states.

Furthermore, using equation (4.4), inequalities (4.14) amount to the positivity of the matrix  $\mathcal{L}_D = [L_{ij}^D]$  of the coefficients of the dissipative term in equation (3.11c) and thus they imply the complete positivity of the time evolution  $\Gamma_t$ .

Let us now discuss the three cases introduced in section 3.

#### 4.1. White noise

As already noticed, the evolution equation (3.11a-c) is now exact. The matrix  $\mathcal{D}^{(3)}$  takes the general form (4.7) so that, provided the inequalities (4.14) are satisfied, the integrated time evolution  $\Gamma_t$  is completely positive.

#### 4.2. Diagonal covariance matrix

In this case one finds

$$\mathcal{D}^{(3)} = -2 \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & \nu \end{pmatrix}. \tag{4.15}$$

The corresponding dynamics is completely positive only when  $1/T_2 \ge 1/2T_1$  ( $a \ge \gamma/2$ ); it is positive, but not completely positive, when  $1/T_2 < 1/2T_1$  ( $a < \gamma/2$ ).

Analytic solutions of the equation of motion corresponding to equation (4.15) are readily calculated; in vectorial representation one has

$$\rho^{0}(t) = \rho^{0} 
\rho^{1}(t) = e^{-2at} \{ \rho^{1} \cos \omega t - \rho^{2} \sin \omega t \} 
\rho^{2}(t) = e^{-2at} \{ \rho^{1} \sin \omega t + \rho^{2} \cos \omega t \} 
\rho^{3}(t) = e^{-2\gamma t} \rho^{3}$$
(4.16)

with  $\omega := \omega_0 + \Delta \omega$ . The difference between complete positivity and positivity shows up in different order relations between the decay diagonal and off-diagonal relaxation, that is either  $a \ge \gamma/2$  or  $a < \gamma/2$ .

However, the true physical meaning of the complete positivity of  $\Gamma_t$  becomes evident when the state  $\rho_{\Psi}$  in equation (2.2), with  $p=-q=1/\sqrt{2}$ , evolves in time according to  $I_2 \otimes \Gamma_t$ . In vectorial representation  $|Q_1\rangle=1/2(1,0,0,1)$ ,  $|Q_2\rangle=1/2(1,0,0,-1)$ ,  $|Q_3\rangle=1/2(0,1,i,0)$  and  $|Q_4\rangle=1/2(0,1,-i,0)$ , thus, using equation (4.16) one obtains

$$\rho_{(2)}(t) = (I_2 \otimes \Gamma_t)[\rho_{\Psi}] = \frac{1}{2}(P_1 \otimes Q_2(t) + P_2 \otimes Q_1(t) - P_3 \otimes Q_4(t) - P_4 \otimes Q_3(t)),$$
(4.17)

with

$$Q_{1}(t) = \frac{1}{2} \begin{pmatrix} 1 + e^{-2\gamma t} & 0 \\ 0 & 1 - e^{-2\gamma t} \end{pmatrix}, \qquad Q_{3}(t) = e^{-t(2a + i\omega)} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$Q_{2}(t) = \frac{1}{2} \begin{pmatrix} 1 - e^{-2\gamma t} & 0 \\ 0 & 1 + e^{-2\gamma t} \end{pmatrix}, \qquad Q_{4}(t) = e^{-t(2a - i\omega)} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

$$(4.18)$$

Therefore

$$\rho_{(2)}(t) = \begin{pmatrix} E_{-}(t) & 0 & 0 & 0\\ 0 & E_{+}(t) & F(t) & 0\\ 0 & F^{*}(t) & E_{+}(t) & 0\\ 0 & 0 & 0 & E_{-}(t) \end{pmatrix}, \qquad E_{\pm} := \frac{1 \pm e^{-2\gamma t}}{4},$$

$$F := -\frac{e^{-t(2a - i\omega)}}{2}.$$
(4.19)

The eigenvalues of the state  $\rho_{(2)}(t)$  at the exit of the interferometer are  $\lambda_{1,2}(t)=E_-(t)$  and

$$\lambda_{\pm}(t) = \frac{1 + e^{-2\gamma t} \pm 2e^{-2at}}{4}.$$
(4.20)

Let  $a < \gamma/2$ , that is let  $\Gamma_t$  be positive but not completely positive. Then, since  $\lambda_-(0) = 0$  and  $d\lambda_+(0)/dt = (2a - \gamma)/2$ , there is a whole range of t where  $\lambda_+(t) < 0$  and  $\rho_{(2)}(t)$  lose physical meaning. On the other hand, if  $a \ge \gamma/2$ ,  $\lambda_+(t) \ge 0$ , for all t.

### 4.3. Single component field correlation

The matrix  $\mathcal{D}^{(3)}$  in equation (4.7) also now has off-diagonal terms

$$\mathcal{D}^{(3)} = -2 \begin{pmatrix} 0 & b & 0 \\ b & \gamma & 0 \\ 0 & 0 & \gamma \end{pmatrix}, \qquad b = -\frac{\Delta \omega}{2}; \tag{4.21}$$

only when these are zero, i.e.  $\Delta \omega = 0$ , is positivity-preserved. This can also be seen by considering the integrated time evolution; in the vectorial representation, one explicitly finds

$$\rho^{0}(t) = \rho^{0}$$

$$\rho^{1}(t) = e^{-\gamma t} \left\{ \rho^{1} \left( \cosh \delta t + \frac{\gamma}{\delta} \sinh \delta t \right) - \rho^{2} \frac{\omega + 2b}{\delta} \sinh \delta t \right\}$$

$$\rho^{2}(t) = e^{-\gamma t} \left\{ \rho^{1} \frac{\omega - 2b}{\delta} \sinh \delta t + \rho^{2} \left( \cosh \delta t - \frac{\gamma}{\delta} \sinh \delta t \right) \right\}$$

$$\rho^{3}(t) = e^{-2\gamma t} \rho^{3}$$

$$(4.22)$$

with  $\delta := \sqrt{\gamma^2 + (4b^2 - \omega^2)}$ . One notes that, besides developing negative eigenvalues because of the lack of positivity, this evolution causes  $\rho^{(1,2)}(t)$  to diverge with  $t \mapsto +\infty$ , when  $\delta > \gamma$ .

Although apparently formal, these results are far from being academic. Indeed, as already stressed at the end of section 2, the entries of  $\rho_{(2)}$  are directly accessible to the experiment<sup>2</sup>. By modulating a background magnetic field close to the stochastic properties investigated in the previous three cases, one might reproduce experimentally the conditions for three different reduced dynamics and check their consequences.

Then, one may conclude that reduced, Markovian time evolutions  $\Gamma_t$  must be not only positive, but also completely positive, since the lack of any of these constraints results in experimentally detectable inconsistencies.

Clearly, the use of one reduced dynamics instead of another depends on the Markovian approximation used to derive it and whether, given the properties of the stochastic field, it was justified or not. It thus seems appropriate to conclude that, whenever a semigroup composition law is expected, the physically appropriate Markovian approximations are those which lead to reduced dynamics consisting of completely positive maps  $\Gamma_t$  [17].

<sup>&</sup>lt;sup>2</sup> For instance, in the case 4.2 above, it follows from equation (2.11) that  $E_{-}(t) = \mathcal{O}_{t}^{1,z}(0,0)$  and  $E_{+}(t) = \mathcal{O}_{t}^{2,z}(0,0)$ , while F(t) coincides with the expression in equation (2.14).

# 5. Noncontextuality and dissipation

We now examine to what extent the Clauser–Horne–Shimony–Holt inequalities (2.10) are modified by the presence of a stochastic magnetic field with covariance matrix as in the cases studied in section 3. We first notice that the mean values (2.9) can be written

$$C_t(\vartheta, \varphi; n) = 2(\mathcal{O}_t^{1,n}(\vartheta, \varphi) - \mathcal{O}_t^{1,-n}(\vartheta, \varphi)) - \text{Tr}_2(\rho_{\text{spin}}(t)B(n)), \tag{5.1}$$

where  $\text{Tr}_2$  denotes the trace over the spin degree of freedom and  $\rho_{\text{spin}}(t) = \text{Tr}_1 \, \rho_{(2)}(t)$ , with  $\text{Tr}_1$  denoting the trace over the translational degree of freedom.

For sake of simplicity, we again consider an initial beam state with  $p = -q = 1/\sqrt{2}$ ; then

$$C_{t}(\vartheta, \varphi; \boldsymbol{n}) = 2(\mathcal{O}_{t}^{1, \boldsymbol{n}}(\vartheta, \varphi) - \mathcal{O}_{t}^{1, -\boldsymbol{n}}(\vartheta, \varphi))$$

$$= \sin^{2}\vartheta \operatorname{Tr}_{2}(Q_{2}(t)B(\boldsymbol{n})) + \cos^{2}\vartheta \operatorname{Tr}_{2}(Q_{1}(t)B(\boldsymbol{n}))$$

$$- \sin 2\vartheta \operatorname{\mathcal{R}e}(e^{-i\varphi} \operatorname{Tr}_{2}(Q_{4}(t)B(\boldsymbol{n}))). \tag{5.2}$$

Furthermore, we take  $h^1 = h^2 = 0$  and  $h^3 = \omega_0/2$  in the Hamiltonian part (4.2) of the evolution equation (4.5).

From equation (4.10) it follows that, in vectorial representation, the time-evolution operator  $\mathcal{G}_t$  acts on initial states  $|\rho\rangle$  as

$$\mathcal{G}_{t} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \mathcal{G}_{11}(t) & \mathcal{G}_{12}(t) & \mathcal{G}_{13}(t) \\
0 & \mathcal{G}_{21}(t) & \mathcal{G}_{22}(t) & \mathcal{G}_{23}(t) \\
0 & \mathcal{G}_{31}(t) & \mathcal{G}_{32}(t) & \mathcal{G}_{33}(t)
\end{pmatrix}.$$
(5.3)

Also, the mean value of an observable  $X = \sum_{\nu=0}^{3} X^{\nu} \sigma_{\nu}$  with respect to  $\rho$  is given by  $\text{Tr}(X\rho) = 2\sum_{\nu=0}^{3} X^{\nu} \rho^{\nu}$ . Furthermore, the observable  $B(n) = Q_n - Q_{-n}$  relative to  $n = (n_1, n_2, n_3)$  corresponds to the vector  $|B(n)\rangle = (0, n_1, n_2, n_3)$ . Thus, one computes

$$\operatorname{Tr}_{2}(Q_{1,2}(t)B(n)) = \pm G(t) \cdot n, \qquad \operatorname{Tr}_{2}(Q_{4}(t)B(n)) = F(t) \cdot n, \qquad (5.4)$$

where

$$G(t) = (\mathcal{G}_{13}(t), \mathcal{G}_{23}(t), \mathcal{G}_{33}(t))$$
 and (5.5a)

$$F(t) = (\mathcal{G}_{11}(t) - i\mathcal{G}_{12}(t), \mathcal{G}_{21}(t) - i\mathcal{G}_{22}(t), \mathcal{G}_{31}(t) - i\mathcal{G}_{32}(t)). \tag{5.5b}$$

Finally, the mean values (5.2) read

$$C_t(\vartheta, \varphi; \mathbf{n}) = \mathbf{n} \cdot [\cos 2\vartheta \mathbf{G}(t) - \sin 2\vartheta \, \mathcal{R}e(e^{-i\varphi} \mathbf{F}(t))]. \tag{5.6}$$

We now discuss the explicit behaviour of  $C_t(\vartheta, \varphi; n)$  in the three cases introduced in section 3, and further analysed in the previous section.

# 5.1. White noise

Though analytic expressions of  $\mathcal{G}_t$  are obtainable in the general case of a stochastic magnetic field with white-noise correlations, these are rather involved and scarcely illuminating. More conveniently, one may suppose that the dissipation  $\mathcal{D}$  in equation (4.3) is small in comparison to the Hamiltonian contribution due to  $H_0$ . In practice, we assume that the parameters a, b, c,  $\alpha, \beta$  and  $\gamma$  are small with respect to  $\omega = \omega_0 + \delta\omega \simeq \omega_0$  and we proceed with a perturbative expansion (for more details compare [18, 19, 21]). To first order in the parameters, the entries

of  $\mathcal{G}_t$  are as reported in the appendix B. Using these, one calculates

$$G_1(t) = -\frac{4|C|}{\omega_0} \sin \frac{\omega_0 t}{2} \cos \left(\frac{\omega_0 t}{2} + \phi_C\right),\tag{5.7a}$$

$$G_2(t) = \frac{4|C|}{\omega_0} \sin \frac{\omega_0 t}{2} \sin \left(\frac{\omega_0 t}{2} + \phi_C\right),\tag{5.7b}$$

$$G_3(t) = e^{-2\gamma t},\tag{5.7c}$$

where  $|C|^2 = c^2 + \beta^2$  and  $\tan \phi_C = \beta/c$ 

$$\mathcal{R}e(e^{-i\varphi}F_1(t)) = e^{-(a+\alpha)t}\cos(\omega_0 t - \varphi) + \frac{|B|}{\omega_0}\sin\omega_0 t\cos(\varphi + \phi_B), \qquad (5.8a)$$

$$\mathcal{R}e(e^{-i\varphi}F_2(t)) = e^{-(a+\alpha)t}\sin(\omega_0 t - \varphi) - \frac{|B|}{\omega_0}\sin\omega_0 t\sin(\varphi - \phi_B), \qquad (5.8b)$$

$$\mathcal{R}e(e^{-i\varphi}F_3(t)) = -\frac{4|C|}{\omega_0}\sin\frac{\omega_0}{2}t\cos\left(\frac{\omega_0}{2}t - \varphi - \phi_C\right),\tag{5.8c}$$

where  $|B|^2 = (a - \alpha)^2 + 4b^2$  and  $\tan \phi_B = 2b/(\alpha - a)$ . It thus follows that

$$C_{t}(\vartheta, \varphi; \mathbf{n}) = n_{1} \left[ -\frac{4|C|}{\omega_{0}} \cos 2\vartheta \sin \frac{\omega_{0}}{2} t \cos \left( \frac{\omega_{0}}{2} t + \phi_{C} \right) \right]$$

$$- \sin 2\vartheta \left( e^{-t(a+\alpha)} \cos(\omega_{0}t - \varphi) + \frac{|B|}{\omega_{0}} \sin \omega_{0}t \cos(\varphi + \phi_{B}) \right)$$

$$+ n_{2} \left[ \frac{4|C|}{\omega_{0}} \cos 2\vartheta \sin \frac{\omega_{0}}{2} t \sin \left( \frac{\omega_{0}}{2} t + \phi_{C} \right) \right]$$

$$- \sin 2\vartheta \left( e^{-t(a+\alpha)} \sin(\omega_{0}t - \varphi) - \frac{|B|}{\omega_{0}} \sin \omega_{0}t \sin(\varphi - \phi_{B}) \right)$$

$$+ n_{3} \left[ e^{-2\gamma t} \cos 2\vartheta + \frac{4|C|}{\omega_{0}} \sin 2\vartheta \sin \frac{\omega_{0}}{2} t \cos \left( \frac{\omega_{0}}{2} t - \varphi - \phi_{C} \right) \right]. \tag{5.9}$$

## 5.2. Diagonal covariance matrix

For the stochastic magnetic fields with correlation matrices as in equation (3.16) we have

$$G(t) = (0, 0, e^{-2\gamma t}), F(t) = e^{-t(2a - i\omega)}(1, -i, 0).$$
 (5.10)

With these expressions one easily derives

$$C_t(\vartheta, \varphi; n) = e^{-2\gamma t} \cos 2\vartheta n_3 - e^{-2\alpha t} \sin 2\vartheta (n_1 \cos(\omega t - \varphi) + n_2 \sin(\omega t - \varphi)). \tag{5.11}$$

#### 5.3. Single component field correlation

The computation is similar in the case of a magnetic field with covariance as in equation (3.21). One finds

$$G(t) = (0, 0, e^{-2\gamma t}),$$
 (5.12a)

$$F(t) = e^{-\gamma t} \left( (\cosh \delta t + i\frac{\omega}{\delta} \sinh \delta t)(1, -i, 0) + \frac{\gamma + 2ib}{\delta} \sinh \delta t(1, i, 0) \right), \tag{5.12b}$$

from which, assuming  $\delta > 0$ , one easily obtains

$$C_t(\vartheta, \varphi; \mathbf{n}) = \mathrm{e}^{-2\gamma t} \cos 2\vartheta n_3$$

$$-e^{-\gamma t}\sin 2\vartheta \left[n_1\left(\left(\cosh\delta t + \frac{\gamma}{\delta}\sinh\delta t\right)\cos\varphi + \frac{\omega + 2b}{\delta}\sinh\delta t\sin\varphi\right) + n_2\left(\left(-\cosh\delta t + \frac{\gamma}{\delta}\sinh\delta t\right)\sin\varphi + \frac{\omega - 2b}{\delta}\sinh\delta t\cos\varphi\right)\right]. \tag{5.13}$$

The lack of positivity preservation which characterizes the time evolution leading to equation (5.13) manifests itself in that the quantities  $C_t(\vartheta, \varphi; n)$  diverge with large t when  $\delta > \gamma$ .

Expressions (5.9), (5.11) and (5.13) agree with those used in [1, 2] when there is no dissipation, namely putting  $a = b = c = \alpha = \beta = \gamma = 0$ 

$$C_t(\vartheta, \varphi; n) = -n_1 \sin 2\vartheta \cos(\omega_0 t - \varphi) - n_2 \sin 2\vartheta \sin(\omega_0 t - \varphi) + n_3 \cos 2\vartheta. \tag{5.14}$$

Notice that the unitary time evolution generated by the Hamiltonian  $H_0$  contributes to a time-varying redefinition of the angle  $\varphi$ .

Concerning the issue of complete positivity versus simple positivity, in expressions (5.9) and (5.11) the two possibilities manifest themselves in different relaxation properties due to whether inequalities (4.14) or (4.8) are fulfilled. No physical inconsistencies may affect the mean values  $C_t(\vartheta, \varphi; n)$ ; indeed, negative probabilities may result in negative mean values of positive observables only if the latter are entangled. In the case of the quantities involved in inequality (2.10), the observables are factorized,  $P_{1,2}(\vartheta, \varphi) \otimes Q_n$  and the positivity of their mean values is preserved even when  $\Gamma_t$  is only positive and not completely positive.

This can be seen as follows. To the Schrödinger time evolution  $\rho_{(2)}(t) = (I_2 \otimes \Gamma_t)[\rho_{(2)}]$ , there corresponds the Heisenberg time evolution of observables  $X_{(2)}(t) = (I_2 \otimes \Omega_t)[X_{(2)}]$ 

$$Tr((I_2 \otimes \Gamma_t)[\rho_{(2)}]X_{(2)}) = Tr(\rho_{(2)}(I_2 \otimes \Omega_t)[X_{(2)}]). \tag{5.15}$$

The maps  $\Omega_t$ , dual to  $\Gamma_t$ , form a semigroup of dynamical maps that transform positive observables into positive observables, if  $\Gamma_t$  preserve the positivity of states. Consequently, even when the initial state  $\rho_{(2)}$  is entangled and  $\Gamma_t$  are positivity-preserving, but not completely positive, it turns out that

$$\operatorname{Tr}(\rho_{(2)}(t)P_{1,2}(\vartheta,\varphi)\otimes Q_n) = \operatorname{Tr}(\rho_{(2)}P_i(\vartheta,\varphi)\otimes \Omega_t[Q_n]) \geqslant 0. \tag{5.16}$$

## 6. Conclusions

Complete positivity is a property of quantum time evolutions which is enjoyed by the standard dynamics of closed quantum systems generated by Hamiltonian operators, but not automatically by the more general reduced dynamics describing the time evolution of open quantum systems in interaction with suitable environments. Complete positivity is intimately related to the phenomenon of quantum entanglement, between two different systems, but also between two different degrees of freedom of the same physical system.

In this paper we have considered the two entangled degrees of freedom, translational and rotational, of a beam of neutrons travelling through an interferometric apparatus devoted to checking the hypothesis of noncontextuality. We have studied the consequences of placing the interferometer in a stochastic, Gaussian magnetic field weakly coupled to the spin degree of freedom that provides an experimentally controllable environment. As explained in section 3, the same Markov approximation naively yields a semigroup of dynamical maps  $I_2 \otimes \Gamma_t$ , where only the spin degree of freedom evolves in time. By varying the decay properties of the external field correlations, these maps turn out to be alternatively completely positive, simply positivity-preserving, not even positivity-preserving.

The noncontextuality tests proposed in [1,2] are based on the Clauser–Horne–Shimony–Holt inequality (2.10) without time dependence, that is with t=0. The presence of a fluctuating magnetic field induces relaxation on the spin degree of freedom with strength and properties depending on those of the field. Typically, the mean values in the inequality are damped and make it more difficult to be violated. However, in the presence of stochastic fields yielding reduced dynamics that do not preserve positivity, the inequality might be dramatically violated because of possible mean values diverging in time.

This latter possibility is a manifestation of the fact that any physically consistent time evolution  $\Gamma_t$  must preserve the positivity of spin states in order that the eigenvalues of the corresponding spin density matrices might at any time be used as probabilities, in agreement with the statistical interpretation of quantum mechanics. If  $\Gamma_t$  preserve the trace of spin density matrices, but not their positivity, spin states may evolve in time in such a way that some of their eigenvalues become negative, while others are greater than one, without upper bounds. It is this physically unacceptable phenomenon that leads to diverging mean values.

The request of positivity preservation by the maps  $\Gamma_t$  with respect to spin states is thus inescapable, but it is not enough to avoid physical inconsistencies when the time-evolution maps  $I_2 \otimes \Gamma_t$  act on states  $\rho_{(2)}$  with correlations between spin and translational degrees of freedom.

Inequality (2.10) does reveal the difference between completely positive and simply positivity-preserving  $\Gamma_t$ , but only as long as the relaxation characteristics are concerned, without any further effect (as the divergence of some contributions to the inequality). In fact, the positive observables in equation (2.10) are factorized, that is they incorporate no entanglement between the translational and spin degrees of freedom. Even if the initial state does incorporate entanglement, it nevertheless follows that the mean values of factorized observables remain positive and bounded.

However, the interferometric apparatus proposed in [1,2], might also be used to measure the entries of the states of the neutron beam at the exit of the interferometer. In this way, one might have access to the spectrum of an initially entangled state after being subjected to the effects of the stochastic magnetic field.

In the case of fluctuating fields yielding reduced dynamics that preserve positivity, but are not completely positive, the theoretical predictions indicate the appearance of negative eigenvalues, that is of negative probabilities, in the spectrum of the entangled exiting state. The fact that they are, in principle, detectable experimentally does not allow us to dismiss such an occurrence as practically negligible. Rather, it forces us to reconsider the Markov approximation used to derive the time evolution and to select as physically consistent only those providing completely positive reduced dynamics.

# Appendix A

$$\rho_{1_4^3}(t) = \frac{\mathcal{O}_t^{1,x}(0,0) - \mathcal{O}_t^{1,-x}(0,0)}{2} \pm i \frac{\mathcal{O}_t^{1,-y}(0,0) - \mathcal{O}_t^{1,y}(0,0)}{2}$$
(A.1)

$$\rho_{2_4^3}(t) = \frac{\mathcal{O}_t^{2,x}(0,0) - \mathcal{O}^{2,-x}(0,0)}{2} \pm i \frac{\mathcal{O}_t^{2,-y}(0,0) - \mathcal{O}_t^{2,y}(0,0)}{2}$$
(A.2)

$$\rho_{\frac{3}{4}1}(t) = \frac{\mathcal{O}_t^{1,z}(\frac{\pi}{4},0) - \mathcal{O}_t^{2,z}(\frac{\pi}{4},0)}{2} \mp i \frac{\mathcal{O}_t^{1,z}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_t^{2,z}(\frac{\pi}{4},-\frac{\pi}{2})}{2}$$
(A.3)

$$\rho_{\frac{3}{4}2}(t) = \frac{\mathcal{O}_t^{1,-z}(\frac{\pi}{4},0) - \mathcal{O}_t^{2,-z}(\frac{\pi}{4},0)}{2} \mp i \frac{\mathcal{O}_t^{1,-z}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_t^{2,-z}(\frac{\pi}{4},-\frac{\pi}{2})}{2}$$
(A.4)

$$\begin{split} \rho_{3\frac{3}{4}}(t) &= \frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},0)}{4} \mp \mathrm{i} \frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},0)}{4} \\ &- \frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},0)}{4} \pm \mathrm{i} \frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},0)}{4} \\ &- \mathrm{i} \frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \mp \frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \\ &+ \mathrm{i} \frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \pm \frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \end{split}$$

$$\begin{split} \rho_{4_{4}^{3}}(t) &= \frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},0)}{4} \pm i \frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},0)}{4} \\ &- \frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},0)}{4} \mp i \frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},0) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},0)}{4} \\ &+ i \frac{\mathcal{O}_{t}^{1,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \mp \frac{\mathcal{O}_{t}^{1,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{1,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \\ &- i \frac{\mathcal{O}_{t}^{2,x}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-x}(\frac{\pi}{4},-\frac{\pi}{2})}{4} \pm \frac{\mathcal{O}_{t}^{2,y}(\frac{\pi}{4},-\frac{\pi}{2}) - \mathcal{O}_{t}^{2,-y}(\frac{\pi}{4},-\frac{\pi}{2})}{4}. \end{split} \tag{A.6}$$

## Appendix B

After consistent absorption in the exponentials of terms linear in t, the entries  $\mathcal{G}_{ij}(t)$ , i, j = 1, 2, 3, of the matrix  $\mathcal{G}_t$  solution of equation (4.5), calculated up to first order in the dissipative term  $\mathcal{D}$ , can be expressed as

$$\mathcal{G}_{11}(t) = e^{-(a+\alpha)t} \cos \omega_0 t + \frac{\alpha - a}{\omega_0} \sin \omega_0 t, \tag{B.1}$$

$$\mathcal{G}_{12}(t) = -\left(e^{-(a+\alpha)t} + \frac{2b}{\omega_0}\right)\sin\omega_0 t,\tag{B.2}$$

$$\mathcal{G}_{13}(t) = -\frac{4}{\omega_0} \sin \frac{\omega_0}{2} t \left( c \cos \frac{\omega_0}{2} t - \beta \sin \frac{\omega_0}{2} t \right); \tag{B.3}$$

$$\mathcal{G}_{21}(t) = \left(e^{-(a+\alpha)t} - \frac{2b}{\omega_0}\right) \sin \omega_0 t, \tag{B.4}$$

$$\mathcal{G}_{22}(t) = e^{-(a+\alpha)t} \cos \omega_0 t + \frac{a-\alpha}{\omega_0} \sin \omega_0 t, \tag{B.5}$$

$$\mathcal{G}_{23}(t) = -\frac{4}{\omega_0} \sin \frac{\omega_0}{2} t \left( \beta \cos \frac{\omega_0}{2} t + c \sin \frac{\omega_0}{2} t \right); \tag{B.6}$$

$$\mathcal{G}_{31}(t) = -\frac{4}{\omega_0} \sin \frac{\omega_0}{2} t \left( c \cos \frac{\omega_0}{2} t + \beta \sin \frac{\omega_0}{2} t \right)$$
 (B.7)

$$\mathcal{G}_{32}(t) = \frac{4}{\omega_0} \sin \frac{\omega_0}{2} t \left( c \sin \frac{\omega_0}{2} t - \beta \cos \frac{\omega_0}{2} t \right)$$
 (B.8)

$$\mathcal{G}_{33}(t) = e^{-2\gamma t}. ag{B.9}$$

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