

# Decoherence, irreversibility, and selection by decoherence of exclusive quantum states with definite probabilities

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(Received 20 February 2002; published 8 May 2002)

The problem investigated in this paper is einselection, i.e., the selection of mutually exclusive quantum states with definite probabilities through decoherence. Its study is based on a theory of decoherence resulting from the projection method in the quantum theory of irreversible processes, which is general enough for giving reliable predictions. This approach leads to a definition (or redefinition) of the coupling with the environment involving only fluctuations. The range of application of perturbation calculus is then wide, resulting in a rather general master equation. Two distinct cases of decoherence are then found: (i) a “degenerate” case (already encountered with solvable models) where decoherence amounts essentially to approximate diagonalization; (ii) a general case where the einselected states are essentially classical. They are mixed states. Their density operators are proportional to microlocal projection operators (or “quasiprojectors”) that were previously introduced in the quantum expression of classical properties. It is found at various places that the main limitation in our understanding of decoherence is the lack of a systematic method for constructing collective observables.

DOI: 10.1103/PhysRevA.65.052119

PACS number(s): 03.65.Yz, 03.65.Db, 05.40.—a

## I. INTRODUCTION

The discovery of decoherence has already much improved our understanding of quantum mechanics. The effect has now been observed experimentally [1]. Many of its consequences have been obtained theoretically, but its foundation, the range of its validity, and its full meaning are still rather obscure. This is due most probably to the fact that it deals with deep aspects of physics, not yet fully investigated.

The intuitive idea of decoherence is rather clear [2]. The wave function of a macroscopic system depends on a very large number of variables and its local phase is very sensitive to boundary conditions, couplings, and initial conditions. Any phase coherence between different components of the wave function is therefore exposed to destruction, after which macroscopic interferences disappear. It is unfortunately very difficult to build up a satisfactory theory on this intuition, because a knowledge of phases remains out of reach for the  $N$ -body methods at our disposal.

### A. Some questions about decoherence

The problems of decoherence are most often stated after making a few simple and pragmatic assumptions. One assumes particularly that a few collective (or relevant) observables can describe the main features of a (generally macroscopic) system, and they are known *a priori*. The system is then split formally into two subsystems: a “collective” one (which is associated with the relevant observables) and an environment, which can be external or internal. Each of these two abstract subsystems has its own Hilbert space,  $\mathcal{H}_c$  or  $\mathcal{H}_e$  and the Hilbert space of the whole system is the product  $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_e$ . The Hamiltonian is accordingly split into three parts, one for each subsystem and one for their coupling,

$$H = H_c \otimes I_e + I_c \otimes H_e + H_1. \quad (1.1)$$

Observers are supposed to have only a direct knowledge of

the collective subsystem. Its properties are expressed by a reduced density operator  $\rho_r$ , which is obtained from the full density operator  $\rho$  through a partial trace on the environment

$$\rho_r = \text{Tr}_e \rho. \quad (1.2)$$

The time evolution of  $\rho_r$  exhibits the various aspects of decoherence. It has been investigated mostly by means of more or less exactly solvable models. Two models were particularly important because they were rather close to reality, at least in specific circumstances. In one of them the environment is replaced by a collection of harmonic oscillators [3–8]. Another model represents decoherence as an accumulation of scattering phase shifts when particles from an external atmosphere collide with a macroscopic object [9]. Much of what is known about decoherence was learned from these models and some of their variants [10].

The conclusions have been accurately summarized by Zurek. He distinguishes three different physical effects resulting from decoherence [10]. There is first a destruction of macroscopic interferences, then some privileged state vectors become selected as alternative physical events, and finally these states evolve classically. The privileged states are also called pointer states in analogy with the position of a pointer on a dial in a measuring apparatus [11]. Most models predict that these states exist and are orthogonal so that they define a Hilbert space basis in which the reduced density operator becomes approximately diagonal after a short while. The existence of this basis is essential since it defines a unique set of alternative events with well-defined probabilities. The name einselection (i.e., the selection of mutually exclusive quantum states with definite probabilities through decoherence) has been coined by Zurek for the mechanism selecting this basis.

These results have so far-reaching consequences for the interpretation of quantum mechanics and other applications such as quantum computing that one must assess their exact degree of generality. How much of them is specific to the models that were used and how much is universal? This question raises several problems.

(1) A basic preliminary problem is concerned with the meaning of collective observables. When an actual physical system is given in practice, it is a rather straightforward matter to guess what coordinates describe most conveniently its macroscopic dynamics (the choice of these “generalized coordinates” goes back to Lagrange). But the question of defining correctly the collective observables for an arbitrary quantum state of the whole system, i.e., to select what is collective and what can be considered as an environment, is much deeper. It will be seen again and again in this paper that it represents the real limit of our understanding.

(2) One may be puzzled by the fact that explicit models yield einselection somewhat too easily. This is because most of them rely on a coupling satisfying the commutation property

$$[H_1, X \otimes I_e] = 0, \quad (1.3)$$

between the coupling Hamiltonian  $H_1$  and a collective coordinate observable  $X$  (which may be supposed unique for simplicity). It is then found that  $\rho_r$  becomes approximately diagonal in the basis  $|x\rangle$  of eigenvectors of  $X$ . It is clear, however, that Eq. (1.3) is very restrictive, at least from a mathematical standpoint, and one cannot assume it to hold universally. What happens then when this condition is not satisfied? Is there still some sort of diagonalization? If so, along which basis? To answer this problem will be the main task of this paper.

(3) Problem (2) is made somewhat tricky because there exists a very large class of systems with collective coordinates for which condition (1.3) holds. They are mechanical nonrelativistic systems (excluding macroscopic electromagnetic effects), described by the position coordinates of hydrodynamics [12–15]. These systems, which are exceptional from a mathematical standpoint, may very well turn to be universal in measurement theory since a measuring device involves practically always some mechanical parts entangled with the rest of the apparatus. As will be shown in Sec. VII, the property (1.3) results from the form of kinetic energies and two-body potentials in nonrelativistic physics. This remarkable feature “explains” why classical mechanics can be formulated in ordinary three-dimensional space although the wave functions are defined on a configuration space [16].

So frequent an occurrence of a very special case may be puzzling from an intuitive standpoint. It raises a conflict between what we consider as general, either when speaking of the physical world or of the mathematics of the theory. This possible source of confusion will be avoided here by referring explicitly to “mathematical generality” when a “general property” or a “general case” will be mentioned, except when otherwise explicitly stated.

(4) One might be lured by models into premature conclusions and a sufficiently wide-ranging theory of decoherence

is necessary for assessing general properties. The construction of such a theory is the fourth problem to be considered here.

(5) Finally, one must consider the attractive approach to einselection by Zurek [10,17]. Einselected states are supposed to be the most predictable (or robust) carriers of information. Given a collective state  $\Psi$  (which may be pure or not) and the corresponding initial density operator  $\rho_\Psi(0) = |\Psi\rangle\langle\Psi|$ , one considers the time-dependent reduced density operator  $\rho_\Psi(t)$ . Its ability to preserve an information content is characterized by some relevant functional of  $\Psi$ , which may be minus the von Neumann entropy or more conveniently the measure of purity

$$c_\Psi(t) = \text{Tr} \rho_\Psi^2(t). \quad (1.4)$$

This quantity is then used to construct a “predictability sieve” distinguishing among the states: The larger the quantity (1.4) is, the more predictable the state  $\Psi$  is supposed to be. Model examples suggest that einselected states do exist and are rather insensitive to a change in the coupling or a redefinition of the environment. A fifth problem consists in evaluating this conjecture in a wider framework.

## B. The present results

These five problems will not of course be solved here completely, but some definite or suggestive answers will be obtained. The most precise results are concerned with einselection and diagonalization, their meaning and their relation. As a preliminary, one needs a sufficiently wide-ranging theory of decoherence, as stated in problem 4. The theory to be used here does not claim to be new. It relies on the familiar idea that decoherence is a special kind of irreversible process. This means that one may expect that the most general theory of decoherence presently at our disposal would derive from the existing quantum theories of irreversible processes. Moreover, the most convenient such theory is the so-called projection method [18–21]. Its main features are recalled in Sec. II and it is applied to decoherence in Sec. III. Although this method was previously introduced elsewhere [15,22,23], some improvements will be required before applying it for the present purpose. These developments are mostly given in the appendices and they may be useful for using the method in other problems.

A very important remark concerning this approach is the possibility of making a definite choice for the coupling Hamiltonian  $H_1$  from which one can easily derive a master equation for  $\rho_r$ . The point is that, given *a priori* a coupling Hamiltonian, one can construct another (time-dependent) one consisting only of fluctuations. Standard perturbation methods can then be applied confidently in most cases. Although this procedure is familiar near equilibrium (it is used for instance in the derivation of the fluctuation-dissipation theorem [24]), it works also far from equilibrium as will be shown in Sec. IV, providing a strong handle on decoherence.

The master equation one obtains in this way is probably the most general one that is accessible with present techniques and therefore the most appropriate one for investigating einselection, as done in Sec. V. One thus finds that, con-

trary to current expectations, two different cases of einselection exist. The first one was encountered with solvable models and is well known, although it is far from being general in a mathematical sense (in the case of an arbitrary coupling). It must be considered on the contrary as a degenerate case for the following reason. If  $n$  is the number of  $X$  observables, decoherence is controlled in the general case by a differential Laplacian-like operator in the  $2n$ -dimensional phase space. In the simplest case  $n=1$ , the decoherence “Laplacian” is associated as usual with a quadratic form [like the two-dimensional Laplacian  $\partial^2/\partial x^2 + \partial^2/\partial p^2$  is associated after a Fourier transform  $(x,p) \rightarrow (\xi,\eta)$  to the quadratic form  $(\xi^2 + \eta^2)$ ]. The decoherence Laplacian is degenerate when it acts on only one variable (for instance the coordinate  $x$  and not the associated momentum  $p$ ) so that the corresponding quadratic form is degenerate (having a zero eigenvalue). In the degenerate case, to which the usual models belong, decoherence essentially amounts to a diagonalization (in the basis einselected by degeneracy).

The nondegenerate case is investigated in Sec. VI. The results are not those expected from Zurek’s predictability sieve, at least as far as I understand it. There are generally two distinct times for decoherence. Typically, in conditions when these times are very different, decoherence selects a basis of privileged states in which  $\rho_r$  begins to become diagonal, but then these “einselected” states do not preserve their probabilities and they begin to share them with neighboring states. When the two decoherence times are similar, not much remains apparently of the idea of einselection. The final outcome of decoherence is rather a tendency towards uniformity where  $\rho_r$  becomes as close to the identity matrix as its finite trace can allow (more precisely, it corresponds to a uniform Wigner function over a rather large region of phase space). Nevertheless, macroscopic interferences are still destroyed and classical behavior may follow.

The question of the different time scales is discussed in Sec. VII and a strong connection is found with the special properties of hydrodynamical variables. The relation between decoherence and dissipation coefficients plays an important role in this discussion. Problem (3) then becomes central because decoherence depends most often in practice on the fact that the space coordinates of a nonrelativistic piece of matter satisfy the condition (1.4) implying degeneracy. One is thus led again to Gell-Mann and Hartle’s ideas concerning the link between coarse graining and the existence of a diagonalization basis [12,13].

Finally, the occurrence of classical dynamics after decoherence is considered in Sec. VIII in both the degenerate and the nondegenerate cases. In the nondegenerate case, although one can still speak of einselected states, they are far from being pure states. They are mixed states whose density operator at a definite time is proportional to a “microlocal projection operator,” which is known in mathematics as the best expression of a classical property involving position and momentum together [25–27]. Finally, the conclusion goes back to the strong connection between the origin of classicality and problem (1), i.e., the construction of collective coordinates. Some proposals for further research are indicated.

Appendix A gives a derivation of decoherence theory from the projection method in irreversible processes. Appendix B is concerned with the relation between decoherence and dissipation coefficients. Appendix C shows how to include the insightful scattering model of decoherence by Joos and Zeh in the framework of the present theory.

## II. A QUANTUM THEORY OF IRREVERSIBLE PROCESSES

One needs a sufficiently wide-ranging theory of decoherence for asserting its general features. Since the loss of phase coherence through decoherence produces disorder, typical of an irreversible process, the most general relevant theory is the projection method, which is now briefly reviewed [18–21].

One considers a system with many degrees of freedom, whose density operator evolves according to the von Neumann–Schrödinger equation,

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho]. \quad (2.1)$$

Some observables are supposed to be particularly relevant for a given problem and one wants only to know the time evolution of their mean values. These relevant observables are denoted by  $A^j$ . Their set may be finite or not, countable or not. One usually includes the identity operator  $I$  in the set and also the conserved quantities such as the total energy  $H$ , although this recipe is not imperative. The “exact” average values of these observables are

$$a^j(t) = \text{Tr}[A^j \rho(t)]. \quad (2.2)$$

The first step of the method consists in introducing a time-dependent test density operator  $\rho_0(t)$  satisfying the following two conditions. (i) It gives the exact average values of the relevant observables,

$$\text{Tr}[A^j \rho_0(t)] = \text{Tr}[A^j \rho(t)] \equiv a^j(t). \quad (2.3)$$

(ii) Its information content is minimal [which means that it does not provide anything else than the quantities  $\{a^j(t)\}$ ]. It can therefore be written as

$$\rho_0(t) = \exp[-\lambda_j(t) A^j], \quad (2.4)$$

where the numbers  $\{\lambda_j\}$  are Lagrange parameters and the Einstein summation convention over repeated indices has been used. Since the identity  $I$  belongs to the set  $\{A^j\}$ , the trace of  $\rho_0$  is normalized.

One will use the name “density” in the present paper for an operator with a finite trace (also called a trace-class operator). It is neither supposed to have a unit trace nor to be necessarily positive. One defines a set of (time dependent) densities

$$s_j = \partial \rho_0 / \partial a^j. \quad (2.5)$$

They satisfy the important orthogonality properties

$$\text{Tr}(s_i A^j) = \delta_i^j, \quad (2.6)$$

amounting essentially to  $\partial a^j / \partial a^i = \delta_i^j$  in view of Eq. (2.3).

The theory makes use of “superoperators,” which act linearly on a density to yield another density. For instance, Eq. (2.1) can be written conventionally as

$$\dot{\rho} = L\rho, \quad (2.7)$$

where  $L$  is the Liouville superoperator. Another important superoperator is defined by

$$P = s_j \otimes A^j, \quad (2.8)$$

which means that when acting on a density  $\mu$ , it gives (with the summation convention)

$$P\mu = s_j \text{Tr}(A^j \mu). \quad (2.9)$$

It is a projection in so far as it satisfies the simple equation

$$P^2 = P, \quad (2.10)$$

resulting from the orthogonality properties (2.6).

One can define a “relevant” (time-dependent) density operator  $\rho_1$  by

$$\rho_1 = P\rho. \quad (2.11)$$

It generates the exact average values  $\{a(t)\}$  since

$$\text{Tr}(A^j \rho_1) = \text{Tr}(A^j P\rho) = \text{Tr}(A^j s_j) \text{Tr}(A^i \rho) = \delta_i^j a^i = a^j. \quad (2.12)$$

(As a matter of fact, it coincides with the test density operator  $\rho_0$ .)

Denoting by  $\mathcal{I}$  the identity superoperator, one also introduces  $\mathcal{Q} = \mathcal{I} - P$ , which satisfies the projection property  $\mathcal{Q}^2 = \mathcal{Q}$  in view of Eq. (2.10), as well as the orthogonality properties  $\mathcal{Q}P = P\mathcal{Q} = 0$ . One defines then another density  $\rho_2 = \mathcal{Q}\rho$  (so that  $\rho = \rho_1 + \rho_2$ ). Applying the two projections  $P$  and  $\mathcal{Q}$  to the evolution equation (2.7) and taking into account the time dependence of these projections, one obtains two coupled evolution equations,

$$\dot{\rho}_1 = PLP\rho_1 + \dot{P}P\rho_1 + PL\mathcal{Q}\rho_2 + \dot{P}\mathcal{Q}\rho_2, \quad (2.13)$$

$$\dot{\rho}_2 = \mathcal{Q}L\mathcal{Q}\rho_2 + \dot{\mathcal{Q}}\mathcal{Q}\rho_2 + \mathcal{Q}LP\rho_1 - \dot{P}P\rho_1. \quad (2.14)$$

A last step would be to eliminate  $\rho_2$  to obtain a master equation for  $\rho_1$  but it will be left for the special case of decoherence.

### III. THE CASE OF DECOHERENCE

The previous theory can be now applied to decoherence and some preliminary considerations will make the task clearer. A first problem is to choose the relevant observables. If one thinks of macroscopic interferences, it is clear that they can involve many different macroscopic observables so that every collective observable is relevant. When the collective observables describe a measuring apparatus, the mea-

sured microscopic observable is also relevant although not collective.

The environment can be defined by its observables, which commute with the collective ones. The resulting splitting of the system into a collective one and an environment is generally time dependent since for instance every new bubble in a bubble chamber or every new spark in a spark chamber generates new collective observables. Decoherence is such a rapid process, however, that the collective environment splitting can often be considered as fixed during the very short time of an individual decoherence process, justifying the expression (1.1) for the Hamiltonian. The coupling  $H_1$  in this equation is responsible for the interactions between the collective system and the environment, including dissipation and decoherence.

The set of relevant observables is completed by the identity operator  $I$  (insuring normalization) and the environment Hamiltonian  $H_e$ , or more properly  $I_c \otimes H_e$ . The total Hamiltonian  $H$  might have been used as relevant in place of  $H_e$  but this choice would have been inconvenient, as will be seen later).

Introducing an arbitrary orthonormal basis  $|k\rangle$  in the collective Hilbert space, the set  $\{|k\rangle\langle k'|\}$  provides a linear basis for the collective operators. A look at the calculations in Sec. II shows that they nowhere use the fact that the  $\{A^j\}$  are Hermitian so that one may use the set of operators  $\{|k\rangle\langle k'|\}$  as relevant “observables.” Alternatively, one might use the set of Hermitian operators

$$\begin{aligned} & \{ (1/2)(|k\rangle\langle k| \pm |k'\rangle\langle k'|); (1/2)(|k\rangle\langle k'|) \\ & \times (\langle k| \mp i\langle k'|) \} \end{aligned}$$

as relevant with identical results. Anyway, the set of relevant observables for a theory of decoherence will be chosen as

$$\{A^{kk'} = |k\rangle\langle k'| \otimes I_e, A^1 = I, A^e = I_c \otimes H_e\}. \quad (3.1)$$

Since none of them connects the collective and the environment Hilbert spaces, the test density operator (2.4) is a tensor product

$$\rho_0 = \rho_c \otimes \rho_e. \quad (3.2)$$

Applying Eq. (2.3) to the operators  $A^{kk'}$ , one finds that

$$\langle k' | \rho_c | k \rangle = \text{Tr}(A^{kk'} \rho_0) \equiv \text{Tr}(A^{kk'} \rho) = \langle k' | \text{tr} \rho | k \rangle = \langle k' | \rho_r | k \rangle, \quad (3.3)$$

so that the collective test density  $\rho_e$  is identical to the conventional reduced density (1.2). The second equality results from Eq. (2.1). A convention for traces that will be used everywhere has also been introduced, the notation  $\text{Tr}$  standing for a trace on the full Hilbert space and  $\text{tr}$  for a trace on the environment.

According to Eq. (2.4), the environment test density  $\rho_e$  is given by

$$\rho_e = \exp(-\beta H_e - \alpha), \quad (3.4)$$

where  $\alpha$  is a Lagrange parameter ensuring normalization and  $\beta$  ensures that the energy  $H_e$  of the environment has its true average value  $E$ . This density is the same as if the environment were in thermal equilibrium but it should be stressed that it is only an auxiliary mathematical quantity providing a correct (time-dependent) value for  $E$  with no assumption about equilibrium.

In Appendix A, the auxiliary densities  $s_j$  are obtained from Eq. (2.5). Denoting, respectively, by  $s_1$  and  $s_2$  the densities associated with  $I$  and  $H_e$ , one gets

$$s_{kk'} = |k'\rangle\langle k| \otimes \rho_e, \quad (3.5)$$

$$s_e = \rho_c \otimes \rho_e (H_e - E) \Delta^{-2}, \quad (3.6)$$

$$s_1 = -E \rho_c \otimes \rho_e (H_e - E) \Delta^{-2}, \quad (3.7)$$

where  $\Delta$  is the uncertainty in energy

$$\Delta^2 = \text{tr}(H_e^2 \rho_e) - E^2. \quad (3.8)$$

When acting on an arbitrary density  $\mu$ , the projection  $P$  is given according to Eq. (2.9) and Eqs. (2.5)–(2.7) by

$$P\mu = \text{tr} \mu \otimes \rho_e + [\rho_c \otimes \{\rho_e (H_e - E) \Delta^{-2}\}] (\text{Tr} H_e \mu - E \text{Tr} \mu), \quad (3.9)$$

from which the relations  $P^2 = P$  and  $\rho_1 = \rho_0$  follow.

#### A. Specifying the coupling

One may now introduce an important remark that will later justify the use of perturbation theory. To begin with, one may notice some arbitrariness in the splitting of the full Hamiltonian  $H$  into three different terms as in Eq. (1.1). A simple recipe for fixing them is to impose that

$$\text{tr} H_1 \rho_e = 0. \quad (3.10)$$

The meaning of this condition can be seen in the example of a cylinder containing a gas. A collective coordinate is specified by the position  $x$  of a piston whereas the environment consists of the gas and the matter of the piston itself. A straightforward definition of  $H_1$  could be the sum of the potential energies between the atoms in the piston and the gas. This interaction is far from being weak, since the confinement of a gas is not a weak effect, but a large part of it consists of a collective energy since  $\text{tr} H_1 \rho_e$  is a collective operator. One can then change the definition of the different parts in  $H$  by including this operator in  $H_c$  and removing it from  $H_1$  or, more precisely, by introducing

$$H'_c = H_c + \text{tr}(H_1 \rho_e),$$

$$H'_1 = H_1 - \text{tr}(H_1 \rho_e) \otimes I_e.$$

The quantity  $\text{tr} H_1 \rho_e$  represents in this example the effect of the gas pressure on the piston. The new expression of  $H_c$  is time dependent (like pressure) but the new expression of  $H_1$  satisfies the condition (3.10). It consists only of the pressure fluctuations resulting from the collisions of the gas molecules with the piston.

The idea of introducing a purely fluctuating coupling and to use perturbation theory for computing its effects is familiar in quantum fluctuation theory [24]. The fact that one can still use it far from equilibrium when dealing with decoherence is due to the possibility of representing everything collectively by the test density. From there on, the condition (3.10) will be assumed.

One may also understand at this point why the choice of  $H_e$  as a relevant observable is more convenient than the total Hamiltonian  $H$ , which is usually recommended [21]. This is because the expression (3.2) for the test density implies the simple rule (3.10) for the coupling, with the benefits just mentioned. Everything would have been more obscure and would have implied much heavier calculations if  $H$  had been chosen as a relevant observable.

#### B. The evolution equations

It is easy to write down explicitly the evolution equations (2.13)–(2.14) for the case of decoherence. It is convenient to split Eq. (2.13) for  $\dot{\rho}_1$  into an equation for  $\dot{\rho}_r$  and another for  $\dot{\rho}_e$  (or for the time evolution of the internal energy). This is done by taking, respectively, the traces of Eq. (2.13) on the environment and the collective Hilbert spaces. As shown in Appendix A, the results are

$$\dot{\rho}_r = -\frac{i}{\hbar} ([H_c, \rho_r] + \text{tr}[H_1, \rho_2]), \quad (3.11)$$

$$\dot{E} + \frac{i}{\hbar} \text{Tr}(H_e [H_1, \rho_1 + \rho_2]) = 0. \quad (3.12)$$

As for the second evolution equation (2.14), it becomes

$$\dot{\rho}_2 = -(i/\hbar)[H, \rho_1 + \rho_2] + (i/\hbar)\text{tr}([H_1, \rho_2]) \otimes \rho_e - \rho_r \otimes \dot{\rho}_e. \quad (3.13)$$

#### IV. A MASTER EQUATION

The most delicate step in the projection method consists always in “solving” the second evolution equation (2.14) for  $\rho_2$  in terms of  $\rho_1$  before inserting the result into Eq. (2.13) [21]. This is much easier when perturbation theory can be used. Perturbation calculus has been used already in the present framework when  $H_1$  is known *a priori* to be small, as often happens in quantum optics [22,23]. It should also presumably be valid in many instances when condition (3.10) is applied and  $H_1$  is a pure fluctuation (although one must acknowledge that a purely fluctuating coupling does not ensure with certainty the validity of perturbation calculus). Anyway, according to Appendix A, the evolution equations (3.11)–(3.13) become at leading order in  $H_1$ ,

$$\dot{\rho}_r = -\frac{i}{\hbar} ([H_c, \rho_r] + \text{tr}[H_1, \rho_2]), \quad (4.1)$$

$$\dot{\rho}_2 = -(i/\hbar)[H_0, \rho_2] - (i/\hbar)[H_1, \rho_2]. \quad (4.2)$$

In the second equation,  $H_0$  denotes the uncoupled Hamiltonian

$$H_0 = H_c \otimes I_e + I_c \otimes H_e \quad (4.3)$$

and Eq. (4.1) is exact whereas Eq. (4.2) is valid at first order in perturbation theory.

The second equation is easily solved after introducing the evolution operator

$$U(t) = \exp(-iH_0 t/\hbar). \quad (4.4)$$

Strictly speaking,  $H_0$  is generally time dependent and the integrand in Eq. (4.4) should be replaced by an integral of  $H_0(t)$  on time. It is difficult, however, to conceive of a case where this external time dependence is not much slower than decoherence and the expression (4.4) is therefore most often valid as it stands. If not, the necessary changes are so trivial that they need not be mentioned here. One thus gets

$$\rho_2(t) = -(i/\hbar) \int_{-\infty}^t dt' U(t-t') [H_1, \rho_1(t')] U^{-1}(t-t'). \quad (4.5)$$

No effect of the initial value of  $\rho_2$  (at time  $-\infty$ ) has been included in Eq. (4.5). This is justified when the environment is initially in thermal equilibrium [since then  $\rho_2(-\infty) = 0$ ]. More generally, however, it may be expected that an initial lack of equilibrium does not influence the decoherence effect, so that Eq. (4.5) is valid for our present purpose. This point was checked in a special case by Paz, Zurek, and co-workers [28,29].

Inserting Eq. (4.5) into Eq. (4.1), one obtains the following “master equation” for decoherence:

$$\begin{aligned} \dot{\rho}_r = & -\frac{i}{\hbar} [H_c, \rho_r] - (1/\hbar^2) \int_{-\infty}^t dt' \text{tr}\{H_1, U(t-t') \\ & \times [H_1, \rho_r(t') \otimes \rho_e(t')] U^{-1}(t-t')\}. \end{aligned} \quad (4.6)$$

The first term on the right-hand side represents the quantum evolution of the reduced density operator under the action of the collective Hamiltonian  $H_c$ . The second term is responsible for decoherence.

This equation is not new but it was derived previously either under the assumption of a small coupling [22,23], or as a guess [15]. It will be used here as a sufficiently general framework for a study of einselection.

The wide range of this master equation is confirmed by its agreement with previous models. This is easily shown when the environment is represented by a collection of harmonic oscillators [3–8]. The key experiment by Brune *et al.* showing the existence of decoherence also belongs to the domain of Eq. (4.6) since  $H_1$  is small in that case [1,30]. In the case of the collision model by Joos and Zeh the calculations are less trivial and they are given in Appendix C as a nontrivial example of the master equation universality.

## V. DECOHERENCE VERSUS DIAGONALIZATION

Models have been extremely useful for understanding decoherence. When the collective subsystem is described by a few position observables  $X$ , decoherence was found to diagonalize the reduced density  $\rho_r$ , in the basis  $|x\rangle$  consisting of eigenvectors of  $X$ . The question to be now considered is therefore: does decoherence always implies some sort of diagonalization? Is there always a selection of privileged “pointer states,” or einselection as defined by Zurek [10]?

One may first select the equation on which this question will be investigated. The idea of diagonalization must be used with some care because the reduced density operator never becomes completely diagonal in view of the first term in Eq. (4.6) representing collective dynamics. For a finite value of the difference  $x - x'$  the matrix elements

$$\rho_r(x, x'; t) = \langle x | \rho_r(t) | x' \rangle, \quad (5.1)$$

vanish exponentially with time, whereas microscopic values of  $x - x'$  are dominated by collective dynamics and they remain finite. This is why there is decoherence on large scale while atomic physics remains perfectly valid at small scale. The question of diagonalization is therefore much clearer if one leaves aside the first term in Eq. (4.6) and considers “pure decoherence” as the behavior of a density operator obeying the truncated equation

$$\begin{aligned} \dot{\rho}_r = & -(1/\hbar^2) \int_{-\infty}^t dt' \text{tr}\{H_1, U(t-t') \\ & \times [H_1, \rho_r(t') \otimes \rho_e(t')] U^{-1}(t-t')\} \\ \equiv & D. \end{aligned} \quad (5.2)$$

The main task will then consist in an analysis of the right-hand side of Eq. (5.2), which has been denoted by  $D$ . It will also be useful to introduce the notation

$$H_1^T = U(t-t') H_1 U^{-1}(t-t'), \quad (5.3)$$

so that one has

$$\begin{aligned} D = & -(1/\hbar^2) \int_{-\infty}^t dt' \text{tr}\{H_1, [H_1^T, U_c(t-t') \rho_r(t') \\ & \times U_c^{-1}(t-t') \otimes \rho_e(t')]\}, \end{aligned} \quad (5.4)$$

where  $U_e^{-1} \rho_e U_e$  has been replaced by  $\rho_e$  in view of Eq. (3.4).

### A. Weyl symbols

One will consider the case when there exists a set of  $n$  collective “position” observables, altogether denoted by  $X$ . The quantity  $D$  is itself a collective operator and it will be convenient to describe it by means of a Weyl symbol [31,25], in analogy with the description of  $\rho_r$  by a Wigner function [32]. The standard Weyl calculus can be slightly generalized to include “operator-valued symbols” acting on the environment as follows.

Let  $A$  denote an arbitrary operator in the full Hilbert space (such as  $H_1$  for instance). Introducing the basis  $\{|x\rangle\}$  in the

collective Hilbert space and an orthonormal basis  $\{|n\rangle\}$  in the environment Hilbert space, the matrix elements of  $A$  can be expressed through a partial Fourier transform

$$\langle x, n | A | x', n' \rangle = \int (2\pi\hbar)^{-n} dp \bar{A}_{nn'} \left( \frac{x+x'}{2}, p \right) \times \exp\{ip(x'-x)\hbar\}. \quad (5.5)$$

Every quantity  $\bar{A}_{nn'}(x, p)$  is a function of  $(x, p)$  and the ordinary Weyl symbol of the matrix element  $A_{nn'} = \langle n | A | n' \rangle$ , which is a collective operator. It will be convenient to consider it as the  $(n, n')$  matrix element of an operator-valued symbol  $\bar{A}(x, p)$ , which is a function of  $(x, p)$  and an operator in the Hilbert space of the environment.

The symbol of the product  $AB$  of two operators  $A$  and  $B$  can then be expressed as a series in powers of  $\hbar$  involving their symbols [31,25],

$$\overline{AB} = \bar{A}\bar{B} - (i\hbar/2)(\bar{A}_p\bar{B}_x - \bar{A}_x\bar{B}_p) - (\hbar^2/24) \times (\bar{A}_{p^2}\bar{B}_{x^2} + \bar{A}_{x^2}\bar{B}_{p^2} - 2\bar{A}_{px}\bar{B}_{px}) + O(\hbar^3). \quad (5.6)$$

The notation has been simplified by omitting the arguments  $(x, p)$  of the symbols and lower indices stand for derivatives [for instance,  $\bar{A}_{xp}$  stands for  $\partial^2\bar{A}(x, p)/\partial x\partial p$ ]. Equation (5.6) is well known in Weyl's calculus when the symbols are ordinary functions. It is easily extended to operator-valued symbols by considering matrix elements and a unique new rule must be added to the case of functions: the order of the operators in the product  $AB$  must be respected in the products of symbols and their derivatives. The symbol of the reduced density operator  $\rho_r$  is the Wigner function, which will be denoted by  $W(x, p)$ . It is not operator valued and commutes with other symbols.

The only further formula one will need from the Weyl calculus is the expression of a complete trace,

$$\text{Tr} A = \int dx dp (2\pi\hbar)^{-n} \text{tr} \bar{A}(x, p). \quad (5.7)$$

### B. Calculation of the decoherence term $D$

It will be convenient to consider from there on the case of a unique coordinate  $X$  ( $n=1$ ) although the generalization to arbitrary values of  $n$  is trivial. Applying Eq. (5.6) to the double commutator in Eq. (5.4), one obtains the symbol  $\bar{D}$  of the decoherence term  $D$  at order  $\hbar^2$ , as shown in Appendix B,

$$\bar{D} = \int_{-\infty}^t dt' [\partial/\partial x (C^{xx} W_x^T + C^{xp} W_p^T) + \partial/\partial p (C^{px} W_x^T + C^{pp} W_p^T)]. \quad (5.8)$$

The function  $W^T(x, p)$  is the symbol of the collective operator

$$U_c(t-t')\rho_r(t')U_c^{-1}(t-t'). \quad (5.9)$$

The various decoherence coefficients are given by

$$C^{xx} = \frac{1}{2} \text{tr} \{ (\bar{H}_{1p} \bar{H}_{1p}^T + \bar{H}_{1p}^T \bar{H}_{1p}) \rho_e \}, \quad (5.10)$$

$$C^{xp} = -\frac{1}{2} \text{tr} \{ (\bar{H}_{1p} \bar{H}_{1x}^T + \bar{H}_{1x}^T \bar{H}_{1p}) \rho_e \}, \quad (5.11)$$

$$C^{px} = -\frac{1}{2} \text{tr} \{ (\bar{H}_{1x} \bar{H}_{1p}^T + \bar{H}_{1p}^T \bar{H}_{1x}) \rho_e \}, \quad (5.12)$$

$$C^{pp} = \frac{1}{2} \text{tr} \{ (\bar{H}_{1x} \bar{H}_{1x}^T + \bar{H}_{1x}^T \bar{H}_{1x}) \rho_e \}. \quad (5.13)$$

It is possible in principle to derive the main consequences of the master equation for decoherence from these equations by using the powerful methods of microlocal analysis [25]. It will be much simpler, however, to rely on a few usual approximations. The first one assumes that the coefficients (5.10)–(5.13) vary slowly with  $(x, p)$  or, more precisely, one neglects the collective evolution  $U_c(t-t')$  in the factors  $U$  and  $U^{-1}$  occurring in the expression (5.3) of  $H_1^T$ . The physical meaning of this approximation is discussed in Appendix B, where the following expression of  $C^{pp}$  is obtained:

$$C^{pp} = \sum_{nn'} \bar{H}_{1xnn'} \bar{H}_{1x'n'} \times \exp[i\omega_{nn'}(t-t')] p_{nn'} \times \cosh(\beta\hbar\omega_{nn'}/2), \quad (5.14)$$

where the states  $|n\rangle$  are the energy eigenstates of  $H_e$  with eigenvalues  $E_n$  and one has written

$$\bar{H}_{1xnn'} = \langle n | \partial \bar{H}_1(x, p) / \partial x | n' \rangle, \quad \omega_{nn'} = (E_n - E_{n'}) / \hbar, \quad p_{nn'} = \exp[-\beta(E_n + e_{n'})/2 - \alpha]. \quad (5.15)$$

Equation (5.14) suggests that the relevant frequencies  $\omega_{nn'}$  in the sum are contained in an interval  $[-\Omega, \Omega]$  characterizing the environment and generally large as compared with the rate of collective dynamics ( $\Omega$  is typically a Debye frequency for an internal environment). Hu, Paz, and Zhang have shown that the master equation is instantaneous (i.e., involves no retardation) in the case an oscillator environment, when the collective Hamiltonian also describes an oscillator [7]. This is due to the linear character of the equations in that case [33]. The resulting master equation has been solved explicitly by Ford and O'Connell [8]. This situation is, however, exceptional and the neglect of retardation is almost always an approximation. The question of its justification is tricky and it would warrant a separate investigation. When retardation effects are unimportant anyway, the integration on  $t'$  in Eq. (5.8) is performed as if the integrand were a  $\delta$  function in time. The time-delayed function  $W'$  is replaced by the ordinary Wigner function  $W$  and Eq. (5.8) becomes

$$\bar{D} = \frac{\partial}{\partial x} (g^{xx} W_x + g^{xp} W_p) + \frac{\partial}{\partial p} (g^{px} W_x + g^{pp} W_p). \quad (5.16)$$

The new coefficients are given by

$$g^{ij} = \int_{-\infty}^t C^{ij}(t-t') dt' \quad (5.17)$$

[with indices  $(i, j) = (x, p)$ ]. Explicit expressions of these coefficients are given in Appendix B, showing that the coefficients  $g^{xx}$  and  $g^{pp}$  are positive symmetric:  $g^{xp} = g^{px}$ , and the quadratic form

$$g^{xx} \alpha^2 + 2g^{xp} \alpha \beta + g^{pp} \beta^2 \quad (5.18)$$

is non-negative. One must then distinguish two significantly different cases according to whether the form (5.18) is degenerate or not, i.e., whether the determinant  $g^{xx} g^{pp} - (g^{px})^2$  is zero or positive.

### C. The degenerate case

The degenerate case was encountered in most models and only one coefficient, namely,  $g^{pp}$ , was different from zero. It is then convenient to go back to the matrix elements  $\rho_r(x, x'; t)$  by inverting the Fourier transform (5.5) so that the pure decoherence master equation (5.2) becomes

$$\frac{\partial}{\partial t} \rho_r(x, x'; t) = -\frac{g^{pp}}{\hbar^2} (x - x')^2 \rho_r(x, x'; t). \quad (5.19)$$

Diagonalization in the basis  $\{|x\rangle\}$  is then obvious when  $g^{pp}$  is a constant since the solution of this equation is

$$\rho_r(x, x', t) = \rho_r(x, x', 0) \exp\left[-\frac{g^{pp}}{\hbar^2} (x - x')^2 t\right].$$

Similarly, when the only nonzero coefficient is  $g^{xx}$ , one may use the momentum basis  $\{|p\rangle\}$  to obtain

$$\frac{\partial}{\partial t} \rho_r(p, p'; t) = -\frac{g^{xx}}{\hbar^2} (p - p')^2 \rho_r(p, p'; t), \quad (5.20)$$

implying again diagonalization.

A simple condition for the coupling implying diagonalization in the position basis is given by Eq. (1.3) [34,15]. Using coarse graining, Gell-Mann and Hartle have shown that this condition is satisfied for mechanical systems when using hydrodynamical observables as relevant [13].

## VI. THE NONDEGENERATE CASE

Quite different results are obtained in the general case when there is no degeneracy. One may note first that the differential operator in the right-hand side of Eq. (5.16) is similar to a Laplacian, which is given by

$$\Delta = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left( \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right), \quad (6.1)$$

in the case of a metric  $ds^2 = g_{ij} dx^i dx^j$  (with  $g_{ij} g^{jk} = \delta_i^k$ ). The factor  $g$  is the determinant of the matrix with elements  $g_{ij}$  or the inverse of  $\det(g^{ij})$ . One could use this remark in principle for a general study of decoherence but it would need the full power of microlocal analysis. Rather than entering into such heavy mathematics, it will be convenient to consider only the case when the coefficients  $g^{ij}$  are constants. A further simplification is obtained by diagonalizing the quadratic form (5.18). This is done by a change of variables after introducing scale-invariant parameters. Let  $L$  be a unit of “length” (i.e., a scale with the dimensionality of  $X$ ) and  $\Pi$  a unit of momentum. The transformation

$$\Pi X' = \Pi X \cos \theta + LP \sin \theta,$$

$$LP' = -\Pi X \sin \theta + LP \cos \theta, \quad (6.2)$$

can be viewed either as an “orthogonal” change of axes in the  $(x, p)$  plane or as a linear canonical transformation. It leaves Weyl’s calculus invariant [25], so that if one chooses  $\theta$  to diagonalize the metric, one obtains a simpler equation for pure decoherence, namely (after dropping the prime indices),

$$\frac{\partial W}{\partial t} = g^{xx} \frac{\partial^2 W}{\partial x^2} + g^{pp} \frac{\partial^2 W}{\partial p^2}. \quad (6.3)$$

### A. General decoherence is not a diagonalization process

The general case of decoherence occurs when the quadratic form (5.18) is nondegenerate. Does then the effect still amount to diagonalization? By looking at the degenerate case, one sees that diagonalization was due to a specific property of the collective operator  $D$ . There was a specific orthonormal (“pointer”) basis  $\{|j\rangle\}$ , such that

$$\langle j|D|j\rangle = 0 \quad \text{for each } j, \quad (6.4)$$

$$\text{Re}\langle j|D|k\rangle < 0 \quad \text{for every pair of indices } j \neq k. \quad (6.5)$$

These relations held true for any density matrix  $\rho_r$  entering in the definition of  $D$ . They must obviously be satisfied if diagonalization takes place, at least if the basis is independent of the preparation  $\rho_r(0)$  and depends only on the decoherence coefficients. They do not hold, however, in general as shown by the following

*No-go theorem.* Whatever the state  $\psi$ , it is impossible for the equation

$$\langle \psi|D(\rho_r)|\psi\rangle = 0 \quad (6.6)$$

to hold for every density matrix  $\rho_r$ ,

*Proof.* According to Eq. (5.16), one can write

$$D(\rho) = \Delta \rho, \quad (6.7)$$

where  $\Delta$  is understood as a superoperator acting on a collective density  $\rho$ . One can write



$$\langle \psi | \Delta \rho | \psi \rangle = \text{Tr}_c(|\psi\rangle\langle\psi| \Delta \rho).$$

If this equation is supposed to be valid for any choice of  $\rho$ , one must have (since the superoperator  $\Delta$  is Hermitian)

$$\Delta |\psi\rangle\langle\psi| = 0.$$

When written explicitly in the position basis, this equation becomes

$$\left\{ g^{xx} \frac{\partial^2}{\partial x^2} - (g^{pp}/\hbar^2) \xi^2 \right\} \psi(x + \xi/2) \psi^*(x - \xi/2) = 0,$$

from which one gets

$$\begin{aligned} \psi(x + \xi/2) \psi^*(x - \xi/2) = & a(\xi) \exp\left( \sqrt{\frac{g^{pp}}{g^{xx}}} (x\xi/\hbar) \right) \\ & + b(\xi) \exp\left( - \sqrt{\frac{g^{pp}}{g^{xx}}} (x\xi/\hbar) \right). \end{aligned}$$

This is, however, impossible (even if the coefficients are distributions) because it would imply that the wave function of the state  $\psi$  increases exponentially for large values of its argument. ■

*Note.* The present theorem forbids the existence of a universal diagonalization basis. The possibility of a  $\rho$ -dependent basis remains open, although it looks very doubtful.

### B. Decoherence in the nondegenerate case

Since decoherence cannot be generally a diagonalization process, one must investigate it anew. Its consequences are most easily obtained when  $x - x'$  is large. It will be more convenient to use the notation  $(x', x'')$  for the arguments of the reduced density matrix  $\rho_r(x', x'')$  in the position representation and to introduce auxiliary variables  $x = (x' + x'')/2$ ,  $\xi = x' - x''$ . This means that we are interested in the case where  $\xi$  is large (macroscopic). After performing a Fourier transform to go back from the variable  $p$  to  $\xi$ , the pure decoherence equation (5.2) becomes

$$\dot{\rho} = g^{xx} \frac{\partial^2 \rho}{\partial x^2} - (g^{pp} \xi^2 / \hbar^2) \rho. \quad (6.8)$$

The time evolution of the function  $\rho(x, \xi) = \rho_r(x + \xi/2, x - \xi/2)$  is therefore given by

$$\begin{aligned} \rho(x, \xi, t) = & \exp(-g^{pp} \xi^2 t / \hbar^2) \frac{1}{\sqrt{4\pi g^{xx} t}} \\ & \times \int dx' \exp[-(x - x')^2 / 4g^{xx} t] \rho(x', \xi, 0). \quad (6.9) \end{aligned}$$

The first factor on the right-hand side shows that  $\rho_r(x + \xi/2, x - \xi/2)$  tends to become diagonal in the position basis, as in the degenerate case. The heat kernel in the integral has, however, a very different effect since it smoothes off the reduced density along the diagonal, so that probabilities that

were initially distinct become mixed together. If the process is stopped at some time  $t$ , its effect is analogous to an imperfect measurement of the position.

The smoothing effect is most clearly seen by considering as initial state a superposition of two distinct wave functions,

$$\rho_r(t=0) = |\psi\rangle\langle\psi|, \quad \text{with } |\psi\rangle = |\psi_1\rangle + |\psi_2\rangle, \quad (6.10)$$

the two wave functions  $\psi_1(x)$  and  $\psi_2(x)$  being clearly separated with clearly different average values for  $X$  or  $P$  or both. One is interested in the interference part of  $\rho_r$  originating from  $|\psi_1\rangle\langle\psi_2|$  and  $|\psi_2\rangle\langle\psi_1|$  in the initial state operator, but one must also now consider the probabilistic part originating from  $|\psi_1\rangle\langle\psi_1|$  and  $|\psi_2\rangle\langle\psi_2|$ . The first factor on the right-hand side of Eq. (6.9) suppresses very rapidly the interference terms in  $\rho_r$  when  $\psi_1(x)$  and  $\psi_2(x)$  have well-separated mean values of the position  $X$ . It also suppresses them, although less rapidly when the values of  $\langle X \rangle$  coincide while those of  $\langle P \rangle$  are significantly different [35]. From the standpoint of macroscopic interferences, there is therefore nothing new.

The smoothing integral in Eq. (6.10) introduces a new effect. It mixes together the probabilities for different values of  $\langle X \rangle$ . If the state (6.10) represents, for instance, the state of a pointer after a measurement, two results that would be distinct for an apparatus with degenerate decoherence can become indistinguishable if decoherence is nondegenerate. This conclusion does not depend on the specific form of  $\psi_1(x)$  and  $\psi_2(x)$ . It also holds for coherent states, which are not therefore properly einselected.

### C. A symmetric form of decoherence

A convenient expression of nondegenerate decoherence can be obtained for any number  $n$  of collective variables. One denotes altogether by  $\{\xi^i\}$  the set of the  $2n$  position and momentum variables and the pure decoherence equation becomes

$$\dot{W} = \frac{\partial}{\partial \xi^i} \left( g^{ij} \frac{\partial W}{\partial \xi^j} \right). \quad (6.11)$$

If the decoherence coefficients  $g^{ij}$  are constants, one may introduce the inverse ‘‘covariant’’ coefficients  $g_{ij}$  satisfying the relations  $g^{ij} g_{jk} = \Delta_k^i$ . They exist only in the nondegenerate case. The solution of Eq. (6.11) is then given by

$$\begin{aligned} W(\xi t) = & (\pi t)^{-n} \int \sqrt{g} d^{2n} \eta \exp[-g_{jk}(\xi^j - \eta^j) \\ & \times (\xi^k - \eta^k) / 4t] W(\eta, 0), \quad (6.12) \end{aligned}$$

where  $g$  is the determinant of the matrix with coefficients  $g_{ij}$ , inverse of the matrix of the decoherence coefficients  $g^{ij}$ . It may be useful to notice that Eq. (6.12) remains approximately valid when the decoherence coefficients are not constants but slowly varying [25].

The effect of decoherence is therefore to smear out the Wigner function in phase space. In this approach, the removal of interference terms is due to the fact that an interference term, localized in phase space with a vanishing inte-

gral, is rapidly reduced to zero under smoothing. One may also notice that the results are unchanged under a linear canonical transformation in phase space, at least when the coefficients are constants. They are only slightly modified when the coefficients are slowly varying under a smooth canonical transformation [25].

## VII. MORE ABOUT DEGENERACY

One may now consider the order of magnitude of the decoherence coefficients. It should be stressed first that the condition (3.1) implying diagonalization was most often imposed *a priori* in the construction of models. If one again considers a unique position observable  $X$ , only one decoherence coefficient,  $g^{pp}$ , is different from zero when this condition is satisfied (as shown in Appendix B). Models have revealed a strong connection between the decoherence coefficient  $g^{pp}$  and the friction coefficient  $\gamma^{pp}$ , which appears in the classical limit of the equation of motion when the collective Hamiltonian is  $H_c = P^2/2m + V(X)$ . Classical motion is then governed by

$$\frac{dp}{dt} = -\partial V/\partial x - \gamma^{pp}p. \quad (7.1)$$

As shown in Appendix B, the spectral densities of the coefficients  $g^{pp}$  and  $\gamma^{pp}$  are very similar and, at high enough temperature, the two coefficients have a simple proportionality relation,

$$g^{pp} = mT\gamma^{pp}. \quad (7.2)$$

What should be considered in that case as a high temperature has been discussed by Hu, Paz, and Zhang [7]. The fact that  $g^{pp}$  enters with a denominator  $\hbar^2$  in the expression (6.9) of decoherence implies a strong effect of decoherence as soon as  $\gamma^{pp}$  is not very small, i.e., when there is a possibility of dissipation.

### A. Rough orders of magnitude

Let us consider a model with an environment of oscillators, the collective system being also an oscillator with frequency  $\omega$  [3–8]. One assumes usually a coupling proportional to the collective position  $X$ ,

$$H_1 = X \sum_i (\lambda_i a_i^\dagger + \lambda_i^* a_i),$$

so that the condition (1.3) is satisfied. More generally, one may consider a coupling with the creation and annihilation operators of the collective oscillator in place of  $X$ , i.e.,

$$H_1 = (X - iP/m\omega) \sum_i \lambda_i a_i + (X + iP/m\omega) \sum_i \lambda_i^* a_i^\dagger.$$

According to Appendix B, one has then typically,

$$g^{xx} \approx g^{pp}/m^2\omega^2. \quad (7.3)$$

According to Eq. (6.9), the decoherence time characterizing the vanishing of nondiagonal interference terms separated by a distance  $\Delta x$  is given as usual by

$$t_{dec} = \frac{\hbar^2}{mT\gamma^{pp}\Delta x^2}, \quad (7.4)$$

whereas the characteristic time after which there the probabilities are mixed up for two different positions on the diagonal separated by the same distance  $\Delta x$  is

$$t_{mix} \approx \frac{m\omega^2\Delta x^2}{\gamma^{pp}T}. \quad (7.5)$$

For reference, it may be recalled that the time necessary for the spreading of a wave packet on the same distance is

$$t_{wp} = \frac{m\Delta x^2}{\hbar}. \quad (7.6)$$

For not too small values of  $\Delta x$ , and a generic coupling (i.e., no degeneracy) one has for the various rates: decoherence is much greater than probability mix up that is much greater than wave packet spreading.

### B. On the existence of pointer states

The main conclusion of the previous sections was that the existence of an exact diagonalization basis is not essential for most physical consequences of decoherence. On the other hand, it will be now shown that there is a very large class of physical systems for which such a basis exists.

Coming back to the case when  $X$  denotes a class of  $n$  collective coordinates, there is exact diagonalization in the basis  $|x\rangle$  if the derivatives of the symbol  $\bar{H}_1$  with respect to the canonically conjugate variables  $p$  vanish. One has then according to Eq. (5.6) and Eqs. (B9)–(B11)

$$[H_1, X] = 0, \quad (7.7)$$

$$g^{xp} = g^{xx} = 0. \quad (7.8)$$

Under the same assumptions, according to Eq. (B17)–(B19), the friction coefficients  $\gamma^{px}$  and  $\gamma^{xx}$  also vanish.

When they do not vanish, the classical equations of motion become

$$dx_i/dt = p_i/m_i - \gamma_{ij}^{px} p_j - \gamma_{ij}^{xx} x_j, \quad (7.9)$$

$$dp_i/dt = F_i - \gamma - i j^{pp} p_j - \gamma_{ij}^{px} x_j, \quad (7.10)$$

where  $F_i$  denotes a force.

These equations look rather unusual and it is important to understand why they are exceptional (or unrealistic). In the case of a mechanical system (with no macroscopic electromagnetic effects) we are familiar with a unique type of friction coefficient ( $\gamma^{pp}$ ) and of decoherence coefficient ( $g^{pp}$ ). The reason was clearly shown by Gell-Mann and Hartle [13], who used as position observables the hydrodynamical variables resulting from a coarse graining. The corresponding

variables can be identified with the center-of-mass positions  $x_i$  of small pieces of matter, small enough from a macroscopic standpoint although containing a large number of atoms. The key feature is then the nonrelativistic form of the Hamiltonian for the particles of matter,

$$H = \sum [p_\alpha - A(x_\alpha)]^2 / 2m_\alpha + \sum V(x_\alpha - x_\beta),$$

where the summations are performed over the particles (indicated by Greek indices). If there is no macroscopic magnetic field (so that one can neglect the magnetic potential  $A$ ), one of the Heisenberg equations of motion, yields the following simple relation between the classical velocity and momentum (denoted by Latin indices)

$$\dot{x}_i = p_i / m_i.$$

Comparing this with Eq. (7.9), one sees that  $\gamma^{px} = \gamma^{xx} = 0$  and, from Eq. (B16), one may expect that  $g^{xp} = g^{xx} = 0$ . Equations (7.9) and (7.10) strongly suggest that this property follows from the Galilean invariance of nonrelativistic mechanics under a change of reference system.

Strangely enough, no realistic example of the nondegenerate case has yet been proposed, except tacitly in unprecise measurements. Examples might be expected, however, in electromagnetic systems (where the magnetic and electric fields replace position and conjugate momentum) but the prospect of producing quantum superpositions of fields and see their decoherence seems rather remote. One must probably attribute the rarity of examples to the fact that decoherence has been mostly studied in the framework of measurement theory. There is almost always (or always) in that case some mechanical part of some apparatus that is entangled with the measurement result and the rest of the system, and it enforces its own einselection on them.

## VIII. CLASSICAL BEHAVIOR

### A. The derivation of classical behavior

Decoherence is in most cases immediately followed by a classical behavior of the collective subsystem [4,10,12,23]. Although this property will not be analyzed in detail in the present work, a few points involving again the problem of einselection are worth mentioning.

Decoherence is described in the nondegenerate case by Eq. (6.12) involving a smearing effect on the Wigner function  $W(x,p)$ . An important consequence is to make this function non-negative so that its interpretation as a density probability in phase space becomes significant [36]. As far as orders of magnitude are concerned, one may consider that a derivative operator  $\partial/\partial x$  acting on  $W$  is of the order of  $(g^{xx}t)^{-1/2}$  for  $t$  large enough (i.e., when decoherence is effective) whereas  $\partial/\partial p$  is of the order of  $(g^{pp}t)^{-1/2}$ . One may then consider more carefully the first term in the master equation (4.6) giving the following contribution to the master equation:

$$\dot{\rho}_r = -\frac{i}{\hbar}[H_c, \rho_r]. \quad (8.1)$$

One can write down this equation in terms of the Wigner function and the Hamilton function  $h(x,p)$ , which are, respectively, the symbols of  $\rho_r$  and of  $H_c$ . It reads to second order in  $\hbar$ ,

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{\partial h}{\partial p} \frac{\partial W}{\partial x} + \frac{\partial h}{\partial x} \frac{\partial W}{\partial p} + \frac{\hbar^2}{24} \left\{ \frac{\partial^3 h}{\partial p^3} \frac{\partial^3 W}{\partial x^3} - 3 \frac{\partial^3 h}{\partial x \partial p^2} \frac{\partial^3 W}{\partial p \partial x^2} \right. \\ & \left. + 3 \frac{\partial^3 h}{\partial p \partial x^2} \frac{\partial^3 W}{\partial x \partial p^2} - \frac{\partial^3 h}{\partial x^3} \frac{\partial^3 W}{\partial p^3} \right\}. \end{aligned} \quad (8.2)$$

One recognizes in the first term on the right-hand side a Poisson bracket of the Hamilton function and the probability density, in agreement with classical physics. This term generates a classical evolution of the Wigner function as if its arguments  $(x,p)$  were moving according to the classical Hamilton equations.

The order of magnitude of the  $W$  derivatives resulting from Eq. (6.12) imply that higher-order corrections in  $\hbar$  are negligible so that after some decoherence the evolution becomes classical. It is somewhat paradoxical that the analysis is more involved in the degenerate case [10]. The difficulty arises from a linear superposition of two initial wave functions with the same  $x$  location but different average values of  $p$ . The destruction of interferences must then wait till the motion due to the difference in the values of  $\langle P \rangle$  separates the wave functions in  $x$  space. A conspiracy of decoherence with the collective dynamics is therefore necessary for producing finally a classical behavior.

### B. Classicality and the choice of a collective subsystem

The previous conclusion of a classical behavior assumed tacitly that the derivatives of the Hamilton functions are not large, but one might then get involved in a circular argument. The collective observables are chosen ordinarily on empirical grounds, from a direct knowledge of the system. One says: ‘‘I look at the system and I clearly see how it can be described by some coordinates, which I replace by quantum observables.’’ Then one concludes after much work: ‘‘See, the description of the system with these variables becomes finally classical.’’ This is certainly not a proof of classicality resting on the basic principles of quantum mechanics, but only a check of consistency. Classical behavior can be proved when the convenient variables for describing it have been selected by means of one’s classical intuition.

The question ‘‘how does one select a collective subsystem?’’ is therefore prior to the question of einselection. One can then look at Eq. (8.2) from a different standpoint. It should give a criterion for choosing the collective observables and not provide a proof that they describe a classical motion. This criterion implies that the derivatives  $\partial/\partial x$  and  $\partial/\partial p$  of the classical Hamilton function in the second and higher terms of Eq. (8.2) are not controlled by factors involving some power of  $\hbar^{-1}$ .

This gross criterion can be presumably much refined in view of Fefferman’s formulation of quantum mechanics through pseudodifferential calculus (microlocal analysis) [37]. He investigated the eigenstates of the complete Hamiltonian  $H$  of an arbitrary quantum system by analyzing its symbol  $\bar{H}$  in the phase space of the constituent particles and, by cutting this space into “distorted boxes,” he was able to diagonalize  $H$  approximately. This is a deep result of abstract mathematics but there has been no direct application of it in physics. Nevertheless, it means that there exists one (or several) privileged way of cutting phase space, into well-defined boxes, according to the possible states of the system. One could then envision that a pair of variables  $(x,p)$  is collective if it defines locally a two-dimensional plane along which  $\bar{H}$  varies very slowly. Such a property is strongly suggested by Feffermann’s construction and it agrees with the small derivatives we just found characterizing classical behavior after decoherence. One may also presume the existence of a whole hierarchy of collective two directions, which would be ordered according to the magnitude of the derivatives.

I will not try to elaborate further on this idea, which was proposed some years ago, although not much progress has been made since [26]. It represents, however, an alternative to Zurek’s predictability sieves (with which it may be related). In any case, it stresses again that the most important problem in a real understanding of decoherence is an explicit construction of the collective observables (with a corresponding explicit definition of the environment). This is closely related with a search for a real theory of the Heisenberg frontier, as also noticed by Zurek [10].

### C. Einselection

Zurek’s concept of predictability sieves was applied successfully to the case of an underdamped collective oscillator interacting with an environment of oscillators [17,40–43]. It was found that Gaussian pure states with various average values  $(x,p)$  of position and momentum are selected in that case as the best carriers of information, suggesting more generally that some sort of coherent states would be einselected by decoherence just before classical motion. There is something puzzling, however, in the fact that the width of these Gaussian states is controlled by the parameters  $(m,\omega)$  of the collective oscillator (it has the same width as the ground-state wave function of the oscillator). When looking at Eq. (6.12), one finds on the contrary that decoherence in the nondegenerate case is insensitive to the characteristics of the collective Hamiltonian and it is completely determined by the coupling Hamiltonian through the decoherence coefficients.

It may be recalled in this connection that a convenient family of einselected states was proposed earlier, although this name was not used [38,39]. These states are closely related to Hörmander’s notion of microlocal projection operators. The symbol  $\bar{P}(x,p)$  of such an operator is zero outside a regular cell  $C$  in the  $(x,p)$  phase space (i.e., a cell whose volume and boundary shape have large characteristic dimensions in terms of the Planck constant).  $\bar{P}(x,p)$  is equal to 1

in  $C$ , except near the boundary where it goes smoothly to zero. The corresponding operator  $P$  is practically a projection [25].

Consider then the integrand of Eq. (6.12) for definite values of  $t$ ,  $\xi=(x,p)$  and  $\eta=(x',p')$ ,

$$\bar{Z}(\xi) = (\pi t)^{-n} \sqrt{g} \exp[-g_{jk}(\xi^j - \eta^j)(\xi^k - \eta^k)/4t]. \quad (8.3)$$

It can be considered as the symbol of a density operator  $Z$  originating at a time  $t$  large enough through nondegenerate decoherence from an initial state localized in the neighborhood of  $\eta$ . Using Eq. (5.6), one finds that  $PZ=Z$  if the cell  $C$  contains a manifold with equation

$$g_{jk}(\xi^j - \eta^j)(\xi^k - \eta^k)/4t = a$$

for a large enough value of  $a$ . (This property remains valid when the decoherence coefficients  $g^{ij}$  are not constant but smoothly varying.)

This means that the normalized mixed states with density matrix  $P/\text{Tr} P$  satisfy the criteria for einselected states. This includes their sifting through predictability sieves [10], since  $\text{Tr} \Xi^2(t) \approx 1$  for a reduced density matrix  $\Xi$  such that  $\Xi(0) = P/\text{Tr} P$ . The sketch of the proof consists in separating diagonalization and mixing according to Eq. (6.9) through a canonical transformation maximizing the rate of diagonalization. The sifting property follows when  $t$  is such that diagonalization has already taken place in the cell  $C$  whereas mixing has not spilled outside  $C$ . This is valid for nondegenerate and degenerate decoherence.

One can then identify einselected states in general with the classically meaningful states, which are defined either as classical properties through the projections  $P$  [39,44] or as quantum states by the density operators  $P/\text{Tr} P$ . The predictability sieve criterion is universally valid. Its stability under a change of definition for the collective subsystem and the environment (i.e., under a shift of Heisenberg’s frontier) cannot be proved, however, along the same lines as long as no objective definition of the collective observables has been found.

## IX. CONCLUSIONS

As suggested by its name, decoherence is a loss of correlation between local phases of a system involving a large number of constituents. It may take in principle many different aspects because “in principle” the set of states of a quantum system is enormous, even much more than its Hilbert space. Empirical physics is, however, interested in the systems really occurring in nature or built in the laboratory, which can be measured or observed.

A wide gap between theory and practice is our inability to characterize mathematically these “real” systems [12]. There is a wide agreement that they always involve some “collective” degrees of freedom but the problem of their definition from first principles is not yet solved. The study of decoherence will probably remain semiempirical as long as the program suggested in Sec. VIII, or an equivalent one, is not completed.

The practical results of the present study were concerned with the three main aspects of decoherence: suppression of macroscopic interferences, einselection, and later classical behavior.

The suppression of macroscopic interferences is a general feature. The interference terms disappear for two collective wave functions with a large enough difference in the average values of position or momentum (or both).

Einselection is the election of definite states representing exclusive events with well-defined probabilities. It is essential in measurement theory and its properties were the main purpose of this paper. Two different cases had to be distinguished, which were, respectively, called degenerate and nondegenerate.

There is something puzzling in this dichotomy if one does not distinguish also between what is most general (or frequent) either from the standpoint of a mathematical theory or of empirical physics. A very large class of physical systems leads to the degenerate form of einselection, which is practically a diagonalization of the reduced density matrix in the basis originating from the collective position coordinates. These systems are truthfully described by hydrodynamical variables after coarse graining [12,13]. Although this condition is still restrictive, it turns out in practice that the mechanical parts of a physical system, which are described by these variables are entangled most often with other degrees of freedom so that degeneracy (with diagonalization) is extended to them. A simpler way of saying this is that most observations and measurements involve or could involve a reading of the position of some mechanical “pointer,” imposing diagonalization as the outcome of decoherence.

A sufficient condition for degeneracy is given by the well known Eq. (1.3), which covers the hydrodynamical case. It is very restrictive, however, from a mathematical standpoint and, in the absence of a criterion defining a realistic system, one had also to investigate the general case of nondegenerate decoherence. The results did not quite agree with the conjecture of predictability sieves [10]. One found a tendency of decoherence to combine an approximate diagonalization with a partial lumping of probabilities rather than a clear mutual exclusion of events, which is typical of unprecise measurements.

The situation was clearer when one looked at the classical behavior after decoherence. There is a simple way to reconcile the present results with the Zurek’s predictability criteria [10]. It consists in identifying the einselected states with the mixed states representing classical properties, which I proposed earlier [44]. The fact that these states are best defined by the mathematics of microlocal analysis [25], as well as Fefferman’s promising approach to the definition of collective observables [37], indicate in my opinion that this framework is the right one.

## APPENDIX A: DECOHERENCE AS AN IRREVERSIBLE PROCESS

### 1. Auxiliary densities

The simplest way for computing the quantities  $s_i$  for decoherence consists in using the observables  $(|k\rangle\langle k'|)$

$+|k'\rangle\langle k|)\otimes I_e$  and  $(1/i)(|k\rangle\langle k'| - |k'\rangle\langle k|)\otimes I_e$  (for  $k \neq k'$ ,  $k > k'$ ) together with the diagonal terms  $|k\rangle\langle k|\otimes I_e$ . They will be denoted altogether by  $A^j$  and they satisfy the relations

$$\text{Tr}_c A^j A^{j'} = \delta^{jj'} \quad (j, j' \neq 1, e). \quad (\text{A1})$$

Rather than the exponential form (2.4) for the test density operator, it is convenient to write it as

$$\rho_0 = \left( \sum_{j \neq 1, e} a^j A^j \right) \otimes \rho_e. \quad (\text{A2})$$

From Eqs. (A1), one sees that the coefficients  $a^j$  in Eq. (A2) are the average values of the observables  $A^j$ . Therefore

$$\partial \rho_0 / \partial a^j = A^j \otimes \rho_e \quad (j \neq 1, e). \quad (\text{A3})$$

After writing  $\rho_0 = \exp(-\alpha - \beta H_e)$ , one obtains

$$\begin{aligned} \partial \beta / \partial E &= -\Delta^2, \quad \partial \alpha / \partial E = E / \Delta^2, \quad \partial \rho_e / \partial \alpha = -\rho_e, \\ \partial \rho_e / \partial \beta &= -H_e \rho_e \end{aligned} \quad (\text{A4})$$

[where  $\Delta$  is defined by Eq. (3.8)]. In view of the definition (2.5) for the auxiliary densities [or equivalently the definition (2.8) of the projection  $P$ ], their expression (3.5)–(3.9) in Sec. III follows immediately from Eqs. (A3) and (A4).

### 2. The evolution equations

In the first evolution equation (2.13), one can compute  $PL\rho_1$  by applying the expression (3.9) giving  $P$  to  $L\rho_1 = -(i/\hbar)[H, \rho_1]$ . Two traces  $\text{tr}[H, \rho_1]$  and  $\text{Tr}(H_e[H, \rho_1])$  enter in the result. Using cyclic invariance of traces together with Eq. (3.10) specifying  $H_1$  and

$$\rho_1 = \rho_r \otimes \rho_e, \quad (\text{A5})$$

one finds that

$$\text{tr}[H, \rho_1] = [H_c, \rho_r],$$

$$\text{Tr}(H_e[H, \rho_1]) = \text{Tr}([H_e, H], \rho_1) = \text{Tr}([H_e, H_1], \rho_1).$$

Therefore

$$\begin{aligned} PL\rho_1 &= (-i/\hbar) \left\{ [H_c, \rho_r] \otimes \rho_e + I_c \otimes \rho_e \frac{H_e - E}{\Delta^2} \right. \\ &\quad \left. \times \text{Tr}(H_e[H_1, \rho_1]) \right\}. \end{aligned} \quad (\text{A6})$$

In order to compute  $\dot{P}\rho_1$ , one remarks that although the quantities  $\rho_e$ ,  $E$ , and  $\Delta$  in Eq. (3.9) are time dependent, the quantity  $\text{Tr}(H_e \rho_1) - E \text{Tr} \rho_1$  vanishes so that one has

$$\dot{P}\rho_1 = \rho_r \otimes \dot{\rho}_e - \dot{E} I_c \otimes \rho_e \frac{H_e - E}{\Delta^2}. \quad (\text{A7})$$

An identical result is obtained for  $\dot{P}\rho$ , so that

$$\dot{P}\rho_2 = 0. \quad (\text{A8})$$

One thus gets the first evolution equation

$$\dot{\rho}_1 = PL\rho_1 + \dot{P}\rho_1 + PL\rho_2, \quad (\text{A9})$$

with the expressions (A6) and (A7) for the first two terms whereas  $PL\rho_2$  is given by Eq. (3.9).

It is convenient to split this equation into one for  $\dot{\rho}_r$  and another for  $\dot{\rho}_e$  (or equivalently for  $\dot{E}$ ). This is obtained by taking, respectively, the trace of Eq. (A9) with respect to the environment and the collective Hilbert space. The environment trace of the second term on the right-hand side of Eq. (A6) vanishes, as well as  $\text{tr} \dot{P}\rho_1$  (because  $\text{tr} \dot{\rho}_e = 0$ ). According to Eq. (3.9), the environment trace of  $PL\rho_2$  reduces to

$$-\frac{i}{\hbar} \text{tr}[H, \rho_2] = -\frac{i}{\hbar} \text{tr}[H_1, \rho_2],$$

where the second equality results from the vanishing of  $\text{tr}[H_e, \rho_2]$  (as the trace of a commutator) and of  $\text{tr}[H_c, \rho_2]$  (because of  $\text{tr} \rho_2 = 0$ ). One obtains thus the basic equation

$$\dot{\rho}_r - \frac{i}{\hbar} ([H_c, \rho_r] + \text{tr}[H_1, \rho_2]). \quad (\text{A10})$$

The trace of Eq. (A9) on the collective Hilbert space reduces to a (potentially infinite) term  $(\text{Tr}_c I_c) \rho_e (H_e - E)$ , multiplied by a number, which must then vanish so that

$$\dot{E} = -\frac{i}{\hbar} \text{Tr}(H_e [H_1, \rho_1 + \rho_2]) = -\frac{i}{\hbar} \text{Tr}(H_e [H_1, \rho_2]), \quad (\text{A11})$$

the last equality resulting from  $\text{Tr}(H_e [H_1, \rho_1]) = \text{Tr}(H_1 [H_e, \rho_1])$ , whereas

$$[H_e, \rho_1] = 0, \quad (\text{A12})$$

since  $\rho_e$  is a function of  $H_e$ .

### 3. The second evolution equation

One can now write down the evolution equation (2.14) for  $\rho_2$ , which is formally

$$\dot{\rho}_2 = QL\rho_2 + QL\rho_1 - \dot{P}\rho_1 \quad (\text{A13})$$

[after taking Eq. (A8) into account]. This will be done according to Sec. IV by considering  $H_1$  as a perturbation. One needs only to compute  $\rho_2$  at first order in  $H_1$  and some terms in Eq. (A13) can be therefore immediately neglected. For instance  $\dot{P}\rho_1$ , as given by Eq. (A7), is negligible because  $\dot{E}$  is of second order [according to Eq. (A11)] and furthermore,

$$\dot{\rho}_e = -\dot{\beta}(H_e - E)\rho_e = \dot{E}\Delta^{-2}(H_e - E)\rho_e \quad (\text{A14})$$

is also of second order [the second equality resulting from Eq. (A4)]. One can also neglect the commutator  $[H_1, \rho_2]$  in  $L\rho_2$  as being of second order.

Let us now consider the quantity  $QL\rho_1 = L\rho_1 - PL\rho_1$ . One has

$$L\rho_1 = -(i/\hbar)[H, \rho_1] = -(i/\hbar)[H_c + H_1, \rho_1], \quad (\text{A15})$$

where the second equality results from Eq. (A12). Then

$$PL\rho_1 = \text{tr}(L\rho_1) \otimes \rho_e + \Delta^{-2}(I_c \otimes H_e - E) \times \rho_1 \{ \text{tr}(I_c \otimes H_e L\rho_1) - E \text{Tr}(L\rho_1) \}. \quad (\text{A16})$$

The last term  $\text{Tr}(L\rho_1)$  vanishes (as a trace of a commutator). The preceding term also vanishes since

$$\begin{aligned} \text{Tr}(I_c \otimes H_e L\rho_1) &= -(i/\hbar) \text{Tr}(I_c \otimes H_e [H, \rho_1]) \\ &= (i/\hbar) \text{Tr}(H [I_c \otimes H_e, \rho_1]) \end{aligned}$$

and the last commutator vanishes. Therefore

$$\begin{aligned} PL\rho_1 &= (-i/\hbar) \text{tr}[H, \rho_1] \otimes \rho_e = (-i/\hbar) [JH_c, \rho_r] \otimes \rho_e \\ &= (-i/\hbar) [H_c \otimes I_e, \rho_1], \end{aligned}$$

where the second equality results from Eqs. (3.10) and (A12). The first term in  $L\rho_1$  as given by Eq. (A15) is therefore cancelled and one is left with the simple equation

$$\dot{\rho}_2 = -(i/\hbar)[H_0, \rho_2] - (i/\hbar)[H_1, \rho_1], \quad (\text{A17})$$

where  $H_0$  is the uncoupled Hamiltonian,

$$H_0 = H_c \otimes I_e + I_c \otimes H_e. \quad (\text{A18})$$

## APPENDIX B: DECOHERENCE AND DISSIPATION

### 1. Derivation of Eq. (5.8)

According to Eq. (5.2), one must evaluate at lowest order in  $\hbar$  the symbol  $\bar{D}$  of the collective operator

$$\begin{aligned} D &= -(1/\hbar)^2 \text{tr}\{H_1, [H_1^T, U(t-t')\rho_r(t') \otimes \rho_e(t') \\ &\quad \times U^{-1}(t-t')]\}. \end{aligned} \quad (\text{B1})$$

Since  $U(t) = U_c(t) \otimes U_e(t)$  [with  $U_c(t) = \exp(-iH_c t/\hbar)$  and  $U_e(t) = \exp(-iH_e t/\hbar)$ ], one can slightly simplify the density operator by writing

$$\begin{aligned} U(t-t')\rho_r(t') \otimes \rho_e(t') U^{-1}(t-t') \\ = U_c(t-t')\rho_r(t') U_c^{-1}(t-t') \otimes \rho_e(t'), \end{aligned} \quad (\text{B2})$$

in view of the equality [resulting from Eq. (A14) and valid up to order  $H_1^2$ ]

$$U_e(t-t')\rho_e(t') U_e^{-1}(t-t') \approx \rho_e(t').$$

Letting  $A$  and  $B$  be two arbitrary operators,  $\bar{A}(x, p)$  and  $\bar{B}(x, p)$  their operator-valued symbols, Eq. (5.5) gives the symbol of the commutator  $[A, B]$ , with the notation of Sec. V,

$$(-i\hbar/2)(\bar{A}_p \bar{B}_x - \bar{A}_x \bar{B}_p - \bar{B}_p \bar{A}_x + \bar{B}_x \bar{A}_p) + O(\hbar^3). \quad (\text{B3})$$

Equation (B3) can be used twice for obtaining the symbol of the double commutator in Eq. (B1). The symbol of the op-

erator  $U_c(t-t')\rho_r(t')U_c^{-1}(t-t')$ , which will be denoted by  $W^T$  is an ordinary function and it commutes with the operator-valued symbols  $\bar{H}_1, \bar{H}_1^T$  and their derivatives. After a straightforward calculation, one gets

$$\begin{aligned} \bar{D} = & \int_{-\infty}^t dt' \left( \frac{\partial}{\partial x} (C^{xx} W_x^T + C^{xp} W_p^T) \right. \\ & \left. + \frac{\partial}{\partial p} (C^{px} W_x^T + C^{pp} W_p^T) \right). \end{aligned} \quad (\text{B4})$$

The coefficients are given by

$$C^{xx} = \frac{1}{2} \text{tr} \{ (\bar{H}_p \bar{H}_p^T + \bar{H}_p^T \bar{H}_p) \rho_e \}, \quad (\text{B5})$$

$$C^{xp} = -\frac{1}{2} \text{tr} \{ (\bar{H}_p \bar{H}_x^T + \bar{H}_x^T \bar{H}_p) \rho_e \}, \quad (\text{B6})$$

$$C^{px} = -\frac{1}{2} \text{tr} \{ (\bar{H}_x \bar{H}_p^T + \bar{H}_p^T \bar{H}_x) \rho_e \}, \quad (\text{B7})$$

$$C^{pp} = \frac{1}{2} \text{tr} \{ (\bar{H}_x \bar{H}_x^T + \bar{H}_x^T \bar{H}_x) \rho_e \}. \quad (\text{B8})$$

## 2. Explicit expressions

The decoherence coefficients after neglecting retardation are obtained by integrating the coefficients (B5)–(B8) on the time  $t'$ . It is convenient to introduce the matrix elements of  $\bar{H}_1$ ,

$$\langle n | \bar{H}_{1i}^T | n' \rangle = \bar{H}_{1inn'} \exp(-i\omega_{nn'}\tau),$$

where the index  $i$  denotes either  $x$  or  $p$ ,  $\tau = t - t'$ , and  $\bar{H}_{1inn'} = \langle n | \bar{H}_{1i} | n' \rangle$ . One has then

$$\begin{aligned} & \frac{1}{2} \text{tr} \{ (\bar{H}_i \bar{H}_j^T + \bar{H}_j^T \bar{H}_i) \rho_e \} \\ & = \sum_{nn'} \bar{H}_{1inn'} \bar{H}_{1jn'n} \exp(i\omega_{nn'}\tau) p_{nn'} \cosh(\beta\hbar\omega_{nn'}/2). \end{aligned}$$

The decoherence coefficients

$$g^{ij} = \int_0^\infty d\tau C^{ij}(\tau)$$

are then given by

$$\begin{aligned} g^{xx} = & \int_0^\infty d\tau \sum_{nn'} \bar{H}_{1pnn'} \bar{H}_{1pn'n} \exp(i\omega_{nn'}\tau) p_{nn'} \\ & \times \cosh(\beta\hbar\omega_{nn'}/2), \end{aligned} \quad (\text{B9})$$

$$\begin{aligned} g^{px} = g^{xp} = & - \int_0^\infty d\tau \sum_{nn'} \bar{H}_{1pnn'} \bar{H}_{1xn'n} \exp(i\omega_{nn'}\tau) p_{nn'} \\ & \times \cosh(\beta\hbar\omega_{nn'}/2), \end{aligned} \quad (\text{B10})$$

$$\begin{aligned} g^{pp} = & \int_0^\infty d\tau \sum_{nn'} \bar{H}_{1xnn'} \bar{H}_{1xn'n} \exp(i\omega_{nn'}\tau) p_{nn'} \\ & \times \cosh(\beta\hbar\omega_{nn'}/2). \end{aligned} \quad (\text{B11})$$

The quadratic form in two real variables  $(\alpha, \alpha')$  with these coefficients is given by

$$\begin{aligned} & g^{xx} \alpha^2 + 2g^{xp} \alpha \alpha' + g^{pp} \alpha'^2 \\ & = \int_0^\infty d\tau \sum_{nn'} |\bar{H}_{1xnn'} \alpha - \bar{H}_{1pn'n} \alpha'|^2 \cos(\omega_{nn'}\tau) p_{nn'} \\ & \times \cosh(\beta\hbar\omega_{nn'}/2) \end{aligned} \quad (\text{B12})$$

and it is clearly non-negative.

## 3. Dissipation coefficients

Let now  $A_k$  ( $k=1$  or  $2$ ) denote either  $X$  or  $P$ . The time derivatives of their average values are given by

$$\begin{aligned} \frac{d\langle A_k \rangle}{dt} = & \frac{i}{\hbar} \text{Tr}([H, A_k] \rho) = \frac{i}{\hbar} \text{Tr}_c([H_c, A_k] \rho_r) \\ & + \frac{i}{\hbar} \text{Tr}([H_1, A_k] \rho_2). \end{aligned} \quad (\text{B13})$$

The first term is due to collective dynamics and the second one represents dissipation effects. Using Eq. (4.5) for  $\rho_2$ , this dissipative term reads

$$-\frac{i}{\hbar^2} \int_0^\infty d\tau \text{Tr} \{ [H_1, A_k] [H_1^T, U(\tau) \rho_r \otimes \rho_e U^{-1}(\tau)] \}. \quad (\text{B14})$$

Equation (5.7) can be used to replace the collective trace by an integration over phase space of the operator symbol. One can use

$$\overline{[H_1, X]} = -i\hbar \bar{H}_{1p}, \quad \overline{[H_1, P]} = i\hbar \bar{H}_{1x}.$$

When computing the symbol of  $[H_1^T, U(\tau) \rho_r \otimes \rho_e U^{-1}(\tau)]$ , one will retain only the term originating from the Poisson bracket between  $H_1^T$  and either  $U(\tau)$  or  $U^{-1}(\tau)$ , because it can be seen that all the other contributions do not contribute to the phase space integral or are of higher order in  $\hbar$ . Finally, denoting by  $\bar{H}_c(x, p)$  the symbol of  $H_c$  (which is the collective Hamilton function), one gets

$$\begin{aligned} & \overline{[H_1^T, U(\tau) \rho_r \otimes \rho_e U^{-1}(\tau)]} \\ & = \frac{i\hbar}{2} \left\{ (\bar{H}_{1p}^T \rho_e - \rho_e \bar{H}_{1p}^T) V'(x) - (\bar{H}_{1x}^T \rho_e - \rho_e \bar{H}_{1x}^T) \frac{P}{m} \right\} \tau W. \end{aligned}$$

In the semiclassical case, when the Wigner function is slowly varying, Eq. (B13) generates the classical equations of motion, which read [after writing  $(p, x)$  in place of  $\langle P \rangle, \langle X \rangle$  and neglecting retardation),

$$\frac{dp}{dt} = -\bar{H}_{cx} - \gamma^{pp}\bar{H}_{cp} - \gamma^{px}\bar{H}_{cx}, \quad (\text{B15})$$

$$\frac{dx}{dt} = -\bar{H}_{cp} - \gamma^{xp}\bar{H}_{cp} - \gamma^{xx}\bar{H}_{cx}. \quad (\text{B16})$$

The coefficients are explicitly given (after performing a partial integration over the time  $\tau$ ) by

$$\begin{aligned} \gamma^{pp} &= \int_0^\infty d\tau \bar{H}_{1xnn'} \bar{H}_{1xnn'} \exp(i\omega_{nn'}\tau) p_{nn'} \\ &\times [\sinh(\beta\hbar\omega_{nn'}/2)/\hbar\omega_{nn'}], \end{aligned} \quad (\text{B17})$$

$$\begin{aligned} \gamma^{px} &= - \int_0^\infty d\tau \bar{H}_{1xnn'} \bar{H}_{1pn'n} \exp(i\omega_{nn'}\tau) p_{nn'} \\ &\times [\sinh(\beta\hbar\omega_{nn'}/2)/\hbar\omega_{nn'}] \\ &= \gamma^{xp}, \end{aligned} \quad (\text{B18})$$

$$\begin{aligned} \gamma^{xx} &= \int_0^\infty d\tau \bar{H}_{1pnn'} \bar{H}_{1pnn'} \exp(i\omega_{nn'}\tau) p_{nn'} \\ &\times [\sinh(\beta\hbar\omega_{nn'}/2)/\hbar\omega_{nn'}]. \end{aligned} \quad (\text{B19})$$

Comparing these results with Eqs. (B9)–(B11), a strong formal similarity appears between the dissipation and the decoherence coefficients. They are even directly proportional at high enough temperature [when  $T \gg \hbar\Omega$  so that  $\cosh(\beta\hbar\omega_{nn'}/2) \approx 1$  and  $\sinh(\beta\hbar\omega_{nn'}/2) \approx \beta\hbar\omega_{nn'}/2$ ], namely,

$$\gamma^{il} \approx g^{ij}/T. \quad (\text{B20})$$

One may also notice that the dissipation of collective energy  $dE_c/dt$  is always negative (or zero), since the quadratic form with coefficients  $\gamma^{ij}$  is non-negative for the same reason as in Eq. (B12). Finally, the equality  $\gamma^{px} = \gamma^{xp}$  is a special case of the Onsager symmetry relations (24).

## APPENDIX C: PREVIOUS MODELS

Much of our knowledge on decoherence was first obtained from a study of simple models. Since the present theory claims a much wider range, it should at least recover these older results. This will be the topic of the present appendix.

### 1. Oscillator bath

A model of environment consisting of a bath of harmonic oscillators has been much investigated. For an atom interacting with radiation in a cavity, the model is exact and its results have been successfully compared with experiment [1]. The atom is represented in that case by a two-state system. When considering a collective system with position  $X$ , the coupling Hamiltonian is typically written as

$$H_1 = X \left( \sum_i (\lambda_i a_i + \lambda_i^* a_i^\dagger) \right), \quad (\text{C1})$$

where the sum is over all the oscillators,  $\lambda_i$  being a coupling constant,  $a_i$  and  $a_i^\dagger$  their annihilation and creation operators.

It is easy to use this coupling in the formulas of Appendix B and to recover the previously known results. The calculations are essentially trivial and need not be given here explicitly. Perhaps more interesting is the question of the range of this model. In addition to their thorough study of it, Caldeira and Leggett suggested that it should be considered as very general [5]. They start from the fact that the number of energy eigenstates  $|n\rangle$  of the environment is extremely large. They introduce formally an oscillator for each such state [i.e., the index  $i$  will stand for  $n$  in Eq. (C1)]. They notice that a state  $|n\rangle$  is either occupied or not, these two possibilities being represented by the ground state and the first excited state of the associated oscillator. Then they argue that higher excited states of the oscillators will play no role because of the smallness of their probability of excitation. They conclude that an oscillator bath can represent almost any environment.

The argument is, however, erroneous, because the coupling resulting from their proposal would not have the very simple form of Eq. (C1) in general, because transitions  $i \rightarrow j$  with  $i \neq j$  are certainly essential and they do not appear in the Hamiltonian (C1). Moreover, the transitions  $i \rightarrow i$  with a change of occupation number are not correctly represented in a quantity such as

$$\text{tr}(H_1 H_1 \rho_e) = \sum_{nn'} \langle n | H_1 | n' \rangle \langle n' | H_1 | n \rangle \rho_{en}.$$

If the occupied state  $|n\rangle$  is considered as the first excited state  $|i,1\rangle$  of an oscillator, the contribution of  $|n'\rangle = |i,2\rangle$  cannot be omitted from the sum if the Hamiltonian (C1) is used. The interest of a theory ignoring the constraints of the oscillator model cannot therefore be disputed.

### 2. The scattering model

Joos and Zeh have proposed a beautiful model of decoherence, when an object with position  $X$  interacts with a bath of particles [9]. Decoherence appeared then as an accumulation of scattering effects. The resulting master equation looked very similar to one occurring in the oscillator model and this was a very strong hint for some universality in the mathematical expression of decoherence. This universal character has been explained in the present paper, but something would still be missing if the scattering model were not also derived. This derivation is nontrivial so that it will be given explicitly.

Let us consider for definiteness a spherical solid object with center  $X$ . As explained in Sec. III, the pressure exerted on it by the outside gas is included in  $H_c$  so that  $H_1$  represents the effect of random collisions of the outside molecules (or photons) on the sphere. Rather than doing a complete calculation, it will be sufficient to look at one term in Eq. (5.4), namely (with  $\hbar = 1$ ),



$$D_1 = - \int_{-\infty}^t dt' \text{tr}\{H_1 U_c(t-t') \rho_r(t') U_c^{-1}(t-t') \otimes \rho_e H_1^T\}. \quad (\text{C2})$$

One may consider first the case of an environment consisting of particles having the same momentum, in a pure state  $|k\rangle: \rho_e = |k\rangle\langle k|$ . The corresponding wave function is a plane wave  $\exp(ikr)$  and, with this normalization, there is one particle per unit volume. Their flux  $\Phi$  is the velocity  $v$  of the particle and a sum over one-particle states  $|k'\rangle$  amounts to an integration over  $dk/(2\pi)^3$ .

A few remarks are useful.

(1) One can neglect the time evolution factors  $U_c(t-t')$ , which are slowly varying.

(2) Introducing momentum eigenstates  $|p\rangle$  of the object and the outgoing scattering states  $|p,k,out\rangle$  associated with the plane waves  $|p,k\rangle = |p\rangle \otimes |k\rangle$ , one can write

$$\langle p_2, k_2, out | H_1 | p_1, k_1 \rangle = \langle p_2, k_2 | T | p_1, k_1 \rangle \delta(p_1 + k_1 - p_2 - k_2), \quad (\text{C3})$$

where  $T$  is the (off energy-shell) collision matrix for the scattering of a particle on the object.

(3) One can use the invariance of the scattering  $T$  matrix under a change of reference frame. For nonrelativistic values of  $p$  and taking into account the large mass of the object (as compared with the particle mass), a Galilean transformation with small velocity gives

$$\begin{aligned} \langle p_2, k_2 | T | p_1, k_1 \rangle &= \langle p_2 - p_1, k_2 | T | 0, k_1 \rangle \langle p_1, k_1 | T | p_2, k_2 \rangle \\ &= \langle 0, k_1 | T | p_2 - p_1, k_2 \rangle. \end{aligned} \quad (\text{C4})$$

(4) In view of the  $\delta$  function in Eq. (C3), it is enough to know  $k_1$  and  $k_2$  for fixing  $p_2 - p_1$  so that the right-hand side of Eq. (C4) can be written more simply  $T(k_1, k_2)$ . Conversely, using Fourier transforms, one can introduce the states  $|x, k\rangle$  corresponding to a localized object, whereas out states  $|x, k, out\rangle$  involve the same value of  $x$  and a scattered particle. One thus gets

$$\langle x', k_2, out | H_1 | x, k_1 \rangle = T(k_1, k_2) \delta(x - x') \exp\{i(k_1 - k_2)x\}. \quad (\text{C5})$$

This result has two important consequences. It shows that  $H_1$  acts like a function of  $X$ , although this property shows up

only when scattering states are used. The imaginary exponential in the right-hand side is moreover typical of the method that was used by Joos and Zeh.

(5) In view of Eqs. (5.3), and (C3), one has

$$\begin{aligned} \langle x, k_1 | H_1^T | x', k_2, out \rangle &= \exp\{i\omega(t-t')\} \delta(x-x') \exp\{-i(k_1 - k_2)x\} \\ &\times T^*(k_1, k_2), \end{aligned} \quad (\text{C6})$$

where

$$\omega = E(k_2) - E(k_1).$$

(6) When throwing out retardation, the integral on  $t'$  of the imaginary exponential in Eq. (C6) gives  $\pi\delta(\omega) - iP(1/\omega)$ , where  $P$  stands for a Cauchy principal part. It may be shown, however, that another term in  $D$  originating from  $H_1^T \rho_1 H_1$  cancels the principal part and one must keep only therefore the delta part.

Finally, the matrix element  $\langle x | D_1 | x' \rangle$  can be easily computed if one uses the orthonormal set of outgoing states  $\{|k', out\rangle\}$  when computing the trace  $\text{tr}$ . One gets

$$\begin{aligned} \langle X | D_1 | x' \rangle &= \int [dk/(2\pi)^3] \pi\delta(\omega) |T(k, k')|^2 \\ &\times \exp\{i(k - k')(x - x')\} \rho_r(x, x'). \end{aligned} \quad (\text{C7})$$

But the quantity  $dk(2\pi)^{-3} \delta(\omega) |T(k, k')|^2$  has a very simple interpretation. It coincides with the product  $d\sigma\Phi$  of the differential cross-section  $d\sigma$  for the scattering  $k \rightarrow k'$  times the flux  $\Phi$  of the environment particles having the given momentum  $k$ . One can then replace the trivial density matrix  $|k\rangle\langle k|$  by a thermal density and introduce the various different particles in the gas, thus obtaining

$$\langle x | D_1 | x' \rangle = \int \pi d\sigma d\Phi \exp\{i(k - k')(x - x')\} \rho_r(x, x'). \quad (\text{C8})$$

Similar results are obtained for the three other terms in  $D$  but it will not be necessary to push the calculation further since, from there on, it becomes identical with the one by Joos and Zeh. Their method was of course simpler than the present one, as one expects from an intuitive approach compared to a technical one. The present calculation shows, however, how universal and versatile the fundamental master equation (4.6) is.

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