

Decoherence and Thermalization

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We present a rigorous analysis of the phenomenon of decoherence for general N -level systems coupled to reservoirs of free massless bosonic fields. We apply our general results to the specific case of the qubit. Our approach does not involve master equation approximations and applies to a wide variety of systems which are not explicitly solvable.

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I. INTRODUCTION

We examine rigorously the phenomenon of quantum decoherence. This phenomenon is brought about by the interaction of a quantum system, called in what follows “the system S”, with an environment, or “reservoir R”. Decoherence is reflected in the temporal decay of off-diagonal elements of the reduced density matrix of the system in a given basis. The latter is determined by the measurement to be performed. To our knowledge, this phenomenon has been analyzed rigorously so far only for explicitly solvable models, see e.g. [1–7]. In this paper we consider the decoherence phenomenon for quite general non-solvable models. Our analysis is based on the modern theory of resonances for quantum statistical systems as developed in [8–13] (see also the book [14]), which is related to resonance theory in non-relativistic quantum electrodynamics [9, 15].

Let $\mathfrak{h} = \mathfrak{h}_S \otimes \mathfrak{h}_R$ be the Hilbert space of the system interacting with the environment, and let

$$H = H_S \otimes \mathbb{1}_R + \mathbb{1}_S \otimes H_R + \lambda v \quad (1)$$

be its Hamiltonian. Here, H_S and H_R are the Hamiltonians of the system and the reservoir, respectively, and λv is an interaction with a coupling constant $\lambda \in \mathbb{R}$. In the following we will omit trivial factors $\mathbb{1}_S \otimes$ and $\otimes \mathbb{1}_R$. The reservoir is taken initially in an equilibrium state at some temperature $T = 1/\beta > 0$. Let ρ_t be the density matrix of the total system at time t . The reduced density matrix (of the system S) at time t is then formally given by

$$\bar{\rho}_t = \text{Tr}_R \rho_t, \quad (2)$$

where Tr_R is the partial trace with respect to the reservoir degrees of freedom. Formulas (1) and (2) describe the situation where a state of the reservoir is given by a well-defined density matrix on the Hilbert space \mathfrak{h}_R . In order to describe decoherence and thermalization we need to consider “true” (dispersive) reservoirs, obtained for instance by taking a thermodynamic limit, or a continuous-mode limit. We refer to [16] for a detailed description of such reservoirs, which is not needed in the presentation of our results here.

Let $\rho(\beta, \lambda)$ be the equilibrium state of the interacting system at temperature $T = 1/\beta$ and set $\bar{\rho}(\beta, \lambda) := \text{Tr}_R \rho(\beta, \lambda)$. There are three possible scenarios for the asymptotic behaviour of the reduced density matrix as $t \rightarrow \infty$:

- (i) $\bar{\rho}_t \rightarrow \bar{\rho}_\infty = \bar{\rho}(\beta, \lambda)$,
- (ii) $\bar{\rho}_t \rightarrow \bar{\rho}_\infty \neq \bar{\rho}(\beta, \lambda)$,
- (iii) $\bar{\rho}_t$ does not converge.

The first situation is generic while the last two are not, although they are of interest, e.g. for energy conserving, or quantum non-demolition interactions, characterized by $[H_S, v] = 0$, see [3, 16].

Decoherence is a basis-dependent notion. It is usually defined as the vanishing of the off-diagonal elements $[\bar{\rho}_t]_{m,n}$, $m \neq n$ in the limit $t \rightarrow \infty$, in a chosen basis. Most often decoherence is defined w.r.t. the basis of eigenvectors of the system Hamiltonian H_S (the energy, or computational basis for a quantum register), though other bases, such as the position basis for a particle in a scattering medium [3], are also used.

Since $\bar{\rho}(\beta, \lambda)$ is generically non-diagonal in the energy basis, the off-diagonal elements of $\bar{\rho}_t$ will not vanish in the generic case, as $t \rightarrow \infty$. Thus, strictly speaking, decoherence in this case should be defined as the decay (convergence) of the off-diagonals of $\bar{\rho}_t$ to the corresponding off-diagonals of $\bar{\rho}(\beta, \lambda)$. The latter are $O(\lambda)$. If these terms are neglected then decoherence manifests itself as a process in which initially coherent superpositions of basis elements ψ_j become incoherent statistical mixtures,

$$\sum_{j,k} c_{j,k} |\psi_j\rangle \langle \psi_k| \longrightarrow \sum_j p_j |\psi_j\rangle \langle \psi_j|, \quad \text{as } t \rightarrow \infty.$$

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In particular, phase relations encoded in the $c_{j,k}$ disappear for large times.

II. GENERAL RESULTS

We consider N -dimensional quantum systems interacting with reservoirs of massless free quantum fields (photons, phonons or other massless excitations) through an interaction $v = G \otimes \varphi(g)$, see also (1) and (6). Here, G is a hermitian $N \times N$ matrix and $\varphi(g)$ is the bosonic field operator smoothed out with the form factor $g(k)$, $k \in \mathbb{R}^3$. For any observable A of the system we set

$$\langle A \rangle_t := \text{Tr}_S(\bar{\rho}_t A) = \text{Tr}_{S+R}(\rho_t(A \otimes \mathbb{1}_R)). \quad (3)$$

Assuming certain regularity conditions on $g(k)$ (allowing e.g. $g(k) = |k|^p e^{-|k|^m} g_1(\sigma)$ where g_1 is a function on the sphere and where $p = -1/2 + n$, $n = 0, 1, \dots$, $m = 1, 2$), we show that the ergodic averages

$$\langle \langle A \rangle \rangle_\infty := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle A \rangle_t dt$$

exist, i.e., that $\langle A \rangle_t$ converges in the ergodic sense as $t \rightarrow \infty$. Furthermore, we show that for $t \geq 0$, and for any $0 < \omega' < \frac{2\pi}{\beta}$,

$$\langle A \rangle_t - \langle \langle A \rangle \rangle_\infty = \sum_{\varepsilon \neq 0} e^{it\varepsilon} R_\varepsilon(A) + O(\lambda^2 e^{-\frac{1}{2}[\min_\varepsilon \{\text{Im } \varepsilon\} + \omega'/2]}), \quad (4)$$

where the complex numbers ε are the eigenvalues of a certain explicitly given operator $K(\omega')$, lying in the strip $\{z \in \mathbb{C} \mid 0 \leq \text{Im} z < \omega'/2\}$. They have the expansions

$$\varepsilon \equiv \varepsilon_e^{(s)} = e - \lambda^2 \delta_e^{(s)} + O(\lambda^4), \quad (5)$$

where $e \in \text{spec}(H_S \otimes \mathbb{1}_S - \mathbb{1}_S \otimes H_S) = \text{spec}(H_S) - \text{spec}(H_S)$ and the $\delta_e^{(s)}$ are the eigenvalues of a matrix Λ_e , called a *level-shift operator*, acting on the eigenspace of $H_S \otimes \mathbb{1}_S - \mathbb{1}_S \otimes H_S$ corresponding to the eigenvalue e (which is a subspace of $\mathfrak{h}_S \otimes \mathfrak{h}_S$). The level shift operators play a central role in the ergodic theory of open quantum systems, see e.g. [16, 17]. By using spectral renormalization group methods [9] one can eliminate the condition $\text{Im} \varepsilon < \omega'/2 < \pi/\beta$ and upgrade our results to hold uniformly in $T = 1/\beta \rightarrow 0$. This will be addressed elsewhere. The operator $K(\omega')$ is a suitable spectral deformation of an operator K . The latter is constructed from the Hamiltonian H , (1), according to a recently developed method for the analysis of open systems far from equilibrium [11–13], which we explain in detail in [16].

The coefficients $R_\varepsilon(A)$ in (4) are linear functionals of A which depend on the initial state ρ_0 and the Hamiltonian H . They have the expansion $R_\varepsilon(A) = \sum_{(m,n) \in I_\varepsilon} \varkappa_{m,n} A_{m,n} + O(\lambda^2)$, where I_ε is the collection of all pairs of indices such that $e = E_m - E_n$, the E_k being the eigenvalues of H_S . Here, $A_{m,n}$ is the (m,n) -matrix element of the observable A in the energy basis of H_S , and the $\varkappa_{m,n}$ are coefficients depending on the initial state of the system (and on e , but not on A and λ).

III. QUBIT

Our results for the qubit can be summarized as follows. Consider a two level system (qubit) with Hamiltonian $H_S = \Delta \sigma_z$, where Δ is the energy gap of the qubit, interacting with the reservoir via linear coupling,

$$v = \begin{bmatrix} a & c \\ \bar{c} & b \end{bmatrix} \otimes \varphi(g), \quad (6)$$

where $\varphi(g)$ is the Bose field operator as above. The form-factor $g \in L^2(\mathbb{R}^3, d^3k)$ contains an ultra-violet cutoff which introduces a time-scale τ_{UV} . This time scale depends on the physical system in question. We can think of it as coming from some frequency-cutoff determined by a characteristic length scale beyond which the interaction decreases rapidly. For instance, for a phonon field τ_{UV} is naturally identified with the inverse of the Debye frequency. We assume τ_{UV} to be much smaller than the time scales considered here.

A key role in the decoherence analysis is played by the infrared behaviour of form factors $g(k)$. We characterize this behaviour by the unique $p \geq -1/2$ satisfying

$$0 < \lim_{|k| \rightarrow 0} \frac{|g(k)|}{|k|^p} = C < \infty. \quad (7)$$

The power p depends on the physical model considered, for quantum-optical systems, $p = 1/2$, and for the quantized electromagnetic field, $p = -1/2$. We can treat $p = -1/2 + n$, with $n = 0, 1, \dots$.

Decoherence in models with interaction (6) with $c = 0$ is considered in [1–6, 16, 19, 20, 23]. This is the situation of a non-demolition (energy conserving) interaction, where $[v, H_S] = 0$, and consequently energy-exchange processes are suppressed. The resulting decoherence is called phase-decoherence. A particular model of phase-decoherence is obtained by the so-called position-position coupling, where the matrix in the interaction (6) is the Pauli matrix σ_z [2, 6, 20, 23]. On the other hand, energy-exchange processes, responsible for driving the system to equilibrium, have a probability proportional to $|c|^{2n}$, for some $n \geq 1$ (and a, b do not enter) [9, 10, 12, 13, 17, 18]. Thus the property $c \neq 0$ is important for thermalization (return to equilibrium).

We express the energy-exchange effectiveness by the function

$$\xi(\eta) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \int_{\mathbb{R}^3} d^3k \coth\left(\frac{\beta|k|}{2}\right) |g(k)|^2 \frac{\epsilon}{(|k| - \eta)^2 + \epsilon^2},$$

where $\eta \geq 0$ represents the energy at which processes between the qubit and the reservoir take place. In works on convergence to equilibrium it is usually assumed that $|c|^2 \xi(\Delta) > 0$. This condition is called the ‘‘Fermi Golden Rule Condition’’. It means that the interaction induces second-order (λ^2) energy exchange processes at the Bohr frequency of the qubit (emission and absorption of reservoir quanta). The condition $c \neq 0$ is actually *necessary* for thermalization while $\xi(\Delta) > 0$ is not (higher order processes can drive the system to equilibrium).

Our analysis allows to describe the dynamics of systems which exhibit *both* thermalization *and* (phase) decoherence. Let the initial density matrix, $\rho_{t=0}$, be of the form $\bar{\rho}_0 \otimes \rho_{R,\beta}$. (Our method does not require the initial state to be a product, see [16].) Denote by $p_{m,n}$ the operator represented in the energy basis by the 2×2 matrix whose entries are zero, except the (n, m) entry which is one. We show that for $t \geq 0$

$$[\bar{\rho}_t]_{1,1} - \langle \langle p_{1,1} \rangle \rangle_\infty = e^{it\varepsilon_0(\lambda)} [C_0 + O(\lambda^2)] \quad (8)$$

$$+ e^{it\varepsilon_\Delta(\lambda)} O(\lambda^2) + e^{it\varepsilon_{-\Delta}(\lambda)} O(\lambda^2) + O(\lambda^2 e^{-t\omega'/2}),$$

$$[\bar{\rho}_t]_{1,2} - \langle \langle p_{1,2} \rangle \rangle_\infty = e^{it\varepsilon_\Delta(\lambda)} [C_\Delta + O(\lambda^2)] \quad (9)$$

$$+ e^{it\varepsilon_0(\lambda)} O(\lambda^2) + e^{it\varepsilon_{-\Delta}(\lambda)} O(\lambda^2) + O(\lambda^2 e^{-t\omega'/2}).$$

Here, C_0, C_Δ are explicit constants depending on the initial condition $\bar{\rho}_0$, but not on λ , and the resonance energies ε have the expansions

$$\begin{aligned} \varepsilon_0(\lambda) &= i\lambda^2\pi^2|c|^2\xi(\Delta) + O(\lambda^4) \\ \varepsilon_\Delta(\lambda) &= \Delta + \lambda^2 R + \frac{i}{2}\lambda^2\pi^2 [|c|^2\xi(\Delta) + (b-a)^2\xi(0)] \\ &\quad + O(\lambda^4) \end{aligned} \quad (10)$$

and $\varepsilon_{-\Delta}(\lambda) = -\overline{\varepsilon_\Delta(\lambda)}$, with the real number

$$\begin{aligned} R &= \frac{1}{2}(b^2 - a^2) \langle g, \omega^{-1}g \rangle \\ &\quad + \frac{1}{2}|c|^2 \text{P.V.} \int_{\mathbb{R} \times S^2} u^2 |g(|u|, \sigma)|^2 \coth\left(\frac{\beta|u|}{2}\right) \frac{1}{u - \Delta}. \end{aligned}$$

The error terms in (8), (9) and (10) satisfy (for small λ):

$$\left| \frac{O(\lambda^2)}{\lambda^2} \right| < C \quad \text{and} \quad \sup_{t \geq 0} \left| \frac{O(\lambda^2 e^{-t\omega'/2})}{\lambda^2 e^{-t\omega'/2}} \right| < C.$$

Remarks. 1) To our knowledge this is the first time that formulas (8)-(10) are presented for models which are not explicitly solvable.

2) Expressions for $[\bar{\rho}_t]_{2,2}$ and $[\bar{\rho}_t]_{2,1}$ are obtained from the relations $[\bar{\rho}_t]_{2,2} = 1 - [\bar{\rho}_t]_{1,1}$ (conservation of unit trace) and $[\bar{\rho}_t]_{2,1} = [\bar{\rho}_t]_{1,2}^*$ (hermiticity of $\bar{\rho}_t$).

3) If the qubit is initially in one of the logic pure states $\bar{\rho}_0 = |\varphi_j\rangle\langle\varphi_j|$, where $H_S\varphi_j = E_j\varphi_j$, $j = 1, 2$, then we find $C_\Delta = 0$, and $C_0 = e^{\beta\Delta/2}(e^{\beta\Delta} + 1)^{-3/2}$ for $j = 1$ and $C_0 = e^{\beta\Delta}(e^{\beta\Delta} + 1)^{-3/2}$ for $j = 2$, see [16].

4) To second order in λ , the imaginary part of ε_Δ is increased by a term $\propto (b-a)^2\xi(0)$ only if $p = -1/2$, where p is defined in (7). For $p > -1/2$ we have $\xi(0) = 0$ and that contribution vanishes. For $p < -1/2$ we have $\xi(0) = \infty$.

5) $\xi(\Delta)$ and R contain purely quantum, vacuum fluctuation terms as well as thermal ones, while $\xi(0)$ is determined entirely by thermal fluctuations. $\xi(\Delta)$ and $\xi(0)$ are increasing in T , and, as $T \downarrow 0$, $\xi(0)$ is linear in T ($p = -1/2$, see (7)) and $\xi(\Delta)$ converges to a fixed nonzero value. The decoherence rate thus increases for decreasing T , and approaches a finite value as $T \downarrow 0$, for $c \neq 0$. A discussion of the decoherence function in terms of the temperature for the explicitly solvable case, $c = 0$, is given in [6].

6) Our proofs in [16] are valid for any fixed nonzero T . There is strong evidence and preliminary results using

the spectral renormalization group technique (see [9] and a remark in Section II) that (4)-(5) and (8)-(10) remain valid in the regime $T \rightarrow 0$. These results are in agreement with the recent experiments in [24], corroborated by earlier experiments on 1D nano-wires and 2D films, showing that the decoherence in 1D nano-wires does not vanish in the limit $T \rightarrow 0$. (The interpretation of the experiments reported in [24] stimulated a lively discussion of whether the decoherence vanishes or not, at $T \rightarrow 0$, in disordered conductors in a weak localization regime, see [25–27]. It is argued in [26, 27] that the Pauli principle for the electrons suppresses the decoherence in the zero temperature limit.)

7) The thermalization and decoherence rates are defined by $\tau_T = [\text{Im}\varepsilon_0(\lambda)]^{-1}$ and $\tau_D = [\text{Im}\varepsilon_\Delta(\lambda)]^{-1}$, respectively. Their ratio is, to second order in perturbation, $\tau_T/\tau_D = \frac{1}{2}[1 + (\frac{b-a}{|c|})^2 \frac{\xi(0)}{\xi(\Delta)}]$. For $\tau_T/\tau_D < 1$, the populations converge to their limiting values faster than the off-diagonal matrix elements, as $t \rightarrow \infty$ (coherence persists beyond thermalization of the populations). For $\tau_T/\tau_D > 1$, the off-diagonal elements converge faster. If the interaction matrix is diagonal ($c = 0$) then $\tau_T/\tau_D = \infty$, if it is off-diagonal (or if $a = b$), then $\tau_T/\tau_D = 1/2$.

8) For energy-conserving interactions, $c = 0$, full decoherence occurs if and only if $b \neq a$ and $\xi(0) > 0$. If either of these conditions is not satisfied, then the off-diagonal matrix elements are purely oscillatory (while the populations are constant), see also [16].

Illustration. Let the initial state of S be given by a coherent superposition in the energy basis,

$$\bar{\rho}_0 = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}. \quad (11)$$

We obtain the following expressions for the dynamics of the reduced matrix elements, for all $t \geq 0$:

$$\begin{aligned} [\bar{\rho}_t]_{m,m} &= \frac{e^{-\beta E_m}}{Z_{S,\beta}} + \frac{(-1)^m}{2} \tanh\left(\frac{\beta\Delta}{2}\right) e^{it\varepsilon_0(\lambda)} \\ &\quad + R_{m,m}(\lambda, t), \quad m = 1, 2, \\ [\bar{\rho}_t]_{1,2} &= \frac{1}{2} e^{it\varepsilon_{-\Delta}(\lambda)} + R_{1,2}(\lambda, t), \\ [\bar{\rho}_t]_{2,1} &= \frac{1}{2} e^{it\varepsilon_\Delta(\lambda)} + R_{2,1}(\lambda, t), \end{aligned}$$

where the numbers ε are given in (10). The remainder terms satisfy $|R_{m,n}(\lambda, t)| \leq C\lambda^2$, uniformly in $t \geq 0$, and they can be decomposed into a sum of a constant part (in t) and a decaying one, $R_{m,n}(\lambda, t) = \langle \langle p_{n,m} \rangle \rangle_\infty - \delta_{m,n} \frac{e^{-\beta E_m}}{Z_{S,\beta}} + R'_{m,n}(\lambda, t)$, where $|R'_{m,n}(\lambda, t)| = O(\lambda^2 e^{-\gamma t})$, with $\gamma = \min\{\text{Im}\varepsilon_0, \text{Im}\varepsilon_{\pm\Delta}\}$. Therefore, convergence of the populations and decoherence occur with rates $\tau_T = [\text{Im}\varepsilon_0(\lambda)]^{-1} \leq \infty$ and $\tau_D = [\text{Im}\varepsilon_\Delta(\lambda)]^{-1} \leq \infty$, respectively. In particular, coherence of the initial state stays preserved on time scales of the order $\lambda^{-2} [|c|^2\xi(\Delta) + (b-a)^2\xi(0)]^{-1}$, c.f. (10).

IV. DISCUSSION

Relation (4) gives a detailed picture of the dynamics of averages of observables. The resonance energies ε and

the functionals R_ε can be calculated for concrete models, to arbitrary precision (by rigorous perturbation theory in λ). See (8)-(10) for explicit expressions for the qubit, and the illustration above for an initially coherent superposition given by (11). In the present work, we use relation (4) to discuss the processes of thermalization and decoherence of a qubit. In [16] we present, besides a proof of (4), applications to energy-preserving (non-demolition) interactions and to registers of arbitrarily many qubits. It would be interesting to apply the techniques developed here to the analysis of the transition from quantum to classical behaviour (see [1, 20]). Our approach can also be useful in applications for cooled nano-mechanical systems [21]. (See also the discussion in [22].)

In the absence of interaction ($\lambda = 0$), we have $\varepsilon = e \in \mathbb{R}$, see (5). Depending on the interaction, each resonance energy ε may migrate into the upper complex plane, or it may stay on the real axis, as $\lambda \neq 0$. The averages $\langle A \rangle_t$ approach their ergodic means $\langle\langle A \rangle\rangle_\infty$ if and only if $\text{Im}\varepsilon > 0$ for all $\varepsilon \neq 0$. In this case the convergence takes place on the time scale $[\text{Im}\varepsilon]^{-1}$. Otherwise $\langle A \rangle_t$ oscillates. A sufficient condition for decay is that $\text{Im}\delta_e^{(s)} < 0$ (and λ small, see (5)).

There are two kinds of processes which drive the decay: energy-exchange processes and energy preserving ones. The former are induced by interactions enabling processes of absorption and emission of field quanta with

energies corresponding to the Bohr frequencies of S (this is the ‘‘Fermi Golden Rule Condition’’ [9, 12, 13, 17, 18]). Energy preserving interactions suppress such processes, allowing only for a phase change of the system during the evolution (‘‘phase damping’’, [1–6, 19]).

Even if the initial density matrix, $\rho_{t=0}$, is a product of the system and reservoir density matrices, the density matrix, ρ_t , at any subsequent moment of time $t > 0$ is not of the product form. The evolution creates the system-reservoir entanglement. We prove formula (4) for $\langle A \rangle_t - \langle\langle A \rangle\rangle_\infty$ for all observables A of any N -level system S in [16]. If the system has the property of return to equilibrium ($\xi(\Delta) > 0$), then $[\bar{\rho}_\infty]_{m,n} = \delta_{m,n} \frac{e^{-\beta E_m}}{\text{Tr}_S(e^{-\beta H_S})} + O(\lambda^2)$. Hence the Gibbs distribution is obtained by first letting $t \rightarrow \infty$ and then $\lambda \rightarrow 0$. A similar observation in the setting of the quantum Langevin equation has been made in [28]. If ρ_0 is an arbitrary initial density matrix on $\mathcal{H}_S \otimes \mathcal{H}_R$ then our method yields a similar result, see [16].

Equations (8), (9) and (10) define the decoherence time scale, $\tau_D = [\text{Im}\varepsilon_\Delta(\lambda)]^{-1}$, and the thermalization time scale, $\tau_T = [\text{Im}\varepsilon_0(\lambda)]^{-1}$. We should compare τ_D with the decoherence time scales and with computational time scales in real systems. The former vary from 10^4 s for nuclear spins in paramagnetic atoms to 10^{-12} s for electron-hole excitations in bulk semiconductors (see e.g. [29]).

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