On Decoherence and Thermalization

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Uses earlier work with M. Merkli, M. Mück,
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and results of Jakšić and Pillet

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Decoherence

Decoherence is reflected in the temporal decay of off-diagonal elements of the reduced density matrix of a quantum system in a given basis due to the interaction with an environment.

Goal: A rigorous analysis of the phenomenon of quantum decoherence for general non-solvable models.

Earlier results: explicitly solvable (non-demolition) models and non-rigorous results the quadratic Markov approximation (Lindblad evolution).

Model

Consider a quantum system interacting with the environment, also called the "reservoir", with the Hamiltonian

$$H = H_{\mathrm{S}} \otimes \mathbb{1}_{\mathrm{R}} + \mathbb{1}_{\mathrm{S}} \otimes H_{\mathrm{R}} + \lambda v,$$

acting on the Hilbert space $\mathcal{H} = \mathcal{H}_{\mathrm{S}} \otimes \mathcal{H}_{\mathrm{R}}$.

We assume that the *systems* in question are *finite dimensional* and the *reservoirs* are described by *free massless quantum fields* (photons, phonons or other massless excitations) with Hamiltonian

$$H_{\mathrm{R}} = \int_{\mathrm{R}^3} a^*(k)|k|a(k)\mathrm{d}^3 k,$$

where $a^*(k)$ and $a(k)$ are bosonic creation/annihilation operators.

Interactions

The interaction:

$$v = G \otimes \varphi(g),$$

where G is a self-adjoint matrix on $\mathcal{H}_{\mathrm{S}}$ and

$$\varphi(g) = \int (a^*(k)g(k) + a(k)g(\bar{k}))d^3k,$$

the field operator on the Fock space $\mathcal{H}_{\mathrm{R}}$,

Reservoirs

It is understood that the reservoir is in the thermodynamic limit of infinite volume and positive densities, in a phase without Bose-Einstein condensate (for massive Bosons).

We assume that intially the system is close to a state in which the reservoir is near equilibrium at temperature $T = 1/\beta > 0$.

(There could also be several reservoirs initailly at different temperatures as in the case of a quantum dot attached to leads. Results below can be extended to this case.)

Reduced Density Matrix

Though we deal with positive densities we think of the state of the total system at time t as a density matrix ρ_t satisfying the von Neumann equation

$$i\partial_t \rho_t = [H, \rho_t].$$

The *reduced density matrix* (of the system S) at time t is then formally given by

$$\overline{\rho}_t = \mathrm{Tr}_{\mathrm{R}}\, \rho_t,$$

where Tr_{R} is the partial trace with respect to the reservoir degrees of freedom.

Decoherence is defined- *in a chosen basis* - as:

$$[\overline{\rho}_t]_{m,n} \to 0, \text{ as } t \to \infty, \ \forall m \neq n.$$

Most often the basis is that of eigenvectors of the system Hamiltonian H_{S} (the energy basis, also called the computational basis for a quantum register).

Thermalization

Let $\rho(\beta, \lambda)$ be the equilibrium state of the interacting system at temperature $T = 1/\beta$. We say that the system is thermolized if If

$$\overline{\rho}_t \longrightarrow \overline{\rho}(\beta, \lambda), \text{ with } \overline{\rho}(\beta, \lambda) := \mathrm{Tr}_{\mathrm{R}} \rho(\beta, \lambda).$$

In this case, the off-diagonal elements of $\overline{\rho}_t$ generically will not vanish, as $t \to \infty$ and the decoherence should be defined as the convergence of the off-diagonals of $\overline{\rho}_t$ to the corresponding off-diagonals of $\overline{\rho}(\beta, \lambda)$.

It is usually assumed tacitely that the latter terms can be neglected (they are, at most, of the order $O(\lambda)$).

Observables

Averages of observables, A, of the *system* (operators on the system Hilbert space $\mathcal{H}_{\mathrm{S}}$) are given in terms of the reduced density matrix as

$$\mathrm{Tr}_{\mathrm{S+R}}(\rho_t(A \otimes \mathbb{1}_{\mathrm{R}})) = \mathrm{Tr}_{\mathrm{S}}(\overline{\rho}_t A) =: \langle A \rangle_t \, .$$

Let $\{\varphi_j\}_{j\geq 1}$ be an orthonormal basis of $\mathcal{H}_{\mathrm{S}}$ diagonalizing H_{S}. The reduced density matrix has matrix elements

$$[\overline{\rho}_t]_{m,n} := \langle \varphi_m, \overline{\rho}_t \varphi_n \rangle = \langle P_{n,m} \rangle_t \ \text{ with } P_{n,m} = |\varphi_n\rangle\langle\varphi_m|.$$

Thus to understand the decoherence and thermalization it suffices to understand behavior of the expectations $\langle A \rangle_t$.

Results 1

Under certain conditions on the interaction, we have:
1) The ergodic averages

$$\langle\langle A\rangle\rangle_\infty := \lim_{T\to\infty} \frac{1}{T}\int_0^T \langle A\rangle_t \, \mathrm{d}t$$

exist, i.e., that $\langle A\rangle_t$ converges in the ergodic sense as $t \to \infty$.
If the system is thermolized then

$$\langle\langle A\rangle\rangle_\infty = \mathrm{Tr_S}(\overline{\rho}(\beta,\lambda)A), \text{ with } \overline{\rho}(\beta,\lambda) := \mathrm{Tr_R}\rho(\beta,\lambda).$$

Results 2

2) $\exists$ complex numbers ε, lying in the strip $\{z \in \mathbb{C} \mid 0 \leq \mathrm{I}mz < \frac{\pi}{\beta}\}$, s.t. for any $t \geq 0$ and for any $0 < \omega' < \frac{2\pi}{\beta}$,

$$\langle A \rangle_t - \langle\langle A \rangle\rangle_\infty = \sum_{\varepsilon \neq 0} \mathrm{e}^{\mathrm{i}t\varepsilon} R_\varepsilon(A) + O\left(\lambda^2 \, \mathrm{e}^{-\frac{t}{2}[\max_\varepsilon\{\mathrm{Im}\,\varepsilon\} + \omega'/2]}\right),$$

where $R_\varepsilon(A)$ are linear functionals of A, given in terms of the initial state, ρ_0, and the Hamiltonian H.

Results 3

3) The complex numbers ε are the *resonances* of a certain explicitly given operator L, which is a 'perturbation' of the Liouville operator $L_S := H_{\mathrm{S}} \otimes \mathbb{1}_{\mathrm{S}} - \mathbb{1}_{\mathrm{S}} \otimes H_{\mathrm{S}}$ of the system and 'bifurcate' from the eigenvalues of L_S as

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

where

$$e \in \mathrm{s}pec(L_S) = \mathrm{s}pec(H_{\mathrm{S}}) - \mathrm{s}pec(H_{\mathrm{S}})$$

and $\delta_e^{(s)}$ are the eigenvalues of a matrix Λ_e, called a *level-shift operator*, acting on the eigenspace of L_S corresponding to the eigenvalue e.
The $\varepsilon \equiv \varepsilon_e^{(s)}$ encode properties of irreversibility of the reduced dynamics of S (decay of observables and matrix elements.)

Two-dimensional systems (Qubits)

Consider a two-dimensional system (qubit), with state space (of pure states) $\mathcal{H}_{\mathrm{S}} = \mathbb{C}^2$, and Hamiltonian $H_{\mathrm{S}} = \mathrm{diag}(E_1, E_2)$, interacting with the Bose field via

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

where $\varphi(g) = \int \varphi(x)g(x)$ is the Bose field operator.

$c = 0$ corresponds to a non-demolition (energy conserving) interaction (v commutes with the Hamiltonian H_{S} and consequently energy-exchange processes are suppressed).

The property $c \neq 0$ is necessary for thermalization.

Decoherence of qubits

Let $\Delta = E_2 - E_1 > 0$ be the energy gap of the qubit. Then

$$[\tau_T]^{-1} = \mathrm{Im}\varepsilon_{diag}(\lambda) = \lambda^2\pi^2|c|^2\xi(\Delta) + O(\lambda^4)$$

$$[\tau_D]^{-1} = \mathrm{Im}\varepsilon_{off-diag}(\lambda) = \frac{1}{2}\lambda^2\pi^2\left[|c|^2\xi(\Delta) + (b-a)^2\xi(0)\right]$$

$$+O(\lambda^4),$$

$$\text{with} \quad \xi(\eta) = 4\coth\left(\frac{\beta\eta}{2}\right)|g(\eta)|^2\eta^2.$$

Exactly solvable models (non-demolition interactions): Palma, Suominen, Ekert, Shao, Ge, Cheng, Mozyrsky, Privman, and others.

Quantum registers

Consider the dynamics of N interacting spins-qubits (quantum register) collectively coupled to a thermal environment. The register Hamiltonian is of the form

$$H_{\mathrm{S}} = \sum_{i,j=1}^{N} J_{ij} S_i^z S_j^z + \sum_{j=1}^{N} B_j S_j^z,$$

where the J_{ij} are pair interaction constants that can take positive or negative values, and $B_j \geq 0$ is an effective magnetic field at the location of spin j.

($B_j = \frac{\hbar}{2}\gamma B_j^z$, where $\hbar$ is the Planck constant, γ is the value of the electron gyromagnetic ratio and B_j^z is an inhomogeneous magnetic field, oriented in the positive z direction.)

Interaction

Consider a *collective coupling*: the distance between the N qubits is much smaller than the correlation length of the reservoir and consequently each qubit feels *the same* interaction with the latter. The collective interaction between S and R consists of energy conserving and energy exchange parts and is given by the operator

$$v = \lambda_1 v_1 + \lambda_2 v_2 = \lambda_1 \sum_{j=1}^{N} S_j^z \otimes \phi(g_1) + \lambda_2 \sum_{j=1}^{N} S_j^x \otimes \phi(g_2).$$

The coupling constants λ_1 and λ_2 measure the strengths of the *energy conserving* (position-position) coupling, and the *energy exchange* (spin flip) coupling, respectively. (Spin-flips are implemented by the S_j^x.)

Collective decoherence

We illustrate our results on a qubit register with $J_{ij} = 0$. For *generic* magnetic fields we show

- $\min \varepsilon_{diag} = O(1)$ in N (thermalization).
- $\min \varepsilon_{off-diag} \propto \lambda_1^2 [\sum_{j=1}^{N} (\sigma_j - \tau_j)]^2$
  (purely energy conserving interactions, $\lambda_2 = 0$).
  This can be as large as $O(\lambda_1^2 N^2)$.
- $\min \varepsilon_{off-diag} \propto \lambda_2^2 \mathfrak{D}(\underline{\sigma} - \underline{\tau})$
  (purely energy exchanging interactions, $\lambda_1 = 0$).
  This cannot exceed $O(\lambda_2^2 N)$.

Here $\underline{\sigma} = \{\sigma_1, \ldots, \sigma_N\} \in \{+1, -1\}^N$ and similarly $\underline{\tau}$ are *spin configurations* labeling the energy basis of eigenvectors $\varphi_{\underline{\sigma}} = \varphi_{\sigma_1} \otimes \cdots \otimes \varphi_{\sigma_N}$ of H_{S} and $\mathfrak{D}(\underline{\sigma} - \underline{\tau}) := \sum_{j=1}^{N} |\sigma_j - \tau_j|$ is the *Hamming distance* between $\underline{\sigma}$ and $\underline{\tau}$.

Collective decoherence*

The above results show:

- *The fastest decay rate of reduced off-diagonal density matrix elements due to the energy conserving interaction alone is of order $\lambda_1^2 N^2$, while the fastest decay rate due to the energy exchange interaction alone is of the order $\lambda_2^2 N$. Moreover, the decay of the diagonal matrix elements is of oder λ_1^2, i.e., independent of N.*
- The same discussion is valid for the interacting register ($J_{ij} \neq 0$).

Earlier results: Altepeter, Hadley, Wendelken, Berglund, Kwiat, Ao, Rammer, Berman, Kamenev, Tsifrinovich, Duan, Guo, Fedorov, Fedichkin, Palma, Suominen, Ekert, Utsunomiya, Master, Yamamoto.

Idea of the proof

- Formulate the problem as an evolution on the Hilbert space $\mathcal{K} := \mathcal{H}_S \otimes \mathcal{H}_S \otimes \mathcal{H}_R \otimes \mathcal{H}_R$:

$$\rho_t \Longleftrightarrow \Psi_t = e^{iLt}\Psi \ \in \ \mathcal{K},$$

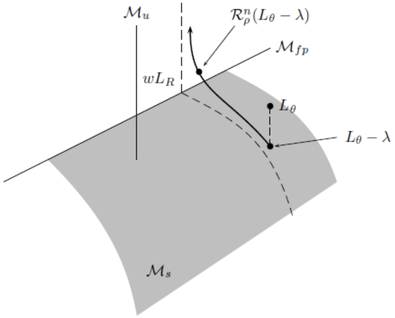
  where L is an unbounded and, in general, non-self-adjoint operator on $\mathcal{K}$ (Liouville operator);
- The exponents $\varepsilon_e^{(s)}$ are the resonances of the generator L;
- Use spectral deformation ($L \to L_\theta$) and renormalization group (RG) technique to analyze L_θ.

Renormalization Group

To find the spectral structure of L_θ we use the spectral renormalization group (RG):

- Pass from a single operator L_θ to a Banach space $\mathcal{B}$ of Liouville-type operators;
- Construct a map, $\mathcal{R}_\rho$, on $\mathcal{B}$, with the following properties:
  (a) $\mathcal{R}_\rho$ is 'isospectral';
  (b) $\mathcal{R}_\rho$ removes the (thermal) reservoir degrees of freedom related to energies $\geq \rho$.
- Relate the dynamics of semi-flow, $\mathcal{R}_\rho^n, n \geq 1$, to spectral properties of individual operators in $\mathcal{B}$.

We show that the flow, $\mathcal{R}_\rho^n$, has the fixed-point manifold $\mathcal{M}_{fp} := \mathbb{C}L_R$, an unstable manifold $\mathcal{M}_u := \mathbb{C}\mathbf{1}$, and a (complex) co-dimension 1 stable manifold $\mathcal{M}_s$ for $\mathcal{M}_{fp}$ foliated by (complex) co-dimension 2 stable manifolds for each fixed point.



Stable and unstable manifolds.

RG and Spectral Properties

Adjust the parameter λ, so that $L_\theta - \lambda$ is in a ρ^n-neighborhood of the stable manifold $\mathcal{M}_s$

$\Longrightarrow L_\theta - \lambda$ is in the domain of $\mathcal{R}_\rho^n$.

$\Longrightarrow L^{(n)}(\lambda) := \mathcal{R}_\rho^n(L_\theta - \lambda) \approx wL_R$, for some $w \in \mathbb{C},\ \mathrm{Re}\ w > 0$, and n sufficiently large

$\Longrightarrow$ Spectral information about $L^{(n)}(\lambda)$.

$\Longrightarrow$ Spectral information about $L^{(n-1)}(\lambda)$ (by 'isospectrality' of $\mathcal{R}_\rho$)

...

$\Longrightarrow$ Spectral information about L_θ.