

Can Environmental Decoherence be Reversed for an Open Quantum System in a Magnetic field ?

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Abstract

A simple model is considered for an open system consisting of an aggregation of magnetic particles (like greigite) in the presence of a magnetic field (H), and interacting linearly with a bath of 3D harmonic oscillators. Using the Feynman-Vernon formalism, as given in Weiss (termed FVW), the time-evolved reduced density matrix (after eliminating the bath d.o.f.'s), is examined for environmental decoherence as defined in the FVW formalism. While decoherence is usually positive for most two-way couplings with the environment, it is found that a *three – way* interaction involving the system plus bath plus H-field all together, can facilitate a *reversal* of sign of this quantity ! This may have implications for quantum coherence based phenomena on the origins of life.

Key words : Decoherence; field-induced aggregate; H-field; 3-way coupling; sign reversal

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1 Introduction : Preliminaries

Decoherence is a ubiquitous phenomenon [1] which arises when one attempts to extend quantum theory to macro systems (and even to meso systems). Since environment has a crucial role for a quantum system, the relevant theoretical framework for the study of decoherence is a theory of open quantum systems which treats the effect of an uncontrollable environment on the quantum evolution. The concept was originally developed to incorporate the effect of friction and thermalization in a quantum formalism, but a correct perspective of decoherence effects requires its time scale to be much shorter than typical ‘relaxation’ phenomena. Rather ironically, decoherence is not so much about *how* a bath d.o.f. affects the system, as *viceversa*, the latter revealing information on the state of the system. The relevance of decoherence is especially acute for quantum information processing tasks where the coherence of many quantum systems must be maintained for a long time. To explain decoherence in a nut-shell, one may crudely assume that the interaction between the quantum system and environment is short-ranged enough to be described by scattering theory for asymptotically ‘free’ states before and after the interaction, so that the detailed anatomy of the collision dynamics itself does not come into

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the picture. Let ρ be density operator for the system which, for simplicity, interacts with a single environment d.o.f. represented by $|\psi\rangle$. Then it can be shown that the *diagonal* elements of ρ remain unchanged by interaction, i.e., $\rho'_{mm} = \rho_{mm}$. But the off-diagonal elements ρ'_{mn} after interaction are no longer equal to ρ_{mn} before interaction. Rather, they get suppressed by a factor $\langle \psi^n | \psi^m \rangle$ whose magnitude is always less than unity. And since the off-diagonal elements are the repository of quantum effects, this suppression is tantamount to loss of *ability* of the system to show quantum behaviour due to the interaction with the environment's quantum d.o.f. [It arises from the correlation between the system plus environment particle]. So, if the environmental d.o.f. is integrated out, this *ability* is lost. Alternatively, the interaction is an information transfer from the system to the environment. The more the overlap $\langle \psi^n | \psi^m \rangle$ deviates from unity, the more an observer could in principle learn about the system by measuring the environmental particle! But this measurement is usually never made, so this alternative principle explains that the wave-like interference phenomenon characterized by the coherence *vanishes* as more information discriminating the distinct "particle-like" system is revealed.

Against this background, we may regard that decoherence that is inherent in the decay of an open quantum system into the surroundings, leads to a destruction of phase correlations within the system. The issue of decoherence of such a system due to its interaction with a thermal bath of harmonic oscillators was first formulated by Feynman and Vernon [2] and addressed subsequently by many workers, notably Grabert-Schramm-Ingold [3] as well as Caldeira-Leggett [4]. The result of many of these studies has been incorporated in a comprehensive book by Weiss [5] which will be taken as a standard reference for the present investigation. We shall freely use the results of ref [5], often under the name FVW, and in the same notation where possible without explanation. Specifically we consider an 'open' system consisting of an aggregation of magnetic particles (such as greigite) in the presence of a magnetic field (H), and interacting linearly with a bath of 3D harmonic oscillators. While several types of two-way interaction of the system with the bath has been adequately covered in FVW, the possibility of new forms of interactions when an external magnetic field is present, and their effect on the resulting decoherence, is the subject of this paper.

In Section 2 we collect the relevant formulae from ref.[5] under the further assumption of slow time variation, so as to simplify the essential formulae, as well as extend them from 1 to 3 dimensions before identifying the decoherence rate. In Section 3 we introduce the H-field and examine the effect of a new form of interaction—a *three-way* coupling involving the system, bath and field. To the best of our knowledge such a *direct* 3-way coupling has not been considered in the literature [5], a novel feature being that the calculated decoherence has a *negative* sign; its origin is of course accounted for, and its order of magnitude estimated. Section 4 discusses the significance of this result and its possible interpretation on the lines of a Froehlich-like mechanism [6].(In Appendix A we re-derive a formula for the problem 3-11 of Feynman-Hibbs [7], since a term appears to be missing in it).

2 Essential Results for System plus Bath Coupling

From Eq (3.11) of Weiss[5], the System-Bath Hamiltonian has the form

$$H = \frac{p^2}{2M} + \sum_1^N \frac{p_\alpha^2}{2m_\alpha} + V(q, x) \quad (2.1)$$

$$V(q, x) = V(q) + \frac{1}{2} \sum_1^N m_\alpha \omega_\alpha^2 \left(x_\alpha - \frac{c_\alpha q}{m_\alpha \omega_\alpha^2} \right)^2 \quad (2.2)$$

This Hamiltonian serves two purposes : A) As the Euclidean Lagrangian (with imaginary Matsubara time [5]) in quantum statistical mechanics for the calculation of the density matrix under thermal equilibrium conditions a la Feynman-Hibbs [7] and Weiss [5]; B) as the Hamiltonian corresponding to a real-time Lagrangian (obtained by changing the sign for the potential term V) which participates in the time-evolution of the density matrix for the joint system-bath complex under non-equilibrium conditions, using real time path integral techniques [4, 5, 7]. The Matsubara time τ is related to the real time t by $t = -i\tau$, and varies in the range

$$0 \leq \tau \leq \hbar\beta = \hbar/kT \quad (2.3)$$

The global density matrix $W(0)$ for the initial state $t=0$ is assumed for simplicity to be in a factorized form in which the system and bath are decoupled [4,5], and the unperturbed bath is in thermal equilibrium, given by (see eq (5.10) of [5]):

$$W(0) = \rho(0) \otimes W_R(0); \quad W_R(0) = Z_R^{-1} \exp\{-\beta H_R\} \quad (2.4)$$

Here ρ is the reduced density matrix for the system whose time evolution $\rho(t)$ is the primary object of interest. To that end note that the global density matrix $W(t)$ evolves from a state $W(0)$ at $t=0$ as (see eq.(5.1) of [5])

$$W(t) = \exp\{-iHt/\hbar\} W(0) \exp\{+iHt/\hbar\} \quad (2.5)$$

We now skip most of the formalism which is outlined in sections (5.1-2) of Weiss [5], and focus on the time evolution $\rho(t)$ of the reduced density matrix after eliminating the bath d.o.f.'s. This quantity can be expressed in terms of the Feynman-Vernon influence functional F_{FV} as follows [5]

$$\rho(q_f q_f'; t) = \int dq_i dq_i' \int Dq Dq' \exp[i(S_S[q] - S_S[q'])/\hbar] F_{FV}[q, q'] \quad (2.6)$$

F_{FV} in turn is made up as a product of two functionals F, F^* :

$$F_{FV}[q, q'] = \int dx_f dx_i dx_i' W_R[x_i, x_i'] F[q; x_f x_i] F^*[q'; x_f x_i'] \quad (2.7)$$

where

$$F[q; x_f x_i] = \int Dx(\cdot) \exp[i(S_R[x]) + S_I[x, q)]/\hbar] \quad (2.8)$$

and a similar expression for the (complex conjugated) quantity $F^*[q'; x_f x_i']$. The quantity $W_R[x_i, x_i']$ in eq(2.7) which also appears in eq (2.4), is the canonocal density matrix for the bath in thermal equilibrium, and its path integral over the (imaginary) Matsubara time τ is (see eq (5.17) of [5]) a product of modes $W_{R\alpha}$ where (see eq (5.17) of [5])

$$W_{R\alpha}[x_i, x_i'] = C_\alpha \exp\left\{ \frac{-m_\alpha \omega_\alpha}{2\hbar \sinh \beta \hbar \omega_\alpha} [(x_{i\alpha}^2 + x_{i\alpha}'^2) \cosh \beta \hbar \omega_\alpha - 2x_{i\alpha} x_{i\alpha}'] \right\} \quad (2.9)$$

Similarly the quantity $F[q; x_f x_i]$ is expressible as a product of its modes F_α whose path integral over real time [7,5] works out as [5]

$$F_\alpha[x_{f\alpha}, x_{i\alpha}] = C_\alpha(t) \exp\left\{\frac{i}{\hbar}\phi_\alpha[q; x_{f\alpha}, x_{i\alpha}]\right\} \quad (2.10)$$

where $C_\alpha(t)$ is a constant, and ϕ_α is given by eq (5.19) of ref [5]. However we prefer to give a simplified expression for ϕ_α and a corresponding quantity ϕ'_α arising from $F^*[q'; x_f x'_i]$ of eq (2.7), based on an (approximate) time independence of q and q' , which may be adapted from eq.(A.7) of Appendix A. The result for ϕ_α , mostly in the notation of ref [5], is

$$\begin{aligned} \phi_\alpha &= \frac{m_\alpha \omega_\alpha}{2 \sin \omega_\alpha t} [(x_{i\alpha}^2 + x_{f\alpha}^2) \cos \omega_\alpha t - 2x_{i\alpha} x_{f\alpha}] \\ &+ c_\alpha (x_{i\alpha} + x_{f\alpha}) q \frac{1 - \cos \omega_\alpha t}{\omega_\alpha \sin \omega_\alpha t} - \frac{c_\alpha^2 q^2 (1 - \cos \omega_\alpha t)^2}{2m_\alpha \omega_\alpha^3 \sin \omega_\alpha t} \\ &+ \frac{c_\alpha^2 q^2}{2m_\alpha \omega_\alpha^2} \left[t - \frac{\sin \omega_\alpha t}{\omega_\alpha} \right] \end{aligned} \quad (2.11)$$

The corresponding quantity ϕ'_α which comes with a negative sign, arising as it does from $F^*[q'; x_f x'_i]$, is given by a similar expression to (2.11), except for

$$x_{i\alpha} \Rightarrow x'_{i\alpha}; \quad q \Rightarrow q'$$

The rest of the calculation which involves the integration over the bath d.o.f.'s, is straightforward though lengthy. Following Weiss [5], introduce the variables

$$\sqrt{2}[z_{i\alpha}; y_{i\alpha}] = x_{i\alpha} \pm x'_{i\alpha} \quad (2.12)$$

The integration in eq(2.6) for the reduced density matrix ρ , over the variables z, y, x_f , all standard gaussian variables, is best carried out successively in this very order. The result for the related Feynman-Vernon influence functional $F_{FV}[q, q']$, eq.(2.7), which subsumes all the pre-exponential factors a la ref [4], is

$$\begin{aligned} F_{FV}[q, q'] &= \exp\{-S_{FV}[q, q']/\hbar\} \\ S_{FV}[q, q'] &= \frac{1}{2} \sum_\alpha \frac{c_\alpha^2 (q - q')^2}{\hbar m_\alpha \omega_\alpha^3} \coth(\beta \hbar \omega_\alpha / 2) (1 - \cos \omega_\alpha t) \\ &- \frac{i}{2} \sum_\alpha \frac{c_\alpha^2 (q^2 - q'^2)}{\hbar m_\alpha \omega_\alpha^3} \left(t - \frac{\sin \omega_\alpha t}{\omega_\alpha} \right) \end{aligned} \quad (2.13)$$

From (2.13) we can identify the decoherence factor [5] as the first term $S_y^{(N)}$ of $S_{FV}[q, q']$ in (2.13), which is seen to be *positive*. It can be recast as an integral over the "spectral density" defined by [4]

$$J(\omega) \equiv \frac{\pi}{2} \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha) \quad (2.14)$$

which allows it to be expressible as [5]

$$S_y^{(N)} = \frac{1}{\pi} \int_0^\infty J(\omega) \frac{q_0^2}{\hbar \omega^2} \coth(\beta \hbar \omega / 2) (1 - \cos \omega t) \quad (2.15)$$

where $q_0 = q - q'$ is the spatial separation of two different localized states [4]. The decoherence rate γ_{decoh} is just the time derivative of $S_y^{(N)}/\hbar$, which simplifies in the regime of high temperature ($\beta = 1/k_B T$) for the ohmic case $J(\omega) = \eta\omega$ as [5]

$$\gamma_{decoh} = \frac{\eta q_0^2}{\pi \hbar^2 \beta} \int_{-\infty}^{+\infty} d\omega \frac{\omega \sin \omega t}{\omega^2 + \omega_0^2} \quad (2.16)$$

where we have inserted an infrared cut-off frequency ω_0 which, although not needed here, will be found useful for later purposes (see below). We also note that the damping rate is negligible compared with the decoherence rate [5]. The integral is now evaluated as a contour integral to give

$$\gamma_{decoh} = \frac{q_0^2 \eta}{\beta \hbar^2} \exp\{-t\omega_0\} \quad (2.17)$$

We now turn to a generalization of this 1D formula to 3D, so as to include the effect of an external magnetic field.

3 Effect of H-field on Decoherence

The generalization of the foregoing result to 3D is merely a matter of replacements like

$$qq' \Rightarrow \mathbf{q} \cdot \mathbf{q}'; \quad qx_{i\alpha} \Rightarrow \mathbf{q} \cdot \mathbf{x}_{i\alpha}$$

in the Hamiltonian (2.1) and the potential term (2.2). More interesting coupling structures arise with the introduction of an external (magnetic) field. While pairwise interactions do not produce any new structures, there is now the possibility of *three – way* interactions which have more interesting features. The simplest form of the latter for a spin-half magnet of moment $\mu\sigma$ is

$$V_3 = \frac{q_0}{\hbar\omega_{i\alpha}} i\mu\sigma \times \mathbf{H} \cdot c_\alpha \mathbf{x}_{i\alpha} \quad (3.1)$$

where the factor i associated with $\mu\sigma$ meets the hermiticity requirement. And the factor in front ensures dimensional homogeneity with the formalism of Section 2. Note the correspondence $q \Leftrightarrow \mathbf{Q}$ where

$$\mathbf{Q} \equiv \frac{q_0}{\hbar\omega_{i\alpha}} i\mu\sigma \times \mathbf{H} \quad (3.2)$$

The formalism now goes through just as in Section 2 (adapted to the 3D form) as indicated above, except for the replacement of $q_0^2 = (q - q')^2$ in (2.15) by

$$\mathbf{Q}^2 = \frac{q_0^2}{\hbar^2 \omega_{i\alpha}^2} \{i\}^2 (\mu)^2 2H^2 \quad (3.3)$$

making use of the result $(\sigma \times H)^2 = 2H^2$. Note that the presence of the factor $\{i\}^2$ in (3.3) renders the quantity *negative* as a whole, thus *reversing* the sign of the decoherence factor! This brings out the central result of this exercise: The 3-way coupling involving the magnetic field gives a contribution to the decoherence with a *reversed* sign. As to the magnitude of the effect vis-a-vis the reference value (2.17), the counterpart of (2.16) reads as

$$\begin{aligned} \gamma_{decoh}^H &= \frac{i^2 \eta q_0^2}{\pi \hbar^2 \beta} \int_{-\infty}^{+\infty} d\omega \frac{2\omega_H^2 \omega \sin \omega t}{(\omega^2 + \omega_0^2)^2} \\ \omega_H^2 &= (\mu)^2 H^2 / \hbar^2 \end{aligned} \quad (3.4)$$

where the effect of the infrared cut-off frequency appears (even more strongly) in the last factor. Evaluation of the integral as a contour integration over the double pole finally gives

$$\gamma_{decoh}^H = \frac{q_0^2 \eta}{\beta \hbar^2} \frac{i^2 \omega_H^2 t}{\omega_0} \exp\{-t\omega_0\} \quad (3.5)$$

The value of t in front of the exponential on the rhs is $t \sim \omega_0^{-1}$, so that the ratio of the two decoherence factors (3.5) to (2.17) finally works out as

$$\gamma_{decoh}^H / \gamma_{decoh} \approx i^2 \omega_H^2 / \omega_0^2 \quad (3.6)$$

The factor i^2 brings out the reverse sign, while the smallness of ω_0 wrt ω_H (note that ω_0 is a small infrared cut-off, while ω_H is a finite quantity) testifies to the enhancement of the (coherence) effect.

4 Discussion

This work was motivated by the need to study the role of a magnetic field in the context of origin of life scenarios [8]. While referring the interested reader for details of the precise mechanism involved therein, suffice it to say that the principal object behind the introduction of a magnetic field is its role in bringing about *coherence* in a system whether it is directed against the dissipating effect of temperature or for generating an environment conducive to a quantum scenario. Taking a simple algebraic viewpoint, the respective signatures of coherence / decoherence must be of *opposite* signs in whatever definitions are employed for their respective measures. Viewed in that light, the result (3.6) is fully consistent with the purported introduction of a magnetic field in the interaction of an open system with its environment, viz., to reduce the effect of decoherence by a reversed sign of the contribution of the magnetic field, taking advantage of a *special 3-way coupling* involving the system, environment and the (external) magnetic field. As to the relative magnitude of the factor ω_H vis-a-vis ω_0 in Eq (3.6), the former, being a finite quantity, easily exceeds the latter which is a small infrared cut-off. Somewhat different approaches [9, 10] directed towards avoiding decoherence for open systems by adjusting external controllable parameters (such as a magnetic field) seem to converge towards similar conclusions, although employing different strategies.

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Appendix A.

Here we outline some simplified expressions for the quantities ϕ_α and ϕ'_α of Section 2, based on an elementary derivation of the classical action for a harmonic oscillator in the presence of a *constant* force f . To that end we first put on record the more general result for a time-dependent force $f(t)$, vide problem 3-11 of Feynman-Hibbs [6], mostly in their

notation, from which the result for $f = \text{const}$ follows as a particular case. [An added reason for this exercise is the appearance of an extra term in the classical action, over and above the result listed in this classic book [7], in the hope of obtaining a verdict on its bona fides from interested experts]. The classical action for this problem is given by [7]

$$S_{cl} = \int_0^T dt \left[\frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 + x f(t) \right] \quad (\text{A.1})$$

which can be transformed via the equation of motion as

$$S_{cl} = \int_0^T dt \left[\frac{1}{2} x f(t) \right] + \frac{1}{2} m [x_b \dot{x}_b - x_a \dot{x}_a] \quad (\text{A.2})$$

where x_a and x_b are the initial and final positions and their dots are the corresponding velocities. Now the solution of the equation of motion may be written as

$$x = c \exp i\omega t + c^* \exp -i\omega t + \frac{1}{m} \frac{1}{D^2 + \omega^2} f(t) \quad (\text{A.3})$$

where the last term – the particular integral PI – is obtained through the following steps

$$\begin{aligned} PI &= \frac{1}{D^2 + \omega^2} f(t)/m = \frac{1}{2im\omega} \left[\frac{1}{D - i\omega} - \frac{1}{D + i\omega} \right] f(t) \\ &= \frac{1}{2im\omega} e^{i\omega t} \int_0^t e^{-i\omega t'} f(t') dt' + c.c. \\ &= \frac{1}{2im\omega} e^{i\omega t} F_\omega(t) - \frac{1}{2im\omega} e^{-i\omega t} F_\omega^*(t) \end{aligned} \quad (\text{A.4})$$

thus defining the integral function $F_\omega(t)$ and its complex conjugate $F_\omega^*(t)$. The constants c and c^* are determined from $x_a = c + c^*$ and

$$x_b = c e^{i\omega T} + c^* e^{-i\omega T} + \frac{1}{2im\omega} [e^{i\omega T} F_\omega(T) - e^{-i\omega T} F_\omega^*(T)]$$

Straightforward substitution in (A.2) and simplification gives

$$\begin{aligned} S_{cl} &= \frac{m\omega}{2 \sin \omega T} [(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b + \frac{2x_b}{m\omega} \int_0^T f(t) \sin \omega t dt \\ &+ \frac{2x_a}{m\omega} \int_0^T f(t) \sin \omega(T-t) dt - \frac{2}{m^2 \omega^2} \end{aligned} \quad (\text{A.5})$$

$$\times \int_0^T dt \int_0^t ds f(t) f(s) \sin \omega(T-t) \sin \omega s] + S(\text{EXTRA}) \quad (\text{A.6})$$

which agrees with Feynman-Hibbs [7] as well as Weiss [5], *except* for the term $S(\text{EXTRA})$ given by

$$S(\text{EXTRA}) = \frac{1}{2m\omega} \int_0^T dt \int_0^t ds f(t) f(s) \sin \omega(t-s) \quad (\text{A.7})$$

Unfortunately we are unable to write off the last term, eq (A.6), from the complete solution given in [7]. We also note that it does not figure in Weiss [4] either, although we could not detect any error in our (repeated) calculations. Its source can be traced to the integral term in (A.2), wherein the complementary part of the x -solution, eq (A.3), contributes an amount

$$\frac{1}{2} [c F_\omega^*(T) + c^* F_\omega(T)]$$

which remains after identifying all the terms of prob 3-10 in Feynman-Hibbs [7].

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