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General theory of the decoherence effect in quantum mechanics

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Abstract

The decoherence effect, which is responsible for vanishing macroscopic quantum interferences, has only been established on special models though it is presumed to be universal (at least when some dissipation may occur). A general theory of the effect is proposed in this work. A master equation for the relevant quantity (reduced density operator) is established by two different methods, a direct one, which is also the simplest one, and another, more general, relying upon Balian's theory of irreversible processes. It shows that decoherence is essentially an irreversible process, not very different from more familiar ones as far as theory is concerned.

The master equation is worked out in detail when there exist convenient collective observables (for which a criterion is given), selecting a preferred basis for the effect to take place. The previously proposed models, including the quantum diffusion model, are found to be special applications of the theory.

1. Introduction

The decoherence effect is a mechanism destroying quantum interferences at a macroscopic level. Like an irreversible process in thermodynamics, it can only be seen in a macroscopic system. It does not affect the full wave function of an isolated system but occurs in the observation or consideration of a subsystem, which is most often associated with classically meaningful (collective) observables. The need to select a "relevant" subsystem and the resulting character of decoherence as a law emerging at a high level of complexity is obviously reminiscent of irreversible statistical mechanics.

One may think of the wave function of a macroscopic system as a function $\psi(x, y)$, where x can be reached by observation (the position of a pointer or similar collective quantities), whereas the totality of the very numerous variables y cannot be measured. One can then express grossly the decoherence effect by considering the various functions of y one obtains for every fixed value of x : They tend to become orthogonal as time increases, essentially because they are too complex for keeping mutual coherence, if they had any. The destruction of quantum interferences in the observation of x is a direct consequence of the effect, which is often described by saying that Schrödinger's cat must then be either dead or alive. A convenient mathematical formulation consists in introducing the density operator $D = |\psi\rangle\langle\psi|$ of the whole system and the reduced density operator

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

where the formal subsystem that is described by y is called the "environment" and Tr_e means a partial trace over it, expressing a lack of observation.

Although some effect of that sort had been suspected [1] and even partly investigated [2] since a long time, the decoherence effect was clearly identified by Zeh [3] who made clear the distinction between decoherence and the noise coming from the environment. One may consider as an example the case when the total hamiltonian of the system is

$$H = H_c \otimes I_e + I_c \otimes H_e + H_1 \quad (1.2)$$

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 relevant (or collective) subsystem

and e the environment. The interaction coupling H_1 is then responsible for noise, dissipation and decoherence. This relation between the first two effects results in the fluctuation-dissipation theorem [4-5]. Other similarities also exist for decoherence.

These similarities were exhibited by the solution of some 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 because of the simple properties of harmonic oscillators, and particularly the possibility of explicit Feynman path integration [15]. Decoherence results from a "master equation" one finds for ρ_C in these models:

$$\begin{aligned} \langle x' | \dot{\rho}_C - \frac{1}{i\hbar} [H_C, \rho_C] | x \rangle = & -\mu (x' - x)^2 \rho_C(x', x) \\ & - \gamma (x' - x) (\partial/\partial x' - \partial/\partial x) \rho_C(x', x) \end{aligned} \quad (1.3)$$

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

$$\mu = \gamma (2mT/\hbar^2), \quad (1.4)$$

in the special case where $H_C = P^2/2m + V(x)$, T being the absolute temperature (supposed to be high enough) in energy units. This occurrence of T and the proportionality of the two coefficients of decoherence and friction show the intimate relation between decoherence and dissipation. The very small term $\hbar^2$ in a denominator shows the tremendous efficiency of decoherence: $\rho_C(x', x)$ becomes very rapidly "almost diagonal"? Complete diagonality in the x -basis is however forbidden by energy conservation and it is limited in Eq.(1.3) by the effect of the commutator in the left-hand side [16, 17].

The importance of a preferred "pointer" basis where diagonalization takes place was made clear by Zurek [18-20], who related it to measurement processes. Another important contribution was made by Joos and Zeh [21] who considered another model of environment, made by an external gas of molecules (atmosphere) or photons. They obtained a master equation very similar to Eq.(1.3). In view of the very different environment models that were used, these converging results strongly suggest that there should exist a general theory of the effect, with no detailed assumptions about the environment, except

for its large number of degrees of freedom. One would expect some sort of decoherence-dissipation theorem as an outcome of such a theory.

The need of such a general theory is motivated by the essential role of decoherence in some of the most general interpretations of quantum mechanics [22-24], by the discussions around the meaning of decoherence in "fundamental" physics [25-28] and, of course, 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 of the effect in action had been seen however with SQUID's [29]. It has now been observed unquestionably in quantum optics [30]. The aim of the present work is to propose the necessary general theory.

A misconception that still seems to exist should perhaps be mentioned for appreciating the need of a general theory. It originated in an interesting remark by Caldeira and Leggett (in [9], Appendix C) . When considering a superconductor, they noticed that one can formally associate an oscillator with each energy level of the environment. Because there are so many levels, the ideal oscillators must be in their ground state or first excited state (which represent a non-occupied or occupied energy level) and they have a negligible probability to be in a higher excited state. One must be careful however not to extend this remark outside the very special case where it holds. Though the representation of the environment itself by oscillators is always correct, the coupling H_1 is almost never linear in the oscillators (p, q) 's, as one may check in the case of a gaseous environment. It would be therefore an error to believe that the oscillator model has a wide range of applicability and, too often, the success of its results have been wrongly considered as justifying its validity. It will be shown here that, on the contrary, Eq.(1.3) is representative of most practical cases, if not all, and its range of validity much exceeds the very restricted range of the oscillator model.

It may be useful, as a preliminary to more formal considerations, to think of a simple example. 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 is in a gedanken cylinder (a geometric abstraction) containing a gas, which constitutes the environment. The piston can maintain the gas molecules on one side if one takes for the interaction hamiltonian $H_1 = \sum_j v(x - x_j)$, where the summation is over the gas molecules

and v is a sufficiently repulsive potential. This example will be helpful for making some ideas clearer.

The theory will be approached in two rather different ways and it will first be described along the easiest one, which is how it was found. The idea was to try using a density operator

$$D_0 = \rho_c \otimes \rho_e, \quad (1.5)$$

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

$$\rho_e = \exp[-\beta (H_e - F)]. \quad (1.6)$$

The quantities β and F are determined by the conditions

$$\text{Tr}_e \rho_e = 1 ; E_e \equiv \text{Tr}_e (H_e \rho_e) = \text{Tr} (H_e D), \quad (1.7)$$

where Tr_e means a trace over the environment Hilbert space $\mathcal{H}_e$ and Tr means a complete trace. Eqs.(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 because of the inelastic collisions of the piston with a molecule (or a small bunch of mutually interacting molecules). The parameters β and F therefore fluctuate. Their time average may also change more slowly because of dissipation. It should be stressed in any case that *one does not assume the environment to be really in thermal equilibrium* and ρ_e is no more than a mathematical device.

A theory, however "general" as it pretends to be, must make some assumptions. The present one will assume an interaction small enough for being considered as a perturbation. Our example shows however that this assumption would be much too strong if applied to H_1 : the repulsive potential v between the piston and a gas molecule must be large for the piston to be worth its name. One therefore introduces the average

$$\Delta H_c = \text{Tr}_e (\rho_e H_1). \quad (1.8)$$

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

$$H'_1 = H_1 - \Delta H_c \otimes I_e, \quad (1.9)$$

is a small quantity. It represents in our example the fluctuating part in the collisions. *The basic assumption of the theory will be that H_1 is small.*

It will be shown in Section 2 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

$$i\dot{D} = [H, D], \quad (1.10)$$

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

$$D_1 = D - D_0, \quad (1.11)$$

inevitably entering in the calculations, cannot be small. It will be found however to act small.

The master equation might be used for interesting investigations but, as shown in Section 3, it becomes much simpler when there exists a preferred basis. A simple sufficient criterion for this will be given : A complete set of commuting observables X in the collective Hilbert space $\mathcal{H}_c$ will be called "microstable" if

$$[X, H_1] = 0. \quad (1.12)$$

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

$$[H, X] = [H_c + \Delta H_c, X]. \quad (1.13)$$

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, 31]. Another interesting example will be given for an induction circuit. This will show that microstable observables can be sometimes extended from classical mechanics to some other domain of classical physics, but not to every domain and not for every problem. This opens an interesting new field, which we have not explored.

The master equation derived from this in Section 4 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 Section 5. 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 much less obvious. This is considered in Section 6. Section 7 will sum up the various assumptions that are introduced in the construction and indicates which result depends on what assumption.

This balance of assumptions and results shows that the framework we used is not yet general enough. A realistic quantum measurement cannot be properly represented by this theory, because the collective, or relevant observables can change with time. In a bubble chamber for instance, every new-born bubble asks for its share of a new Hilbert space $\mathcal{H}_C$. Consistent histories could deal with this situation but, their consistency would follow from decoherence and this remains to be shown. There are also some questions about the theory itself : Why does the guess (11.5) work; why does D_1 act small though not being small ? To improve the theory, one must understand the key of its success.

There exists fortunately an answer to these expectations and these questions. It is offered by the general theory of quantum irreversible processes [32, 33], to which we shall turn in Section 8. It will be shown in Section 9 that the initial approach is in fact a special case of these methods. If one recalls that the larger framework is not restricted in principle to systems that are near equilibrium nor to a family of fixed relevant observables, it seems that one has really obtained the correct framework for a general theory of decoherence.

2. 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

$$\rho_C = \text{Tr}_E D, \quad (2.1)$$

$$d(\beta F)/dt - (d\beta/dt) \text{Tr}_e H_e = d(\beta F)/dt - (d\beta/dt) E_e = 0, \quad (2.2)$$

$$\text{Tr}_e [H'_1, \rho_e] = 0, \quad (2.3)$$

$$\text{Tr}_e D_1 = 0. \quad (2.4)$$

The first relation is the definition of the reduced density operator ρ_c . 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

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

where

$$\Omega = \text{Tr}_e [H'_1, D_1]. \quad (2.6)$$

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

$$i \dot{D}_1 = [H, D_1] + [H'_1, D_0] + A, \quad (2.7)$$

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

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

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

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

$$i\dot{D}'_1 = [H, D'_1] + B, \quad (2.10)$$

$$B = -i \beta (E_e - H_e) D_0 + [H'_1, D_0] \quad (2.11)$$

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

$$U(t, t') = T \exp\left(-i \int_{t'}^t H(t'') dt''\right) \quad (2.13)$$

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

$$D'_1(t) = -i \int_0^t U(t, t') B(t') U^\dagger(t, t') dt', \quad (2.14)$$

Eq.(2.9) gives, at first order in perturbation theory

$$D'_1 - D_1 = \int_0^t U(t, t') \rho_e \otimes \Omega(t') U^\dagger(t, t') dt'. \quad (2.15)$$

Introducing the quantity $\Omega' = \text{Tr}_e [H'_1, D'_1]$, Eq. (2.15) gives

$$\Omega' - \Omega = - (i/\hbar) \text{Tr}_e \left\{ [H'_1, \int_0^t U(t, t') \rho_e \otimes \Omega(t') U^\dagger(t, t') dt'] \right\}.$$

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.(2.14) 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

$\text{Tr} O D_1$ 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

$$\begin{aligned} \dot{\rho}_c + i [H_c + \Delta H_c, \rho_c] = \\ - \int_0^t \text{Tr}_e \{ [H'_1(t), U_c U_e(t, t')] [H'_1(t'), D_0(t')] U_c^\dagger U_e^\dagger(t, t')] \} dt'. \end{aligned} \quad (2.16)$$

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

3. Microstable bases and their meaning.

The master equation (2.16) 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 to look 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 $\mathcal{H}_e$ in H_e . As a matter of fact, the most useful basis in $\mathcal{H}_c$ may be sometimes 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 the most general case. 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

$$[H'_1, X] = 0. \quad (3.1)$$

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

$$-i\dot{X} \equiv [H, X] = [H_C + \Delta H_C, X]. \quad (3.2)$$

When X represents a set of position coordinates $\{X_i\}$ with a kinetic energy $(1/2) (M^{-1})_{ij} P_i P_j$, 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 solids 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 $\sum (p_\alpha^2/2m_\alpha + v_{\alpha\beta})$. 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 semi-classical physics has only reached presently a description of classical physics in configuration space (See however [31]), and one did not remember how surprised Schrödinger was to find that wave functions are defined in a configuration place .

Another interesting example is offered by an induction loop, such as the ones that are used in a superconducting quantum interference device [29]. 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 [34]. 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

$$\langle x \ n | H'_1 | x' \ n' \rangle = \delta(x-x') V_{nn'}(x). \quad (3.3)$$

The master equation (2.16) suggests the introduction of convenient correlation functions that are defined by

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

$$G(x', x, t - t') = \text{Tr}_e \{ V(x', t) \rho_e U_e(t, t') V(x, t') U_e^\dagger(t, t') \} \quad (3.5)$$

One does not need to take care in these expressions of the slightly fluctuating character of ρ_e nor of its regular 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 [35, 36], so that these functions depend only upon $t - t'$. More explicitly, one has

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

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

$$G(x', x, \tau) = F(x, x', -\tau) = F^*(x', x, \tau), \quad (3.7)$$

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 $(1/2)(x' + x)$ 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.

4. Decoherence

The existence of a microstable basis will now be used to extract the effects of decoherence and dissipation from the master equation (2.16). 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

$$U_c(t - t') \approx I - i (H_c + \Delta H_c) (t - t') \quad (4.1)$$

is certainly sufficient. One can moreover keep only the terms in Eq.(2.16) that are at most linear in $t - t'$. One can therefore write the master equation as

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

where the index d stands for decoherence and f for friction. These two terms correspond respectively to the leading terms one obtains in Eq.(2.16) by putting $U_c(t - t') = I$ 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

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

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

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

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

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

One can introduce the real and imaginary parts of the function $F(x', x, \tau)$ by $F = F_1 + i F_2$, with the symmetry properties following from Eq.(3.7)

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

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

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

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

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

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

The decoherence effect is most easily seen if one takes advantage of the sort 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 letting the slow dependence upon $(x' + x)$ unwritten, one has

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

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

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

the decoherence coefficients μ_{ij} being given by

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

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

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

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

$$\langle x' | \rho_c(t) | x \rangle \approx \langle x' | \rho_c(0) | x \rangle \exp(-\mu (x' - x)^2 t) \quad (4.13)$$

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].

5. 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.(2.16) by

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

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 $(1/2) (M^{-1})_{ij} P_i P_j + V(X)$. The conjugation of these three assumptions is somewhat restrictive, though still frequently met, but our aim is only to clarify the meaning of the results. 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

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

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

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 $\rho_c(x', x)$ to a quasi-diagonal form. This means that one can write

$$\int_0^\infty F_2(x', x, \tau) \tau \delta\tau = a + (M\gamma/4) (x' - x)^2, \quad (5.2)$$

still leaving aside a possible smooth dependence on $(x + x')$, and neglecting terms of higher order in $(x' - x)^2$ that are 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

$$R_f = - \gamma (x' - x) (\partial/\partial x' - \partial/\partial x) \rho_c(x', x). \quad (5.3)$$

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

$$d\langle P \rangle / dt = - \langle \partial V / \partial x \rangle - \gamma \langle P \rangle. \quad (5.4)$$

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

$$\int_0^\infty F_2(x', x, \tau) \tau d\tau = (\beta/2) \int_0^\infty F_1(x', x, \tau) d\tau. \quad (5.5)$$

and since

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

one has $\mu = 2MT\gamma$. Reintroducing explicitly Planck's constant and several degrees of freedom, one obtains

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

6. 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 (2.16) involves also the kind of double commutator that was postulated in the quantum diffusion model [37- 40]. 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 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 , used in ρ_n , is made of free incoming plane waves $\phi_p(x) = \exp(ipx)$, 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-know Lippmann-Scwinger relation in scattering theory [41] , one has

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

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. Since there on, the calculation can proceed as it was done by Joos and Zeh.

One cannot fail to mention a most important aspect of decoherence, which is very frequently a semi-classical behavior of the collective subsystem. This question has been considered however with great care by Gell-Mann and Hartle[31] and there is nothing essential to add to their work.

7. 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 (2.16).

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 section 5 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 von Neumann famous model [42] 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 p_c as a relevant quantity and this does not necessarily demands 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, as long as no counter-example is found.

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 [32 - 33] 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 [33]. 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.

8. An approach using the theory of irreversible processes

The theory of irreversible processes is now far from being restricted to systems near thermal equilibrium. We shall rely upon its formulation by Balian and coworkers [32 - 33]. 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 Hilbert space H and the dual space of densities made of operators that are not necessarily supposed to be positive nor with trace 1. Duality (linear functionals) is expressed by a "scalar product" between an operator A and a density Δ denoted by

$$(A ; \Delta) \equiv \text{Tr} A \Delta. \quad (8.1)$$

The relevant observables we shall use are

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

collectively denoted by A^i . Though $|x\rangle\langle x'|$ is not an observable, it is a combination of the observables $(1/2)(|x\rangle\langle x'| + |x'\rangle\langle x|)$ 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

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

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

$$D_0 = \exp(-\lambda_i A^i), \quad (8.4)$$

the parameters λ_i being determined by the conditions $\text{Tr} A^i D_0 = a^i$. 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 indicates 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 presently in practice the total hamiltonian H . The first requirement is already satisfied since I is a linear combinations 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

$$E_0 = \exp[- \int \lambda_{xx'} A^{xx'} dx dx' - \beta (H_e + H'_1)]$$

These two reference densities are related in perturbation theory by

$$E_0 = D_0 - \beta \int_0^1 D_0^{1-u} H'_1 D_0^u du \\ + \beta^2 \int D_0^{1-u-v} H'_1 D_0^u H'_1 D_0^v du dv$$

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 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

$$\dot{D} = \mathcal{L} D, \quad (8.5)$$

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

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

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

$$s_i = \partial D_0 / \partial a^i, \text{ i. e. } s_{xx'} = |x'\rangle \langle x| \otimes \rho_e, \quad s_e = \rho_c \otimes (H_e - E_e) \Delta_2. \quad (8.7)$$

$$\Delta_2 = \text{Tr}_e H_e^2 \rho_e - E_e^2. \quad (8.8)$$

They satisfy the orthogonality relations

$$(A^i; s_j) \equiv \text{Tr } A^i s_j = \delta^i_j. \quad (8.9)$$

In view of Eq.(8.9), the superoperator

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

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

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

Explicitly, one has

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

Our previous densities D_0 and D_1 are given by

$$D_0 = \mathcal{P}D, \quad D_1 = QD, \quad D = D_0 + D_1. \quad (8.13)$$

9. The master equation

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

$$\dot{D}_0 - \mathcal{P} \mathcal{L} \mathcal{P} D_0 = \mathcal{P} \mathcal{L} D_1 + \dot{\mathcal{P}} Q D_1, \quad (9.1)$$

$$\dot{D}_1 - Q \mathcal{L} Q D_1 = - \dot{\mathcal{P}} Q D_1 - \dot{\mathcal{P}} D_0 + Q \mathcal{L} \mathcal{P} D_0. \quad (9.2)$$

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

$$\dot{\mathcal{P}} Q \Delta = - i (1/\Delta E_e^2) \rho_c (E_e - H_e) \rho_e \text{Tr}([H'_1 H_e] \Delta). \quad (9.3)$$

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). Putting $D_2 = - \dot{\mathcal{P}} D_0 + Q \mathcal{L} \mathcal{P} D_0$ and using $\mathcal{P} D_0 = D_0$, which gives $\dot{\mathcal{P}} D_0 = Q \dot{D}_0$, one gets

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

Eq.(9.2) becomes

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

One may notice that $Q D_2 = D_2$. Introducing the operator^(b)

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

the solution of Eq.(9.5) at first order in H'_1 (which will turn out to be enough), is given by

$$D_1 = D_a + D_b, \quad (9.7)$$

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

$$D_b = \int_0^t dt' \mathcal{W}(t, t') (-\dot{\mathcal{P}} Q(t')) \int_0^{t'} dt'' \mathcal{W}(t', t'') Q(t'') D_2(t''). \quad (9.9)$$

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 $H'1$),

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

It does not look particularly simple. It might also be noticed that, since $\mathcal{P}$ and Q , according to Eq.(8.12), depend upon ρ_c , the master equation looks non-linear. Non-linearity is in fact 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 $\rho_c = \text{Tr}_e D$ imply that the present equation must be linear, which is of course verified by the explicit calculation to follow.

As a matter of fact, one is not directly interested in D_0 but in $\rho_c = \text{Tr}_e D_0$. This gives the reduced master equation (see the Appendix)

$$\dot{\rho}_c - (1/i) [H_c + \Delta H_c, \rho_c] = (1/i) \text{Tr}_e [H, D_a + D_b] + (1/i) \text{Tr}_e [H, \dot{\mathcal{P}} Q D_a]. \quad (9.11)$$

The calculations indicated in the Appendix, to second order in $H'1$, show that this equation coincides with the master equation (2.16) one already obtained by a direct method.

10. Conclusions

Two different methods have been proposed for obtaining a master equation for decoherence. The direct method was explained in the Introduction and a rather detailed summary of its results was given in Section 7. The second method, though applied here with the same assumptions, relies on a general theory of irreversible processes, showing that the method can cover, at least in principle, the problems one must solve for a realistic and complete account of quantum measurements. The effect of decoherence has thus been shown to be a particularly interesting irreversible process, though only one such process. This is an important epistemic finding since it shows, as noted elsewhere [24] that the reflections about the "practical for all purposes" or "fundamental" meaning of decoherence [25 - 27] cannot be distinguished from the similar problems that arose in statistical mechanics since the work of Boltzmann.

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

Acknowledgements

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Appendix : The proof of some intermediate results.

Staightforward, even if tedious, algebraic calculations will no be given explicitly. There are however some intermediate steps that may require some care and they are given in the present Appendix.

Why $\dot{\beta}$ does not affect decoherence (Section 2).

Some terms involving the derivative $\dot{\beta}$ of the inverse temperature were neglected in Section 2. This is justified when there exists a system of microstable observables X . as follows.

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

$$\dot{E}_e = - \dot{\beta} \Delta_2 = \text{Tr } H_e \dot{D} = - i \text{Tr } (H_e [H, D]) = - i \text{Tr } (H_e [H'1, D]) , \quad (\text{A.1})$$

where $\Delta_2 = \text{Tr}_e(H_e^2 \rho_e) - E_e^2$ and the last equality is easily obtained by introducing a basis $|x\rangle$. 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 the equation (A.1) 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.(A.1) that $\dot{\beta}$ is a quantity of second order. Another proof, following from the approach by irreversibility, is a consequence of the calculations at the end of this Appendix and shows that the assumption of a microstable basis is not necessary.

The proof of Eq.(9.3)

One has obviously

$$\dot{\mathcal{P}} Q \Delta = \dot{\mathcal{P}} \Delta - \dot{\mathcal{P}} \mathcal{P} \Delta. \quad (\text{A2})$$

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

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

This gives

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

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).

The proof of Eq.(9.11)

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

$$\text{Tr}_e \mathcal{P} \mathcal{L} \Delta = (1/i) \text{Tr}_e [H, \Delta]. \quad (\text{A.5})$$

This gives, in view of some vanishing traces,

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

According to Eq.(8.12), one has $\text{Tr}_e \mathcal{P} \Delta = \text{Tr}_e \Delta$ so that $\text{Tr}_e Q \Delta = 0$.

Therefore, $\text{Tr}_e \dot{\mathcal{P}} D_0 = \text{Tr}_e Q \dot{D}_0 = 0$.

Derivation of the master equation from Eq.(9.11)

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

$$D_2 = (1/i) [H, D_0] - (1/i) \rho_e \text{Tr}_e [H, D_0]$$

$$- A \{ \text{Tr}(\text{He}\dot{D}_0) - (1/i) \text{Tr}(\text{He}[H, D_0]) \} \quad (\text{A.6})$$

with

$$A = D_0 (H_e - E_e)/\Delta_2. \quad (\text{A.7})$$

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

$$\text{Tr}(\text{He}\dot{D}_0) = \rho_c \dot{E}_e,$$

and

$$\dot{E}_e = \text{Tr}(\text{He}\dot{D}) = (1/i) \text{Tr}(\text{He}[H, D]) = (1/i) \text{Tr}(\text{He}[H'_1, D]) .$$

The coefficient of A in Eq.(A.6) is therefore $(1/i) \text{Tr}(\text{He}[H'_1, D_1])$. This gives

$$D_2 = (1/i) [H'_1, D_0] - (1/i) A \text{Tr}(\text{He}[H'_1, D_1]) , \quad (\text{A.8})$$

which implies

$$\text{Tr}_e D_2 = 0 \quad (\text{A.9})$$

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

$$\begin{aligned} i\dot{F} = i Q \mathcal{L} Q F &= [H, F] - \rho_e \text{Tr}_e[H, F] - [H, \rho_e \text{Tr}_e F] \\ &+ \rho_e [H_c + \Delta H_c, \text{Tr}_e F] - [H, A] \cdot \text{Tr}(H - E_e)F. \end{aligned} \quad (\text{A.10})$$

This implies $\text{Tr}_e \dot{F} = 0$ and in view of Eq.(A.9),

$$\text{Tr}_e F = 0. \quad (\text{A.11})$$

This leaves one with

$$i\dot{F} = [H, F] - \rho_e \text{Tr}_e[H, F] - [H, A] \cdot \text{Tr}(HF), \quad (\text{A.12})$$

which implies

$$\begin{aligned} i \frac{d}{dt} \text{Tr}(HF) &= - \text{Tr}(H \rho_e \text{Tr}_e[H, F]) = - \text{Tr}_c((H_c + \Delta H_c) \cdot \text{Tr}_e[H'_1, F]) \\ &= - \text{Tr}((H_c + \Delta H_c) [H'_1, F]), \end{aligned} \quad (\text{A.13})$$

but from Eq.(A.7), one sees that $\text{Tr}HD_2$ is at most of first order in H'_1 so that $\text{Tr}(HF)$ is also at most of first order. On the other hand, in view of Eq.(A.10), one has $\text{Tr}_e[H, F] = \text{Tr}_e[H'_1, F]$. Eq.(A.10) becomes therefore

$$i\dot{F} - [H, F] = - \rho_e \text{Tr}_e[H, F] - [H, A] \cdot \text{Tr}(HF) = - B, \quad (\text{A.14})$$

where B is of first order in H'_1 . This equation can be solved at first order to give

$$\begin{aligned} D_a(t) &= U(t, t') D_2(t') U^\dagger(t, t') \\ &\quad - (1/i) \int_{t'}^t U(t, t'') B(t'') U^\dagger(t, t'') dt''. \end{aligned} \quad (\text{A.15})$$

The end of the calculation is straightforward and it is convenient to use the expression (A.6) for D_2 . One finds that the second term in Eq.(A.15) gives a negligible contribution to the master equation (of third order in H'_1). Similarly the contributions $(1/i) \text{Tr}_e[H, D_b]$ and $(1/i) \text{Tr}_e[H, \dot{\mathcal{P}} Q D_a]$ to Eq.(9.11) are negligible.

Footnotes and References

(a) Laboratoire associé au CNRS.

(b) It should be noticed that the "memory kernel" used by Balian is our $\mathcal{W} Q$, which he calls $\mathcal{W}$.

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