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General theory of the decoherence effect in quantum mechanics

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The decoherence effect, which may be held responsible for the vanishing of macroscopic quantum interferences, has only been exhibited in special models though it is presumed to be universal (at least when there is a possibility of dissipation). A more general model encompassing the already known ones is proposed in the present work. A master equation for the reduced density operator is established by means of two different methods. A direct method, which is given first, is simple but too specific. A second method relies on the projection method in the theory of irreversible processes. It is in principle very general and not confined to a special model. It shows that decoherence is a typical irreversible process from a theoretical standpoint. The master equation is worked out in detail when there exist convenient, so-called microstable collective observables (for which a criterion is given), selecting a preferred basis in which diagonalization occurs. For macroscopic mechanics, this basis is given by the position coordinates in three-dimensional space of relatively small parts in an object. Previously proposed models, including the quantum diffusion model, are found to be special cases of the present theory. [S1050-2947(97)08609-5]

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I. INTRODUCTION

The decoherence effect is a mechanism destroying quantum interferences at a macroscopic level. It has remarkable analogies with irreversible processes as they are known in thermodynamics. The two kinds of effects occur only in a macroscopic system in which a relatively small number of degrees of freedom are accessible to observation. These degrees of freedom parametrize a ‘‘collective’’ or ‘‘relevant’’ subsystem for which new rules of physics emerge from an inner complexity. It therefore seems interesting to look at decoherence with the methods that have been successful for irreversible processes.

For explaining most simply the decoherence effect, one may think of the wave function of a macroscopic system as a function $\psi(x,y)$, where x can be observed (being, e.g., the position of a pointer or similar collective quantities), whereas the many variables y representing microscopic observables cannot all be measured. One can then express grossly the decoherence effect by considering the various functions of y one obtains associated with different fixed values of x: They tend to become orthogonal as time increases, because they are too complex for keeping mutual coherence for every value of y, even if they had some coherence at the beginning. The destruction of quantum interferences when observing x is a direct consequence of this inner orthogonality. It is often vividly described by saying that, after decoherence, Schrödinger's cat must be either dead or alive and cannot be seen as a superposition of ‘‘dead’’ and ‘‘alive’’ states.

A convenient mathematical formulation consists in introducing the density operator $D=|\psi\rangle\langle\psi|$ of the whole system and the reduced density operator

$$\rho_c(x',x)=\int \psi(x',y)\psi^*(x,y)dy=\langle x'|\mathrm{Tr}_e D|x\rangle, \tag{1.1}$$

where the formal subsystem that is described by y is called the ‘‘environment’’ and Tr_e means a partial trace over it. Taking the trace in Eq. (1.1) is equivalent to a nonobservation of the environment.

The importance of taking the environment into account in a quantum measurement has been realized early and almost since the beginnings of quantum mechanics (see, for instance, [1]). Its effect was investigated as a source of noise [2] before being identified with a phase loss by Zeh [3]. One may consider as an example the case when the total Hamiltonian of the system is

$$H=H_c\otimes I_e+I_c\otimes H_e+H_1, \tag{1.2}$$

I_c and I_e being the unit operators in the Hilbert spaces $\mathcal{H}_c$ and $\mathcal{H}_e$, where the index c denotes the collective (or relevant, or reduced) subsystem and e the environment. The interaction coupling H_1 is then held to be responsible for noise, dissipation, and decoherence. The common origin for the first two effects results in the fluctuation-dissipation theorem [4,5]. Other similarities were also found for decoherence.

These similarities were apparent in the solution of specific models [6]. Particularly important is a model where the environment is represented by a collection of harmonic oscillators and H_1 is linear in the canonical variables (p,q) of the oscillators [7–14]. This model can be solved explicitly because of the simple properties of harmonic oscillators, allowing, for instance, explicit Feynman path integration [15]. Decoherence results from a ‘‘master equation’’ one finds for ρ_c, namely,

$$\left\langle x'\left|\dot{\rho}_c-\frac{1}{i\hbar}[H_c,\rho_c]\right|x\right\rangle=-\mu(x'-x)^2\rho_c(x',x) -(\gamma/2)(x'-x)(\partial/\partial x'-\partial/\partial x) \times\rho_c(x',x). \tag{1.3}$$

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The ‘‘decoherence coefficient’’ μ is very large and it is related to the friction coefficient γ (occurring in the classical relation $\dot{v}=-\gamma v$) by

$$\mu=\gamma(mT/\hbar^2), \tag{1.4}$$

in the special case when $H_c=P^2/2m+V(x)$, T being the absolute temperature (supposed to be high enough) in energy units. This occurrence of temperature and the proportionality of the two coefficients for decoherence and friction indicate an intimate relation between the two effects and a relation with irreversible processes. Most important is the very small denominator $\hbar^2$ in Eq. (1.4) showing a tremendous efficiency of decoherence: $\rho_c(x',x)$ becomes very rapidly ‘‘almost diagonal’’ though complete diagonality is forbidden by energy conservation and is limited by the commutator in the left-hand side of Eq. (1.3) [16,17].

The importance of a preferred ‘‘pointer’’ basis for diagonalization was emphasized by Zurek [18–20], who made clear its relation with measurement processes. Another important contribution was made by Joos and Zeh [21], who considered another model of environment consisting of an external gas of (atmosphere) molecules or photons. They obtained a master equation practically identical with Eq. (1.3). In view of the very different models of environment that had been used, these converging results strongly suggest that there should exist a general theory of the effect, relying on no detailed assumptions about the environment except for the large number of degrees of freedom. One would expect some sort of decoherence-dissipation theorem as an outcome of such a theory.

The search for such a general theory is motivated by the essential role of decoherence in the consistency of an interpretation of quantum mechanics [22–27], by some questions raised about the meaning of decoherence in ‘‘fundamental’’ physics [28–30], and, of course, by the experimental evidence for the effect. It was often said that decoherence is the most efficient effect in physics, to a point where observation always comes too late, after the effect has reached completion. Some strong indications for the effect in action have first been seen in superconducting quantum interference devices (SQUID’s) [31] and it has now been observed unquestionably in quantum optics [32]. The aim of the present work is to propose the necessary general theory, or at least the correct framework for it.

Does one need a general theory or does it already exist? Caldeira and Leggett (in [9], Appendix C) have shown that the oscillator model can sometimes apply for nontrivial reasons and therefore have a larger range of application than expected. In the case of a superconductor, they noticed that one can formally associate an oscillator with each energy level E_n of the environment, with a frequency E_n/h. These ideal oscillators represent a non-occupied or occupied energy level E_n if they are in their ground state or first excited state and, in view of the very large number of energy levels, the formal oscillators have a negligible probability to be in a higher excited state. This remark is helpful for justifying the theoretical analysis of the Paris experiment [32]. One must be careful, however, not to extend this idea too far. Though one can always use a model of environment by ideal oscillators, their external coupling H_1 is only exceptionally linear in the oscillator variable (p,q)’s, as one may check easily in the case of a gaseous environment.[1] It would therefore be an error to believe that the oscillator model has a really large range of applicability and, too often, the success of its results has been wrongly attributed to its own validity. It will be shown that in fact Eq. (1.3) *is* rather general, much more than the model through which it was discovered.

Before entering into more formal considerations, it may be useful to introduce a simple example, as follows. A gedanken piston, with mass m, has only one degree of freedom, which may be taken as its position x. A spring acts on the piston so that $H_c=P^2/(2m)+U(x)$. The piston can move inside an ideal cylinder (a geometric abstraction) containing a gas, which constitutes the environment. The piston can keep the gas molecules on one side if the interaction Hamiltonian H_1 is equal to $\Sigma_J v(x-x_j)$, where the summation goes over the gas molecules and v is a sufficiently repulsive potential. This example will be used for making some ideas clearer.

Most of the present paper will be concerned with the model given by the Hamiltonian (1.2). The theory will be given in two different ways, opposing simplicity and generality. It will first be described according to the easiest approach, through which it was discovered. The idea was to try using a density operator

$$D_0=\rho_c\otimes\rho_e, \tag{1.5}$$

where ρ_c is the exact reduced density and ρ_e is formally an equilibrium density

$$\rho_e=\exp[-\beta(H_e-F)]. \tag{1.6}$$

The quantities β and F are determined by the conditions

$$\mathrm{Tr}_e\rho_e=1, \quad E_e\equiv\mathrm{Tr}_e(H_e\rho_e)=\mathrm{Tr}(H_eD), \tag{1.7}$$

where Tr_e means a trace over the environment Hilbert space $\mathcal{H}_e$ and Tr means a complete trace. Equations (1.7) mean that the correct value of the environment energy E_e is obtained from D_0. One should notice, however, that this energy, in our example, fluctuates with the inelastic collisions of the piston with gas molecules. The parameters β and F therefore fluctuate. Their time average may also change because of dissipation, though at a much slower pace. It should be stressed in any case that *one does not assume the environment to be really in thermal equilibrium* and the introduction of ρ_e is no more than a mathematical device.

The assumptions of the model we use are contained in Eq. (1.2) and in the following condition for applying perturbation calculus: Our example indicates why H_1 is most often too large for a perturbation: the repulsive potential v between the

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[1] For an environment consisting of a bath of independent particles, let one denote by $|pi\rangle$ the state of particle i with momentum p and by v the interaction potential of this particle with the collective subsystem, when this subsystem is at position $x=0$. The coupling H_1 with ideal oscillators when the object is at position x is then given by $\Sigma_i\langle pi|v|qi\rangle\exp[i(p-q)x]a_{pi}a^\dagger_{qi}$. It is not linear in the creation and annihilation operators a_{pi}, $a^\dagger_{pi}$ and it can be even more complex in general.

piston and a gas molecule must be large for the piston to keep molecules on one side. One can therefore introduce an average interaction

$$\Delta H_c = \mathrm{Tr}_e(\rho_e H_1). \tag{1.8}$$

This interaction can be interpreted in our example as giving the pressure force exerted by the gas on the piston. The remaining interaction

$$H_1' = H_1 - \Delta H_c \otimes I_e \tag{1.9}$$

is a much smaller quantity. It represents in our example the fluctuating part in the collisions. *The basic assumption of the examples we give will be that* H_1' *is small enough for being treated as a perturbation.*

It will be shown in Sec. II how one can derive a master equation for ρ_c from this assumption, by using second-order perturbation theory in H_1' for the basic evolution equation

$$i\dot{D} = [H, D] \tag{1.10}$$

(in units where $\hbar = 1$). It might look rather surprising that a perturbation calculation can work, because the quantity

$$D_1 = D - D_0, \tag{1.11}$$

inevitably entering in the calculations, cannot be small. It will be found however to ''act small,'' suggesting that something more general than the model can still lie behind.

The master equation can be used for useful investigations such as the Paris experiment [32], for instance. It will be shown, however, in Sec. III that the master equation becomes much simpler when there exists a special basis. This occurs when there exists a complete set of commuting ''microstable'' observables X in the collective Hilbert space $\mathcal{H}_c$ such that

$$[X, H_1'] = 0. \tag{1.12}$$

Another way of expressing this is to say that the time derivatives of X one obtains from the full Hamiltonian or the collective effective one coincide, namely,

$$[H, X] = [H_c + \Delta H_c, X]. \tag{1.13}$$

In our example, this is true for the piston position and both quantities (1.13) coincide with P/m. More generally, a microstable observable is one preserving the usual proportionality between momentum and velocity. The center-of-mass position of a piece of solid or fluid matter is of that type and this explains why classical mechanics, when derived from quantum mechanics, can be described in ordinary three-dimensional space. (This argument is not completely new [20,33].) Another interesting example will be given for an induction circuit, showing that microstable observables can sometimes be extended outside classical mechanics to another domain of classical physics, but not to every domain and not for every problem. This remark opens an interesting new field, which we have not explored.

The master equation derived from this approach in Sec. IV exhibits the main features one suspected from the models, though it is of course much more general. The relation of decoherence to friction is shown in Sec. V. Though the theory trivially agrees with the results of an oscillator model for the environment, the fact that it also encompasses the particle model [21] and therefore acts truly as a common framework, is less obvious and is shown in Sec. VI. Section VII will sum up the various assumptions that are introduced in the construction and indicates which result depends on what assumption.

This summary of assumptions and results will show why the model we used first is not yet general enough. For instance, a realistic quantum measurement cannot be properly and completely described by such a model, because the collective, or relevant observables can be generated in the course of time: In the case of a bubble chamber, every newborn bubble asks for its share of a new Hilbert space $\mathcal{H}_c$. There are also some questions about the theory itself: Why does the guess (1.5) work? Why does D_1 act small though not being small? To improve the first draft of the theory, one must understand what is the real key for its success.

One can get an answer to these questions by using the general method of projection superoperators in the theory of quantum irreversible processes [34,35], to which we turn in Sec. VIII. It will be shown in Sec. IX that the initial approach we used in our model is in fact a special case of this method.

Every master equation that is known for any irreversible process can be derived from some version of the projection method. Some master equations hold because of perturbation theory, or from short memory approximations or other reasons [35]. They do not assume the vicinity of thermal equilibrium nor that the relevant observables be given once and for all. A general theory of the decoherence effect consists therefore simply in applying the known theory of irreversible processes to the special ''relevant'' observables showing decoherence. The present paper shows one rather far-ranging example of this method, but it will be interesting to investigate other situations one also meets in real measurements.

II. A MASTER EQUATION FOR DECOHERENCE

One will assume that the environment is in thermal equilibrium at an initial time 0, which implies $D_1(0) = 0$. Though this assumption is not necessary, it allows one to dispose of some uninteresting terms that have nothing to do with decoherence.

One may first notice three consequences of the definitions, namely,

$$\rho_c = \mathrm{Tr}_e D, \tag{2.1}$$

$$d(\beta F)/dt - (d\beta/dt)\mathrm{Tr}\rho_e H_e = d(\beta F)/dt - (d\beta/dt)E_e = 0, \tag{2.2}$$

$$\mathrm{Tr}_e[H_1', \rho_e] = 0, \tag{2.3}$$

$$\mathrm{Tr}_e D_1 = 0. \tag{2.4}$$

The first relation is the definition of the reduced density operator. The second one follows from Eq. (1.6) and the third one from Eqs. (1.8) and (1.9). The last one follows from Eqs. (2.1), (1.5), and (1.11).

Taking the trace of Eq. (1.10) over the environment, one gets

$$i\dot{\rho}_c = [H_c + \Delta H_c, \rho_c] + \Omega, \tag{2.5}$$

where

$$\Omega = \mathrm{Tr}_e[H_1', D_1]. \tag{2.6}$$

Proof. The time derivative of ρ_e in $\mathrm{Tr}_e\dot{D}_0$ vanishes because of Eq. (2.1). One has $\mathrm{Tr}_e[H_c, D_0] = [H_c, \rho_c]$ and $\mathrm{Tr}_e[H_e, D_0]$ vanishes as the trace of a commutator. Then $\mathrm{Tr}_e[H_1, D_0] = [\Delta H_c, \rho_c]$ from Eq. (1.8). One has $\mathrm{Tr}_e[H_c, D_1] = 0$ because of Eq. (2.4) and $\mathrm{Tr}_e[H_c, D_1] = 0$ as a trace of a commutator, so that $\mathrm{Tr}_e[H, D_1]$ is reduced to Ω. Similar straightforward algebraic calculations will be omitted from here on.

The density operator D_1 occurring in Ω is *a priori* very complicated. The basic equation (1.10) becomes in fact an equation for D_1 when using Eqs. (1.11), (1.5), and (2.5). This gives

$$i\dot{D}_1 = [H, D_1] + [H_1', D_0] + A, \tag{2.7}$$

$$A = -i\dot{\beta}(E_e - H_e)D_0 + \rho_e \otimes \Omega. \tag{2.8}$$

The quantity $[H_1', D_0]$ is of first order in the small quantity H_1'. Though $\dot{\beta}$ can be considered to be small (at least when there are microstable observables, as shown in the Appendix), one has no idea of the importance of the second term in Eq. (2.8) since one does not know Ω, except that it is at most of first order according to Eq. (2.6). One therefore introduces an auxiliary operator D_1' through the equation

$$i(\dot{D}_1' - \dot{D}_1) - [H, D_1' - D_1] = \rho_e \otimes \Omega. \tag{2.9}$$

Since $D_1(0) = 0$, one has $\Omega(0) = 0$ and $D_1'(0)$ can be taken to be zero. Using $D = D_0 + D_1$, together with Eqs. (1.5), (2.1), and (2.3), Eq. (1.10) becomes

$$i\dot{D}_1' = [H, D_1'] + B, \tag{2.10}$$

$$B = -i\dot{\beta}(E_e - H_e)D_0 + [H_1', D_0]. \tag{2.11}$$

To solve Eq. (2.9), one introduces the evolution operator

$$U(t,t') = T\ \exp\left[-i\int_{t}^{t} H(t'')dt''\right], \tag{2.12}$$

where T means a time ordered product. Similar evolution operators U_e and U_c are defined by replacing H, respectively, by H_e and $H_c + \Delta H_c$. One thus gets

$$D_1'(t) = -i\int_0^t U(t,t')B(t')U^\dagger(t,t')dt'. \tag{2.13}$$

Equation (2.9) gives, at first order in perturbation theory,

$$D_1' - D_1 = \int_0^t U(t,t')\rho_e \otimes \Omega(t')U^\dagger(t,t')dt'. \tag{2.14}$$

Introducing the quantity $\Omega' = \mathrm{Tr}_e[H_1', D_1']$, Eq. (2.14) gives

$$\Omega' - \Omega = -(i/\hbar)\mathrm{Tr}_e\left\{\left[H_{1t}', \int_0^t U(t,t')\rho_e \otimes \Omega(t')U^\dagger(t,t')dt'\right]\right\}.$$

The integral is necessarily of a higher order than Ω because of the occurrence of H_1' and therefore $\Omega' = \Omega$, up to corrections of a higher order. The quantity Ω' is obtained from the auxiliary density operator D_1', which in view of Eq. (2.13) is a small quantity of first order so that Ω itself is of second order. This is a very remarkable result since it means that in some sense, D_1 acts small though it is not small. As a matter of fact, there are certainly some operators O in the complete Hilbert space that would have an average value $\mathrm{Tr}OD_1$ of the order of their norm $\|O\|$, which is a reasonable way of expressing that D_1 is not small. However, as it happens in irreversible processes, the matrix elements of D_1 are extremely numerous and do not favor the collective observables. This is at least an intuitive manner of understanding the present result.

Finally, one has obtained a master equation that is, up to terms of third order and higher,

$$\dot{\rho}_c + i[H_c + \Delta H_c, \rho_c] = -\int_0^t \mathrm{Tr}_e\{[H_1'(t), U_cU_e(t,t') \times [H_1'(t'), D_0(t')]U_c^\dagger U_e^\dagger(t,t')]\}dt'. \tag{2.15}$$

One has replaced $U(t,t')$ by $U_c(t,t')U_e(t,t')$, abbreviated here as $U_cU_e(t,t')$. This master equation contains the two effects of decoherence and dissipation and one must now extract this physical meaning.

III. MICROSTABLE BASES AND THEIR MEANING

The master equation (2.15) is not transparent. One can get, however, an inspiration from the ideas of Zurek [18–20] and from the results of known models. This suggests a search for convenient bases. One therefore introduces a complete set X of commuting observables in $\mathcal{H}_c$ with eigenvectors $|x\rangle$ together with the basis $|n\rangle$ of the eigenvectors of H_e in $\mathcal{H}_e$. As a matter of fact, the most useful basis in $\mathcal{H}_c$ may sometimes be of a different type and it was found convenient, in the case of the electromagnetic field, to use the overcomplete basis of coherent states [14]. We shall not consider this case however, nor shall we try to investigate the master equation in all cases. We shall rather develop the consequences of this equation when there exists what was called in the Introduction a set of microstable observables. This is defined as a complete set of commuting observables satisfying the commutation relation.

$$[H_1', X] = 0. \tag{3.1}$$

The observables X may have a continuous or a discrete spectrum. When discussing a spin measurement, for instance, the spin observable that is measured should be included in the set X (H_c containing the interaction Hamiltonian between the spin and the rest of the collective system). The discussion will be limited, however, to ordinary collective observables, with a continuous spectrum. The physical meaning of the assumption (3.1) is made clearer if one writes it as

$$-i\dot{X}\equiv[H,X]=[H_c+\Delta H_c,X]. \tag{3.2}$$

When X represents a set of position coordinates $\{X_i\}$ with a kinetic energy $\frac{1}{2}(M^{-1}\}_{ij}P_iP_j$, this means that the familiar relation $P_i=M_{ij}\dot{X}_j$ remains valid in spite of the presence of the environment. The assumption is therefore valid in ordinary mechanics, when a macroscopic system that is made of solid parts and fluid parts is described, *à la* Newton, as consisting of small macroscopic parts. The relation (3.2) for the center-of-mass coordinates X of these small parts and their momentum follows in that case from the fact that H can be written in terms of all the constitutive particles α (electrons and nuclei) as $\Sigma(p_\alpha^2/2m_\alpha+v_{\alpha\beta})$. Since classical physics is known to follow from decoherence, the present theory implies that classical mechanics can be described as taking place in three-dimensional space. This remark would look trivial if one did not realize that semiclassical physics has only presently reached a description of classical physics in configuration space (see, however, [33]), and one did not remember how surprised Schrödinger was to find that wave functions are defined in a configuration place.

The origin of this important result is to be found in invariance under a change of inertial reference system. In a change of inertial frame with a nonrelativistic velocity v (with no translation for the origin of space or time nor a change in the direction of axes), the position observables change according to $x_k(t)\rightarrow x_k+vt$. Using the fact that momentum operators are the generators of infinitesimal space translations and using the Lie algebra of the Galilei group, it can be shown that individual momenta are transformed according to $p_k\rightarrow p_k+m_kv$. The relation (3.2) follows then from the equation $\dot{P}=0$ in the inertial reference system where the center of mass of a piece of matter is instantaneously at rest.

Another interesting example is offered by an induction loop, such as the ones that are used in a superconducting quantum interference device [31]. The role of X is taken by the magnetic flux Φ through the loop, P being $-CV$ where V is the potential difference across the terminals of the loop and C the capacity [36]. The relation between momentum and velocity is given by $V=-d\Phi/dt$ and this is insensitive to the presence of an environment since it is a direct consequence of Maxwell's equations, so that the magnetic flux is a microstable observable.

When X is microstable, Eq. (3.1) implies that H_1' is diagonal in $\mathcal{H}_c$, namely,

$$\langle xn|H_1'|x'n'\rangle=\delta(x-x')V_{nn'}(x). \tag{3.3}$$

The master equation (2.15) suggests the introduction of convenient correlation functions that are defined by

$$F(x',x,t,t')=\mathrm{Tr}_e\{V(x',t)U_e(t,t')V(x,t')U_e^\dagger(t,t')\rho_e\}, \tag{3.4}$$

$$G(x',x,t-t')=\mathrm{Tr}_e\{V(x',t)\rho_eU_e(t,t')V(x,t')U_e^\dagger(t,t')\}. \tag{3.5}$$

One does not need to take care in these expressions of the slightly fluctuating character of ρ_e nor of its smooth variation with time, which is slow. These are second-order effects. We shall not consider moreover the possibility of short-time hysteresis, as it may occur in solid friction [37,38], so that these functions depend only upon $t-t'$. More explicitly, one has

$$F(x',x,t-t')=\sum_{nn'}V_{nn'}(x',t)V_{n'n}(x,t')\rho_ne^{-i\omega_{n'n}(t-t')}, \tag{3.6}$$

with $\rho_n=\exp[-\beta(E_n-F)]$, E_n being an eigenvalue of H_e. One may also notice the useful relations

$$G(x',x,\tau)=F(x,x',-\tau)=F^*(x',x,\tau). \tag{3.7}$$

One will be particularly interested in values of x and x' that are macroscopically close. One expects the correlation functions to behave typically in a standard fashion: $F(x',x)$ depends only slowly, i.e., on a macroscopic scale, upon the gross position of the system [which is described by $\frac{1}{2}(x'+x)$ for degrees of freedom in space]. It depends strongly, however, upon $x-x'$, and moreover upon $(x'-x)^2$, in view of simple invariance arguments. [More properly, it depends in general upon the differences $(x_i'-x_i)^2$ for the various degrees of freedom.] As for its dependence upon time, the typical time scale of $F(t-t')$ is given by fluctuations, for instance, the time between successive collisions in the case of an external environment. This is most often extremely short. In any case, the present remarks about $F(x',x,t-t')$ should not be considered as universally valid and they must be checked against the real physics of the system under consideration. They have been mentioned here for a better understanding of probably the most frequent cases.

IV. DECOHERENCE

The existence of a microstable basis will now be used to extract the effects of decoherence and dissipation from the master equation (2.15). The right-hand side of this equation involves the collective propagation operator $U_c(t-t')$. Because of the very-short-time scale of the correlation functions, the approximation

$$U_c(t-t')\approx I-i(H_c+\Delta H_c)(t-t') \tag{4.1}$$

is certainly sufficient. One can moreover keep only the terms in Eq. (2.15) that are at most linear in $t-t'$. One can therefore write the master equation as

$$\dot{\rho}_c+i[H_c+\Delta H_c,\rho_c]=R_d+R_f, \tag{4.2}$$

where the index d stands for decoherence and f for friction. These two terms correspond, respectively, to the leading terms one obtains in Eq. (2.15) by setting $U_c(t-t')=I$ and to the terms linear in $t-t'$ resulting from Eq. (4.1). We shall first consider the decoherence term R_d, which is given by

$$\langle x'|R_d|x\rangle=-\int_0^tK(x',x,t-t')\rho_c(x',x,t)dt',$$

where the kernel is given directly in terms of the correlation functions by

$$K(x',x,\tau)=F(x',x',\tau)-G(x',x,\tau)-G(x,x',-\tau)+F(x,x,-\tau). \tag{4.3}$$

In view of the relations (3.7), this can be written in terms of a unique correlation function as

$$K(x',x,\tau)=F(x',x',\tau)-F^*(x',x,\tau)-F(x,x',\tau)+F^*(x,x,\tau). \tag{4.4}$$

One can introduce the real and imaginary parts of the function $F(x',x,\tau)$ by $F=F_1+iF_2$, with the symmetry properties following from Eq. (3.7),

$$F_1(x,x',-\tau)=F_1(x',x,\tau), \quad F_2(x,x',-\tau)=-F_2(x',x,\tau). \tag{4.5}$$

The explicit expression of these functions, in view of Eq. (3.6), is

$$F_1(x',x,t-t')=\frac{1}{2}\sum_{nn'} V_{nn'}(x',t)V_{n'n}(x,t')\times(\rho_n+\rho_{n'})e^{-i\omega_{n'n}(t-t')}, \tag{4.6}$$

$$F_2(x',x,t-t')=\frac{1}{2i}\sum_{nn'} V_{nn'}(x',t)V_{n'n}(x,t')\times(\rho_{n'}-\rho_n)e^{-i\omega_{n'n}(t-t')}, \tag{4.7}$$

with $\omega_{n'n}=E_{n'}-E_n$. At temperatures high enough for having $\beta\omega_{n'n}\ll 1$ for the significant contributions, it may be noticed that

$$F_2(x',x,t-t')\approx-\frac{\beta}{2i}\sum_{nn'} V_{nn'}(x',t)V_{n'n}(x,t')\times(\rho_n+\rho_{n'})\omega_{n'n}e^{-i\omega_{n'n}(t-t')}. \tag{4.8}$$

The decoherence effect is most easily seen if one takes advantage of the short memory of the correlation function for integrating directly $F(t-t')$ over t' in R_d. In view of the assumed dependence of the correlation function upon $(x-x')^2$ and leaving the slow dependence upon $(x'+x)$ unwritten, one has

$$\int_0^\infty F_1(x',x,\tau)d\tau=f((x'_i-x_i)^2). \tag{4.9}$$

For x and x' macroscopically close and when retardation effects are negligible, one has

$$\int_0^\infty K(x',x,\tau)d\tau=\mu_{ij}(x'_i-x_i)(x'_j-x_j), \tag{4.10}$$

the decoherence coefficients μ_{ij} being given by

$$\mu_{ij}=2\, f''_{ij}(0). \tag{4.11}$$

The contribution of the leading terms in the master equation is therefore

$$\langle x'|\dot{\rho}_c+i[H_c+\Delta H_c,\rho_c]|x\rangle=-\mu_{ij}(x'_i-x_i)(x'_j-x_j)\times\langle x'|\rho_c|x\rangle. \tag{4.12}$$

It will soon be shown (and already known from models) that the decoherence coefficients are large, except when there is no dissipation. Considering only one degree of freedom, it is then clear that the reduced density operator will behave as

$$\langle x'|\rho_c(t)|x\rangle\approx\langle x'|\rho_c(0)|x\rangle\exp[-\mu(x'-x)^2t] \tag{4.13}$$

and become practically diagonal, except for values of x and x' so close that the effect of $[H_c+\Delta H_c,\rho_c]$ becomes comparable to the decoherence effect (4.12) or larger [16,17].

V. DISSIPATION

One must now evaluate the second term R_f in the master equation, which was attributed to friction and comes from the terms linear in $(H_c+\Delta H_c)$ $(t-t')$. It is given according to Eq. (2.15) by

$$R_f=i\int_0^t \mathrm{Tr}_e[H'_1(t),[H'_c,U_e(t,t')[H'_1(t'),D_0(t')]U_e^\dagger(t,t')]]\times(t-t')dt', \tag{5.1}$$

where we have written H'_c for short in place of $H_c+\Delta H_c$.

This quantity is easy to evaluate if one makes the following assumptions. (i) One can neglect the time dependence of F_1 and F_2 coming directly from the products $V_{nn'}(x',t)V_{n'n}(x,t')$. (ii) The temperature is high enough for Eq. (4.3) to be used. (iii) $H_c+\Delta H_c$ can be written as $\frac{1}{2}(M^{-1})_{ij}P_iP_j+V(X)$. The conjugation of these three assumptions is somewhat restrictive, though still frequently met. Our aim is, however, only to clarify the meaning of the results, and specific applications to cases where these assumptions do not hold should better be investigated for their own sake.

We shall make the calculation for only one degree of freedom. One can first replace H'_c by its kinetic part in Eq. (5.1). The various parts of the triple commutator can be evaluated by using

$$\langle x'|P^2A|x\rangle=-\frac{\partial^2}{\partial x'^2}\langle x'|A|x\rangle,$$

$$\langle x'|AP^2|x\rangle=-\frac{\partial^2}{\partial x^2}\langle x'|A|x\rangle.$$

One notices that decoherence is much more rapid than dissipation. Although this result will be a consequence of the present calculation, one may anticipate it and consider that R_f is noticeable only after decoherence has reduced the matrix elements ρ_c (x',x) to a quasidiagonal form. This means that one can write

$$\int_0^\infty F_2(x',x,\tau)\tau d\tau=a+(M\gamma/2)(x'-x)^2, \tag{5.2}$$

still leaving aside a possible smooth dependence on $(x+x')$, and neglecting terms of higher order in $(x'-x)^2$ that are anyway suppressed by the exponential decoherence factor in Eq. (4.13). The meaning of γ in Eq. (5.2) will soon become clear. A straightforward algebraic calculation gives

$$R_f = -(\gamma/2)(x'-x)(\partial/\partial x' - \partial/\partial x)\rho_c(x',x). \tag{5.3}$$

When this is used to evaluate the rate of momentum change (noticing that R_d does not contribute), one gets the familiar expression of friction

$$d\langle P\rangle/dt = -\langle \partial V/\partial x\rangle - \gamma\langle P\rangle. \tag{5.4}$$

Using Eqs. (4.6) and (4.8), one gets on the other hand

$$\int_0^\infty F_2(x',x,\tau)\tau d\tau = (\beta/2)\int_0^\infty F_1(x',x,\tau)d\tau \tag{5.5}$$

and since

$$\mu = 2\int_0^\infty \partial^2 F_1(x,x,\tau)/\partial x \partial x' d\tau,$$

one has $\mu = MT\gamma$, a relation that may also be understood as implying that a thermal equilibrium distribution satisfies Eq. (1.3), which is the final result when there is a microstable basis. Reintroducing explicitly Planck's constant and several degrees of freedom, one obtains

$$\mu_{ij} = (M\gamma)_{ij}T/\hbar^2. \tag{5.6}$$

VI. THE CONNECTION WITH PREVIOUS WORKS

The results one has obtained agree, as one would expect, with the special case of the oscillator model. The master equation (2.15) involves also the kind of double commutator that was postulated in the quantum diffusion model [39–42]. In this model, the stochastic character of $H_1'(t)$ is described by a Brownian noise and the quantum diffusion model can therefore be considered as belonging mostly to the present theory.

This is not so obvious for the results of the external environment model [21], though their coincidence with those of the oscillator model was the main hint for the existence of a common background. To obtain them from the present theory, one may proceed as follows. The relevant system is an object that is surrounded by a gaseous environment made of particles. In the case of molecules, the interaction between the object and a particular molecule is a potential, which is the sum v of the interaction potentials between that molecule and all the atoms in the object. Considering for simplicity that the molecules do not interact together (or each molecule is considered during its last mean free path towards the object), each colliding molecule can be individualized within the environment. The summation in Eq. (3.6) can then be split into independent summations over the various molecules.

In order to take care of the time distribution of the collisions, one may consider the scattering of one molecule on the object. In the summation over the indices nn' that was written in Eq. (3.6), one can use two different bases for n and n'. The basis $|n\rangle$, used in ρ_n, is made of free incoming plane waves $\phi_p(y) = \exp(ipy)$, if y represents the position of the molecule. For the basis n', however, one uses the full scattering waves ψ_p. The matrix elements $H'_{1nn'}$ are therefore given by $\langle \phi_p|v|\psi_p'\rangle$. According to the well-known Lippmann-Schwinger relation in scattering theory [43], one has

$$\langle \phi_p|v|\psi_p'\rangle = -\frac{4\pi}{2m} f(p,p'), \tag{6.1}$$

where m is the mass of the molecule and $f(p,p')$ is the scattering amplitude for a collision where the momentum p goes to p'. This is how the scattering amplitude is found to enter the calculations in the present theory, explaining the central role it plays in the approach by Joos and Zeh. From there on, the calculation can proceed as it was done by Joos and Zeh and it needs not be developed.

One cannot fail to mention a most important aspect of decoherence, which is very frequently a semiclassical behavior of the collective subsystem. This question has been considered, however, with great care by Gell-Mann and Hartle [33] and there is nothing essential to add to their work.

VII. SUMMARIZING THE RESULTS

One may conclude this first approach to the theory of decoherence by recalling the various assumptions that were made along the way and which results hold under what conditions.

(1) The choice of the collective subsystem is made once and for all.

(2) The Hamiltonian can be separated as in Eq. (1.2).

(3) The fluctuating part H_1' of the coupling is small enough to be treated as a perturbation.

(4) One can use the test density D_0 given by Eqs. (1.5) and (1.6).

One then obtains the master equation (2.15).

(5) There exists a system of microstable collective observables X.

The decoherence effect is then described by Eqs. (4.2) and (4.4).

(6) The correlation functions have the behavior (4.9).

(7) Retardation effects are negligible.

The decoherence effect is then described by Eq. (4.12).

(8) The assumptions made in Sec. V are used.

At a time when decoherence has already taken place, friction effects can be written as in Eq. (5.3) and the coefficients of decoherence and friction are related by Eq. (5.6).

One can now evaluate and criticize each assumption. Assumption (1) is convenient for discussing simple models of a quantum measurement, for instance, the famous von Neumann model [44] to which one adds an interaction of the "pointer" with an environment. It does not apply to realistic measurements, when, for instance, new bubbles or any other macroscopic real records are created.

Assumption (2): One would prefer to select only ρ_c as a relevant quantity and this does not necessarily demand the expression (1.2) for H. It often happens that the environment Hamiltonian H_e depends upon the collective observables. In the example of the piston, H_e depends in fact upon the piston position.

Assumption (3) seems to be essential for the whole approach and it also looks quite reasonable.

Assumption (4) does not hold when the piston is submitted to the action of a gas pressure on both sides. One should then make room for two different ''temperatures'' on the two sides and, more generally, resort to an expression of the test density ρ_e analogous to the one describing local thermal equilibrium rather than full equilibrium. It seems that this is only a technical complication with no special difficulty.

Assumption (5) is known to be wrong for an electromagnetic collective system. One can use, however, a basis of coherent states that will play the role of our microstable basis. There exist certainly more general situations, which would require a more systematic investigation of Eq. (4.9).

From there on [assumptions (6) and (7)], our analysis was only meant for some clarity rather than generality. Specific examples, where the assumptions do not hold, should be treated for their own sake. One could write in particular a more elaborate relation between the coefficients of friction and decoherence at low temperature, but it is not very illuminating. Here again, the peculiarities of a specific application should be preferred.

To go further, one should also understand better why the present method works, if only to remove some unnecessary assumptions. This will be our next topic. It will be shown that, at least in principle, one can overcome the limits of assumptions (1) and (2), which are too narrow for a full theory of measurement. The general theory of irreversible processes [34,35] will be used for that purpose. Though this second approach is much more general, it is well known that the mathematical techniques for using the formalism of irreversible processes must be adapted to every special problem one wants to investigate [35]. This is why we shall only consider the essentials by recasting our first approach in the new framework [with Assumptions (1) and (2) explicit], to obtain again the same master equation. Even if this is a very limited achievement, it shows that this second way of looking at the theory provides the right framework for a thorough treatment of decoherence.

VIII. ANOTHER APPROACH THROUGH THE THEORY OF IRREVERSIBLE PROCESSES

The theory of irreversible processes is by now far from being restricted to systems near thermal equilibrium. We shall rely upon its formulation by Balian and co-workers [34,35]. The idea is to select some ''relevant'' quantities for which to obtain an evolution equation while leaving ignored the details of other quantities, much larger in number. This is also obviously the basic idea of decoherence. Rather than recalling the theory itself, we shall reconstruct it as it applies to the present problem, which has some peculiar features that are more easily grasped in that way.

We still keep the structure of two coupled systems e and c, with the Hamiltonian (1.2), all the notations being kept the same. A basis $|x\rangle$ in $\mathcal{H}_c$ is introduced, not necessarily associated with microstable observables nor necessarily observables with continuous spectra. One considers the algebra of operators in the full Hibert space $\mathcal{H}$ and the dual space of densities made of operators that are not necessarily supposed to be positive nor with trace 1. Duality (i.e., the introduction of linear functionals) is expressed by a ''scalar product'' between an operator A and a density Δ denoted by

$$(A;\Delta)\equiv \mathrm{Tr}\, A\Delta. \tag{8.1}$$

The relevant observables we shall use are

$$A^{xx'}=|x\rangle\langle x'|\otimes I_e, \quad A^e=I_c\otimes H_e, \tag{8.2}$$

collectively denoted by A^i. Though $|x\rangle\langle x'|$ is not an observable, it is a combination of the observables $\frac{1}{2}(|x\rangle\langle x'|+|x'\rangle\langle x|)$ and $(1/2i)(|x\rangle\langle x'|-|x'\rangle\langle x|)$ and it is more convenient to take it in that form. The averages of these quantities with the exact total density D are

$$a^i=\mathrm{Tr}A^iD, \text{ i.e., } a^{xx'}=\langle x'|\rho_c|x\rangle, \quad a^e=E_e. \tag{8.3}$$

Balian's theory starts with the introduction of a reference density operator D_0 that is defined by

$$D_0=\exp(-\lambda_i A^i), \tag{8.4}$$

the parameters λ_i being determined by the conditions $\mathrm{Tr}\, A^iD_0=a^i$. It coincides in the present case with our previous D_0 with $\lambda_e=\beta$ [see Eq. (1.5)]. Though Eq. (8.4) is usually motivated by information theory, Eq. (1.5) is enough to show that D_0 is the simplest reference one can use for acceding to the reduced density operator and this will be enough for our purpose.

A significant remark should, however, be made. Balian mentions that it is convenient to include the identity operator I among the relevant observables and he insists upon the idea of introducing also every conserved quantity, which would be in the present case the total Hamiltonian H. The first requirement is already satisfied since I is a linear combination of the $A^{xx'}$. When considering H in the form $H_c+\Delta H_c+H_e+H_1'$, one realizes that $H_c+\Delta H_c$ is a combination of the $A^{xx'}$ so that the recommended reference density would be

$$E_0=\exp\left(-\int \lambda_{xx'}A^{xx'}dx dx'-\beta(H_e+H_1')\right).$$

The two reference densities are related in perturbation theory by

$$E_0=D_0-\beta\int_0^1 D_0^{1-u}H_1'D_0^u du + \beta^2\int D_0^{1-u-v}H_1'D_0^uH_1'D_0^v du\, dv,$$

with a similar relation giving D_0 in terms of E_0. When trying to use E_0, as is usually done in Balian's theory, one is inevitably led to use these cumbersome relations and the theory loses much of its elegance. Quite fortunately, it turns out that one can also start directly from D_0, which is much simpler than E_0, at the price of rederiving the equations that will follow rather than using directly Balian's formulas. This is our main reason for starting from scratch, with the advantage of not supposing the reader familiar with the theory of irreversible processes.

The basic evolution equation (1.10) for D is conveniently written in the form

$$\dot{D}=\mathcal{L}D, \tag{8.5}$$

where $\mathcal{L}$ is a (Liouvillian) linear operator acting linearly in the space of densities (superoperator). Acting on an arbitrary density Δ, it gives

$$\mathcal{L}\Delta=(1/i)[H,\Delta]. \tag{8.6}$$

One can then introduce a set of densities s_i that are defined by

$$s_i=\partial D_0/\partial a^i, \quad \text{i.e.,} \quad s_{xx'}=|x'\rangle\langle x|\otimes\rho_e,$$

$$s_e=\rho_c\otimes(H_e-E_e)\Delta_2, \tag{8.7}$$

$$\Delta_2=\mathrm{Tr}_e H_e^2\rho_e-E_e^2. \tag{8.8}$$

They satisfy the orthogonality relations

$$(A^i;s_j)\equiv\mathrm{Tr}A^i s_j=\delta^i j. \tag{8.9}$$

In view of Eq. (8.9), the superoperator

$$\mathcal{P}=s_iA^i, \quad \mathcal{P}\Delta=s_i\ \mathrm{Tr}(A^i\Delta) \tag{8.10}$$

(with the usual convention of summation over repeated indices) is a projection operator, i.e., $\mathcal{P}^2=\mathcal{P}$. The operator $\mathcal{Q}=I-\mathcal{P}$ (where $I\Delta=\Delta$) is also a projection operator and one has

$$\mathcal{P}^2=\mathcal{P}, \quad \mathcal{Q}^2=\mathcal{Q}, \quad \mathcal{P}\mathcal{Q}=\mathcal{Q}\mathcal{P}=0. \tag{8.11}$$

Explicitly, one has

$$\mathcal{P}\Delta=\rho_e\mathrm{Tr}_e\Delta+\rho_c(H_e-E_e)(1/\Delta_2)\mathrm{Tr}H_e\Delta. \tag{8.12}$$

Our previous densities D_0 and D_1 are given by

$$D_0=\mathcal{P}D, \quad D_1=\mathcal{Q}D, \quad D=D_0+D_1. \tag{8.13}$$

IX. THE MASTER EQUATION

Differentiating Eq. (8.13) with respect to time and using Eq. (8.5), one gets

$$\dot{D}_0=\mathcal{P}\mathcal{L}\mathcal{P}D_0=\mathcal{P}\mathcal{L}D_1+\dot{\mathcal{P}}\mathcal{Q}D_1, \tag{9.1}$$

$$\dot{D}_1-\mathcal{Q}\mathcal{L}\mathcal{Q}D_1=-\dot{\mathcal{P}}\mathcal{Q}D_1-\dot{\mathcal{P}}D_0+\mathcal{Q}\mathcal{L}\mathcal{P}D_0, \tag{9.2}$$

where one used $\dot{\mathcal{Q}}=-\dot{\mathcal{P}}$ and Eq. (8.11). Usually, when one starts from the total Hamiltonian H, rather than H_e, one finds that $\dot{\mathcal{P}}\mathcal{Q}=0$. This is not so in the present case and one has (as shown in the Appendix)

$$\dot{\mathcal{P}}\mathcal{Q}\Delta=-i(1/\Delta E_e^2)\rho_c(E_e-H_e)\rho_e\mathrm{Tr}([H_1'H_e]\Delta). \tag{9.3}$$

The occurrence of H_1' implies that this is a small quantity that can be treated as a perturbation.

One can then solve Eq. (9.2). Setting $D_2=-\dot{\mathcal{P}}D_0+\mathcal{Q}\mathcal{L}\mathcal{P}D_0$ and using $\mathcal{P}D_0=D_0$, which gives $\dot{\mathcal{P}}D_0=\mathcal{Q}\dot{D}_0$, one gets

$$D_2=\mathcal{Q}(-\dot{D}_0+\mathcal{L}D_0), \tag{9.4}$$

Eq. (9.2) becomes

$$\dot{D}_1-\mathcal{Q}\mathcal{L}\mathcal{Q}D_1=-\dot{\mathcal{P}}\mathcal{Q}D_1+D_2. \tag{9.5}$$

One may notice that $\mathcal{Q}D_2=D_2$. Introducing the operator[2]

$$\mathcal{W}(t,t')\equiv T\ \exp\left(\int_{t'}^{k}\mathcal{Q}\mathcal{L}\mathcal{Q}(t'')dt''\right), \tag{9.6}$$

the solution of Eq. (9.5) at first order in H_1' (which will turn out to be enough) is given by

$$D_1=D_a+D_b, \tag{9.7}$$

$$D_a=\int_0^t\mathcal{W}(t,t')\mathcal{Q}(t')D_2(t')dt', \tag{9.8}$$

$$D_b=\int_0^t dt'\mathcal{W}(t,t')$$

$$[-\dot{\mathcal{P}}\mathcal{Q}(t')]\int_0^{t'}dt''\mathcal{W}(t',t'')\mathcal{Q}(t'')D_2(t''). \tag{9.9}$$

It may be noticed that the choice of a definite direction of time in the integrals marks the place where irreversibility enters. Since D_2, as given by Eq. (9.4), is expressed in terms of D_0, the introduction of Eq. (9.7) into Eq. (9.1) gives the required master equation (at second order in H_1'),

$$\dot{D}_0-\mathcal{P}\mathcal{L}\mathcal{P}D_0=\mathcal{P}\mathcal{L}(D_a+D_b)+\dot{\mathcal{P}}\mathcal{Q}D_a. \tag{9.10}$$

It does not look particularly simple. It might also be noticed that, since $\mathcal{P}$ and $\mathcal{Q}$, according to Eq. (8.12), depend upon ρ_c, the master equation looks nonlinear. Nonlinearity is an intrinsic feature of irreversible processes in general, but it does not occur in the present case. As a matter of fact, the linearity of the evolution equation for D together with the relation $\rho_c=\mathrm{Tr}_eD$ imply that the present equation must be linear, which is of course verified by the explicit calculation to follow.

One is not directly interested in D_0 but in $\rho_c=\mathrm{Tr}_eD_0$. Taking the trace of Eq. (9.10) over the environment, one gets the reduced master equation, as shown in the Appendix,

$$\dot{\rho}_c-(1/i)[H_c+\Delta H_c,\rho_c]=(1/i)\mathrm{Tr}_e[H,D_a+D_b]$$

$$+(1/i)\mathrm{Tr}_e[H,\dot{\mathcal{P}}\mathcal{Q}D_a]. \tag{9.11}$$

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[2] It should be noticed that the ‘‘memory kernel’’ used by Balian is our $\mathcal{W}\mathcal{Q}$, which he calls $\mathcal{W}$.

The calculations in the Appendix show that, to second order in H_1', this equation coincides with the master equation (2.15) that was already obtained by a direct method.

X. CONCLUSIONS

Two different methods have been proposed for obtaining a master equation for decoherence, when one can select a small interaction coupling. The direct method was explained in the Introduction and a rather detailed summary of its results was given in Sec. VII. The second method, though applied here under the same assumptions, relies on a general theory of irreversible processes. It can cover, at least in principle, a much wider range of applications than the one developed here and it will be interesting to try it on a fully realistic and complete quantum measurement. The effect of decoherence has been shown to be a particularly interesting irreversible process, though only one such process from the standpoint of theory. This is an important epistemic finding since it shows, as noted elsewhere [26], that the discussions about the ''practical for all purposes'' or ''fundamental'' meaning of decoherence [28–30] cannot be distinguished from the similar problems that arose in statistical mechanics since Boltzmann.

One may add that decoherence had always been previously studied in rather special models, leading to similar results though an inability to explain these similarities. The reason is that these results are in fact much more general and they are now established on firm and precise foundations.

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APPENDIX: THE PROOF OF SOME INTERMEDIATE RESULTS

Straightforward, even if tedious, algebraic calculations will not be given explicitly. There are, however, some intermediate steps that may require some care and they are given in the present Appendix.

1. Why $\dot{\beta}$ does not affect decoherence (Sec. II)

Some terms involving the derivative $\dot{\beta}$ of the inverse temperature were neglected in Sec. II. This is justified when there exists a system of microstable observables X as follows.

Deriving Eq. (1.7) with respect to time, one has

$$\begin{aligned}\dot{E}_e &= -\dot{\beta}\Delta_2 = \mathrm{Tr} H_e \dot{D} = -i\,\mathrm{Tr}(H_e[H,D])\\ &= -i\,\mathrm{Tr}(H_e[H_1',D]),\end{aligned} \tag{A1}$$

where $\Delta_2 = \mathrm{Tr}_e(H_e^2\rho_e) - E_e^2$ and the last equality is easily obtained by introducing a basis $|xn\rangle$. One writes $D = D_0 + D_1$. When there exists a system of microstable observables X, the trace of $H_e[H_1',D]$ vanishes. One can then use Eq. (2.7) for D_1, using the fact that A is negligible because Ω, though depending upon D_1, is known to be a quantity of second order. As for the first term $-i\dot{\beta}(E_e - H_e)D_0$ in A, it would only give a negligible correction to Eq. (A1) for $\dot{\beta}$. One is thus left with

$$i\dot{D}_1 = [H,D_1] + [H_1',D_0],$$

from which it follows with Eq. (A1) that $\dot{\beta}$ is a quantity of second order. Another proof, using the approach by irreversibility, is a consequence of the calculations at the end of this Appendix, showing that the assumption of a microstable basis is not necessary.

2. The proof of Eq. (9.3)

One has obviously

$$\dot{\mathcal{P}}\mathcal{Q}\Delta = \dot{\mathcal{P}}\Delta - \dot{\mathcal{P}}\mathcal{P}\Delta. \tag{A2}$$

One cannot easily use Eq. (8.12) for computing $\dot{P}$ because this would involve the unknown quantity $\dot{\rho}_c$. One therefore uses the definition (8.10) of $\mathcal{P}$, which gives

$$\dot{\mathcal{P}}\Delta = \dot{s}_i \mathrm{Tr}(A^i\Delta) + s_i \mathrm{Tr}\dot{A}^i\Delta. \tag{A3}$$

This gives

$$\begin{aligned}\dot{\mathcal{P}}\mathcal{Q}\Delta &= \dot{s}_i(\mathrm{Tr}A^i\Delta - \mathrm{Tr}A^i s_j \mathrm{Tr}A^j\Delta)\\ &\quad + s_i(\mathrm{Tr}\dot{A}^i\Delta - \mathrm{Tr}\dot{A}^i s_j \mathrm{Tr}A^j\Delta).\end{aligned} \tag{A4}$$

The identities (8.9) remove the term in $\dot{s}_i$. The time derivatives of operators are given by $\dot{A}^i = i[H,A^i]$ and, using Eqs. (8.2) and (8.6), one gets Eq. (9.3).

3. The proof of Eq. (9.11)

In view of Eqs. (9.10) and (8.12), one has

$$\mathrm{Tr}_e\mathcal{P}\mathcal{L}\Delta = (1/i)\mathrm{Tr}_e[H,\Delta]. \tag{A5}$$

This gives, in view of some vanishing traces,

$$\mathrm{Tr}_e\mathcal{P}\mathcal{L}\mathcal{P}D_0 = (1/i)[H_c + \Delta H_c, \rho_c].$$

According to Eq. (8.12), one has $\mathrm{Tr}_e\mathcal{P}\Delta = \mathrm{Tr}_e\Delta$ so that $\mathrm{Tr}_e\mathcal{Q}\Delta = 0$. Therefore $\mathrm{Tr}_e\dot{\mathcal{P}}D_0 = \mathrm{Tr}_e\mathcal{Q}\,\dot{D}_0 = 0$.

4. Derivation of the master equation from Eq. (9.11)

Using Eqs. (9.4) and (8.6), one finds

$$\begin{aligned}D_2 &= (1/i)[H,D_0] - (1/i)\rho_e\mathrm{Tr}_e[H,D_0] - A\{\mathrm{Tr}(H_e\dot{D}_0)\\ &\quad - (1/i)\mathrm{Tr}(H_e[H,D_0])\},\end{aligned} \tag{A6}$$

with

$$A = D_0(H_e - E_e)/\Delta_2. \tag{A7}$$

It will be useful to show that D_2 is a quantity of first order in H_1. This results from

$$\mathrm{Tr}(H_e\dot{D}_0)=\rho_c\dot{E}_e\,,$$

and

$$\dot{E}_e=\mathrm{Tr}(H_e\dot{D})=(1/i)\mathrm{Tr}(H_e[H,D])=(1/i)\mathrm{Tr}(H_e[H_1',D]).$$

The coefficient of A in Eq. (A6) is therefore $(1/i)\mathrm{Tr}(H_e[H_1',D_1])$. This gives

$$D_2=(1/i)[H_1',D_0]-(1/i)A\,\mathrm{Tr}(H_e[H_1',D_1]), \tag{A8}$$

which implies

$$\mathrm{Tr}_eD_2=0 \tag{A9}$$

and shows that D_2 is of first order in H_1'.

One must now compute $F(t)\equiv D_a(t)=\mathcal{W}(t,t')D_2(t')$. A direct calculation gives

$$\begin{aligned}i\dot{F}=i\mathcal{QLQ}F=[H,F]-\rho_e\mathrm{Tr}_e[H,F]-[H,\rho_e\mathrm{Tr}_eF]\\ +\rho_e[H_c+\Delta H_c\,,\mathrm{Tr}_eF]-[H,A]\mathrm{Tr}(H-E_e)F.\end{aligned} \tag{A10}$$

This implies $\mathrm{Tr}_e\dot{F}=0$ and in view of Eq. (A9),

$$\mathrm{Tr}_eF=0. \tag{A11}$$

One is thus left with

$$i\dot{F}=[H,F]-\rho_e\mathrm{Tr}_e[H,F]-[H,A]\mathrm{Tr}(HF), \tag{A12}$$

which implies

$$\begin{aligned}i\,\frac{d}{dt}\,\mathrm{Tr}(HF)&=-\mathrm{Tr}(H\rho_e\mathrm{Tr}_e[H,F])\\ &=-\mathrm{Tr}_c\{(H_c+\Delta H_c)\mathrm{Tr}_e[H_1',F]\}\\ &=-\mathrm{Tr}\{(H_c+\Delta H_c)[H_1',F]\},\end{aligned} \tag{A13}$$

but from Eq. (A7), one sees that $\mathrm{Tr}HD_2$ is at least of first order in H_1' so that $\mathrm{Tr}(HF)$ is also at least of first order. On the other hand, in view of Eq. (A10), one has $\mathrm{Tr}_e[H,F]=\mathrm{Tr}_e[H_1',F]$. Equation (A10) becomes therefore

$$i\dot{F}-[H,F]=-\rho_e\mathrm{Tr}_e[H,F]-[H,A]\mathrm{Tr}(HF)=-B, \tag{A14}$$

where B is of first order in H_1'. This equation can be solved at first order to give

$$\begin{aligned}D_a(t)=U(t,t')D_2(t')U^\dagger(t,t')\\ -(1/i)\int_{t'}^{t}U(t,t'')B(t'')U^\dagger(t,t'')dt''.\end{aligned} \tag{A15}$$

The end of the calculation is straightforward and it is convenient to use the expression (A6) for D_2. One finds that the second term in Eq. (A15) gives a negligible contribution to the master equation (of third order in H_1'). Similarly the contributions $(1/i)\mathrm{Tr}_e[H,D_b]$ and $(1/i)\mathrm{Tr}_e[H,\dot{\mathcal{P}}\mathcal{Q}D_a]$ to Eq. (9.11) are negligible.

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