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To the memory of Michael Solomyak

ON SOME PROPERTIES OF THE TIME EVOLUTION OF QUADRATIC OPEN QUANTUM SYSTEMS

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The paper is aimed at revisiting some mathematical properties that appear in open quantum systems with quadratic Hamiltonians. In particular, a discussion is included of some properties related to the notions of purity, separability, and entanglement, introduced by physicists in quantum information theory. The results are applied, among other things, to coupled harmonic oscillators appearing in the quantum Brownian motion. Moreover, the master equation is revisited, which was obtained for the time evolution of an open system coupled to an environment modeled by any quadratic Hamiltonians.

§1. Introduction

The general setting considered here is a quantum system (S) interacting with an environment (E). The total system $(S) \cup (E)$ is assumed to be an isolated quantum system and we are interested in dynamical properties of (S) alone, which is an open system because of its interactions with (E). In particular, during the time evolution, the energy of (S) is not preserved and its evolution is not determined by a Schrödinger or Liouville–von Neumann equation unlike for the total system $(S) \cup (E)$. A detailed presentation concerning the quantum dynamics of open systems can be found in the book [5].

The Hilbert space of the total system $(S) \cup (E)$ is the tensor product $\mathcal{H} = \mathcal{H}_S \widehat{\otimes} \mathcal{H}_E$[1], and its Hamiltonian $\widehat{H}$ is decomposed as follows:

$$\widehat{H}_V(t) = \underbrace{\widehat{H}_S \otimes \mathbf{1} + \mathbf{1} \otimes \widehat{\mathbf{H}}_{\mathbf{E}}}_{\widehat{H}_0} + \widehat{H}_I(t) = \widehat{H}_0 + \widehat{V}(t). \tag{1.1}$$

Key words: quantum information theory, entanglement, master equation, Schrödinger equation, quantum Brownian motion.

[1]Here $\widehat{\otimes}$ means that the tensor product is the Hilbert space obtained by completion of the algebraic tensor product

A basic example is the quantum Brownian motion, coupling two harmonic oscillators with bilinear potential $V_g(t)$:

$$\widehat{H}_S = \frac{1}{2}(-\partial^2_{x^2} + {\omega_1}^2 x^2), \quad \widehat{H}_E = \frac{1}{2}\sum_{2\leqslant j\leqslant N+1}(-\partial^2_{y_j^2} + {\omega_j}^2 y_j^2), \tag{1.2}$$

$$V_g(t,x,y) = x \cdot \sum_{2\leqslant j\leqslant N+1} g_j(t) y_j, \quad x, y_j, g_j(t) \in \mathbb{R}, \tag{1.3}$$

where $\mathcal{H}_S = L^2(\mathbb{R})$, $\mathcal{H}_E = L^2(\mathbb{R}^N)$.

The whole system $(S) \cup (E)$ is isolated by assumption and its evolution obeys the Schrödinger (or Liouville–von Neumann) equation with the Hamiltonian $\widehat{H}$. Assuming that at time $t = 0$ the system (S) and the environment (E) are decorrelated, the problem is to understand the evolution of the system (S) alone in the Hilbert space $\mathcal{H}_S$ when an interaction with the environment is switched on.

All Hamiltonians here are selfadjoint operators on their natural domain, $\widehat{H}$ and $\widehat{H}_I = \widehat{V}$ are defined in $\mathcal{H}$, $\widehat{H}_S$ in $\mathcal{H}_S$, $\widehat{H}_E$ in $\mathcal{H}_E$. Quantum observables are denoted with a hat accent, the corresponding classical observables (also named Wigner functions or Weyl-symbols) are written without hat accent.

We shall assume that the interacting potential $\widehat{V}$ has the following form

$$\widehat{V}_g(t) = \sum_{1\leqslant j\leqslant N} g_j(t)\widehat{S}_j \otimes \widehat{E}_j \tag{1.4}$$

where $\widehat{S}_j$ and $\widehat{E}_j$ are selfadjoint operators in $\mathcal{H}_S$ and $\mathcal{H}_E$ respectively. Assumptions on their domains will be given later.

Recall that a density matrix $\widehat{\rho}$ is a positive trace class operator with trace one ($\mathrm{tr}\widehat{\rho} = 1$). Let $\widehat{\rho}_0$ be a state of the total system $(S) \cup (E)$ in the Hilbert space $\mathcal{H}$ at the initial time. The time evolution of $\widehat{\rho}$ obeys the following Liouville–von Neumann equation:

$$\dot{\widehat{\rho}} = i^{-1}[\widehat{H}, \widehat{\rho}], \quad \widehat{\rho} : t \mapsto \widehat{\rho}(t), \quad \widehat{\rho}(0) = \widehat{\rho}_0. \tag{1.5}$$

Time derivatives are denoted by a dot, $[\,\cdot\,,\,\cdot\,]$ denotes the commutator of two observables.

We assume that for $t = 0$ the system and the environment are decoupled, which means that

$$\widehat{\rho}(0) = \widehat{\rho}_S(0) \otimes \widehat{\rho}_E(0),\ \widehat{\rho}_{S,E}(0) \text{ are density matrices in } \mathcal{H}_{S,E}. \tag{1.6}$$

The time evolution $\widehat{\rho}(t)$ is given by the propagator $\mathcal{U}_V(t,s)$ generated by the Hamiltonian $H_V(t)$. For $V = 0$ we have $\mathcal{U}_0(t,s) = \mathrm{e}^{-i(t-s)\widehat{H}_S} \otimes \mathrm{e}^{-i(t-s)\widehat{H}_E}$. So we have $\widehat{\rho}(t) = \widehat{\rho}_S(t) \otimes \widehat{\rho}_E(t)$, $t \in \mathbb{R}$, where $\rho_{S,E}(t) = \mathcal{U}^*_{S,E}\rho_{S,E}(0)\mathcal{U}_{S,E}$. In particular, if $\rho_S(0)$ is a pure state, then $\rho_S(t)$ is pure for any $t \in \mathbb{R}$. When the interaction is switched on, $\rho_S(t)$ is defined as the partial trace of $\widehat{\rho}(t)$ over the environment degrees of freedom and one question is to check if $\rho_S(t)$ is pure or not for $t \neq 0$.

Let us recall some definitions concerning some properties of density matrix states.

Definition 1.1. Let $\widehat{\rho}$ be a state in the Hilbert space $\mathcal{H}$, i.e., a nonnegative operator in $\mathcal{H}$ with trace 1.

(i) $\widehat{\rho}$ is a pure state if and only if $\widehat{\rho}$ is the orthogonal projector on a unit vector ψ of $\mathcal{H}$.

(ii) $\widehat{\rho}$ is a mixed state if it is not a pure state.

(iii) Let $\widehat{\rho}$ be a state in $\mathcal{H}_S \otimes \mathcal{H}_E$; $\widehat{\rho}$ is a separable state if there exist a probability space $(\Omega, \mathbf{P})$ and mesurable families of states: $\omega \mapsto \widehat{\rho}_\omega^{(S,E)}$ from Ω in $\mathfrak{S}^1(\mathcal{H}_{S,E})$ such that

$$\widehat{\rho} = \int\limits_\Omega \widehat{\rho}_\omega^{(S)} \otimes \widehat{\rho}_\omega^{(E)} P(d\omega)^2 \tag{1.7}$$

(iv) $\widehat{\rho}$ is entangled if it is not separable.

It is easy to see that a density matrix $\widehat{\rho}$ is a mixed state if and only if $\widehat{\rho}$ has an eigenvalue $\lambda \in]0,1[$. To decide if a state is pure or not we consider the purity function

$$\mathcal{P}_\rho(t) = \mathrm{tr}(\widehat{\rho}(t)^2)$$

We clearly have $0 \leqslant \mathcal{P}_\rho(t) \leqslant 1$. It is not difficult to see that $\rho(t)$ is pure if and only if $\mathcal{P}_\rho(t) = 1$. Suppose that at time $t = 0$ the state $\widehat{\rho}$ is pure. So 0 is a maximum for p_{ur}, so we have $\ddot{\mathcal{P}}_\rho(t)(0) \leqslant 0$. If furthermore $\ddot{\mathcal{P}}_\rho(0) < 0$, then for some $\varepsilon > 0$, the state $\widehat{\rho}(t)$ is mixed whenever $0 < t < \varepsilon$.

For isolated (closed) systems, if the initial state is pure, then it stays pure at every time, as it can easily be seen by using equation (1.5).

So our first step in this paper is to compute the second derivative $\ddot{\mathcal{P}}_S(t)(0)$ for the purity of the reduced system $\widehat{\rho}_S$ when $\widehat{\rho}_S(0)$ is pure. In particular, for a large class of models, including the Quantum Brownian Motion, we shall prove that for the state of the reduced system we have $\ddot{\mathcal{P}}_S(0) < 0$. So for these models there is an indication that the state of the reduced system may be immediately decoherent and entangled with the environment.

Our second goal is to consider the separability (ou entanglement) property of the mixed state $\widehat{\rho}(t)$. We explain here results obtained by physicsts: the

[2] In physicist literature only discrete probability laws are considered, but it seems necessary to extend the definition to any probability law

necessary Horodecki condition which turns out to be sufficient for Gaussian states and this can be applied to the quantum Brownian motion [33, 12].

Our third goal is to compute the time evolution $\widehat{\rho}_S(t)$ of the state of the system. We know that $\widehat{\rho}_S(t)$ does not satisfy a Liouville–von Neumann equation because the system is open so diffusion termes appear. We shall give a proof that for any time dependent quadratic systems, $\widehat{\rho}_S(t)$ obeys an exact "master equation" similar to a Fokker–Planck type equation, with time dependent coefficients, and from this equation we can get an explicit formula for $\widehat{\rho}_S(t)$. Similar results were obtained by different methods in [10, 11, 14].

We recall a mathematical definition for the reduced evolution $\rho_S(t)$ and related properties. This can be done by introducing partial trace (or relative trace) over the environment for a state $\widehat{\rho}$ of the global system.

Definition 1.2. Let $\widehat{A}$ be a trace class operator in $\mathcal{H}_S \otimes \mathcal{H}_E$. We denote by $\mathrm{tr}_E\widehat{A}$ a unique trace class operator on $\mathcal{H}_S$ satisfying, for every bounded operator $\widehat{B}$ on $\mathcal{H}_S$,

$$\mathrm{tr}_S\Big((\mathrm{tr}_E\widehat{A})\widehat{B}\Big) = \mathrm{tr}\Big(\widehat{A}(\widehat{B}\otimes \mathbf{1_E})\Big), \tag{1.8}$$

We have denoted by "tr" the trace in the total space $\mathcal{H}$, and by $\mathrm{tr}_{S,E}$ the trace in $\mathcal{H}_{S,E}$, respectively. Of course we have the "Fubini property:" $\mathrm{tr}_S(\mathrm{tr}_E\widehat{A}) = \mathrm{tr}\widehat{A}$. Moreover, we have $\mathrm{tr}_E(\widehat{B}\otimes\widehat{C}) = \widehat{B}\cdot(\mathrm{tr}_E\widehat{C})$ if $\widehat{B}$ and $\widehat{C}$ are trace class operators in $\mathcal{H}_S$ and $\mathcal{H}_E$ respectively.

If $\widehat{\rho}$ is a density matrix in $\mathcal{H}$, then $\mathrm{tr}_E\widehat{\rho}$ is a density matrix in $\mathcal{H}_S$, called the reduced density matrix or the reduced state. From (1.8) we can compute the matrix element of $\mathrm{tr}_E\widehat{A}$ by the formula

$$\langle\psi, (\mathrm{tr}_E\widehat{A})\varphi\rangle = \mathrm{tr}\left(\widehat{A}(\Pi_{\psi,\varphi}\otimes \mathbf{1_E})\right), \quad \psi,\, \varphi\in\mathcal{H}_S.$$

The partial trace was first introduced by L. Landau (1927) and then more recently in quantum mechanics to explain *entanglement* and *decoherence* (see [28, 30] for more details).

Let

$$\Psi\in\mathcal{H}_S\otimes\mathcal{H}_E, \quad \Psi = \sum_{1\leqslant j\leqslant N}\psi_j\otimes\eta_j,$$

where Ψ is a pure state in $\mathcal{H} = \mathcal{H}_S\otimes\mathcal{H}_E$. Let us compute the partial trace of Π_Ψ in $\mathcal{H}_E$. Applying Definition 1.2, we easily get

$$\mathrm{tr}_E(\Pi_\Psi) = \sum_{1\leqslant j,k\leqslant N}\langle\eta_j,\eta_k\rangle\Pi_{\psi_j,\psi_k} \tag{1.9}$$

where Π_{ψ_j,ψ_k} is a rank one operator in $\mathcal{H}_S : \Pi_{\psi_j,\psi_k}(\varphi) = \langle\psi_j,\varphi\rangle\psi_k$. The decoherence phenomenon [37, 25] means that there exists a (nonorthonormal) basis $\{\eta_j\}$ such that $|\langle\eta_j, \eta_k\rangle|$ becomes very small for $j \neq k$, so that $\mathrm{tr}_E(\Pi_\Psi)$ is very close to

$$\sum_{1\leqslant j\leqslant N} p_j \Pi_{\psi_j}, \quad p_j = \langle\eta_j, \eta_j\rangle$$

hence quantum interferences between the states ψ_j of the system (S) are destroyed.

Formula (1.8) is an operator version of the Fubini integration theorem as we can see in the Weyl quantization setting.

Let $\mathcal{H}_S = L^2(\mathbb{R}^d)$, $\mathcal{H}_E = L^2(\mathbb{R}^N)$. Denote $z = (x,\xi) \in \mathbb{R}^{2d}$, $u = (y,\eta) \in \mathbb{R}^{2N}$, $A = \sigma_w \widehat{A}$ the Weyl symbol of $\widehat{A}$ in the Schwartz space $\mathcal{S}(\mathbb{R}^{2(d+N)})$ (see [8] for more details); then the Weyl symbol of $\mathrm{tr}_E \widehat{A}$ is

$$\sigma_w(\mathrm{tr}_E \widehat{A})(z) = (2\pi)^{-N} \int_{\mathbb{R}^{2N}} A(z,u)du. \tag{1.10}$$

Our main applications here concern the Weyl-quadratic case where:

- H_S and H_E are quadratic Hamiltonians (generalized harmonic oscillators) respectively in the phase spaces $\mathbb{R}^{2d}$, $\mathbb{R}^{2N}$;
- $\widehat{H}_S$ and $\widehat{H}_E$ are quantum Hamiltonians (Weyl quantization of H_S, respectively H_E) in $L^2(\mathbb{R}^d)$, respectively $L^2(\mathbb{R}^N)$;
- $\widehat{\rho}_S$ is the projector to $\psi \in \mathcal{S}(\mathbb{R}^d)$;
- ρ_E is a Gaussian with 0 mean;
- S_j, respectively E_j is a linear form on $\mathbb{R}^{2d}$, respectively $\mathbb{R}^{2N}$ (bilinear coupling).

In applications one considers thermal equilibrium states for the environment: $\widehat{\rho}_E = Z(\beta)^{-1}\mathrm{e}^{-\beta\widehat{H}_E}$, where H_E is a quadratic form, positive definite, and $\beta = \frac{1}{T}$, $T > 0$, is the temperature, $Z(\beta) = \mathrm{tr}(\mathrm{e}^{-\beta\widehat{H}_E})$. In this setting it is possible to find the exact time dependent master equation satisfied by $\widehat{\rho}_S(t)$, as we shall see in the second part of this paper.

This paper is a revised version of the preprint [29].

§2. Studying the purity

2.1. Assumption and statements. Let us consider the following abstract setting. We fix a selfadjoint and positive operator K_0 in $\mathcal{H}$ and we define the scale of abstract Sobolev space $\mathcal{H}^s = \mathrm{Dom}(K_0^s)$ if $s \geqslant 0$ and $\mathcal{H}^s$ is the dual of $\mathcal{H}^{-s}$ if $s \leqslant 0$. Define $\mathcal{H}^\infty = \bigcap_{s\in\mathbb{R}} \mathcal{H}^s$ and $\mathcal{H}^{-\infty} = \bigcup_{s\in\mathbb{R}} \mathcal{H}^s$. Moreover, we assume that K_0^{-1} is in the Schatten class $\mathfrak{S}^{p_0}(\mathcal{H})$. For definitions and properties of Schatten classes we refer to [19]. We introduce the following definition.

Definition 2.1. A linear operator $A : \mathcal{H}^{\infty} \to \mathcal{H}^{-\infty}$ is said to be of order $m \in \mathbb{R}$ if, for any $k \in \mathbb{R}$, we have $A \in \mathcal{L}(\mathcal{H}^{k+m}, \mathcal{H}^{k})$.

Now we introduce our assumptions on the Hamiltonian (1.1).

- [A0] H_S and H_E are selfadjoint operators in $\mathcal{H}_S$, respectively $\mathcal{H}_E$. Moreover, $\widehat{H}_0 := \widehat{H}_S \otimes \mathbf{1} + \mathbf{1} \otimes \widehat{H}_E$ is an operator of order m_0 in $\mathcal{H}$, is a symmetric operator in $\mathcal{H}^{\infty}$ and is such that $[H_0, K_0]K_0^{-1}$ is of order 0.
- [A1] $\widehat{V} = \widehat{V}(t)$ is of order m_0 such that $\widehat{V} \in \mathbb{C}^0(I_0, \mathcal{L}(\mathcal{H}^{k+m_0}, \mathcal{H}^{k}))$, for every k and $\widehat{V}$ is symmetric on $\mathcal{H}^{\infty}$, for $t \in I_0 :=]-T_0, T_0[$ for some $T_0 > 0$. Moreover $[\widehat{V}(t), K_0]K_0^{-1} \in \mathbb{C}^0(I_0, \mathcal{L}(\mathcal{H}^{k}, \mathcal{H}^{k}))$, for all k.
- [A2] The initial state $\widehat{\rho}(0)$ is of order r, with $r < -p_0 - km_0$, for some $k \geqslant 3$.

We have the following preliminary results. The first result is a direct consequence of the paper [27].

Proposition 2.2. *Assume that conditions* [A0] *and* [A1] *are satisfied. Then* $\widehat{H}_V(t)$ *has a unique selfadjoint extension in* $\mathcal{H}$. *In particular,* $\mathcal{H}_0$ *is essentially selfadjoint. Moreover, the time dependent Hamiltonian* $\widehat{H}_V(t)$ *defines a unitary propagator* $\mathcal{U}_V(t,s)$ *in* $\mathcal{H}$ *and* $(t,s) \mapsto \mathcal{U}_V(t,s)$ *is continuous from* $I_0 \times I_0$ *into* $\mathcal{L}(\mathcal{H}^k)$, *for any* $k \in \mathbb{N}$.

Then the time evolution of an initial matrix density $\widehat{\rho}(0)$ is well defined and is given by

$$\rho(t) = \mathcal{U}_V(t,0)^* \widehat{\rho}(0) \mathcal{U}_V(t,0). \tag{2.11}$$

It is useful to compute the second derivative of the purity of the state ρ_S of the system. Assume that $\rho_S(0)$ is pure and that its purity $\mathcal{P}_S(t)$ is C^3 in a neighborhood of 0. Then we have

$$\mathcal{P}_S(t) = 1 + \frac{\ddot{\mathcal{P}}_S(0)}{2} t^2 + O(t^3), \quad t \searrow 0.$$

So if $\ddot{\mathcal{P}}_S(0) < 0$, then $\widehat{\rho}(t)$ becomes a mixed state for t close to 0, $t \neq 0$.

Theorem 2.3. *Assume that conditions* [A0], [A1], *and* [A2] *are satisfied. Then* $t \mapsto \widehat{\rho}(t)$ *is* C^k *from* I_0 *into* $\mathfrak{S}^1(\mathcal{H})$. *Assume furthermore that* $k \geqslant 2$ *and that* $\rho_S(0)$ *is a pure state in* $\mathcal{H}_S$. *Then we have the following formula for the second derivative of* $\mathcal{P}_S(t)$ *at* 0:

$$\ddot{\mathcal{P}}_S(0) = -4 \mathrm{tr} \left(\widehat{V} \widehat{\rho}(0) \widehat{V} (\widehat{\rho}_S^{\perp}(0) \otimes \mathbf{1}) \right), \tag{2.12}$$

where $\widehat{\rho}_S^{\perp} = \mathbf{1} - \widehat{\rho}_{\mathbf{S}}$

Now we get a more explicit formula for the separable interactions (1.4).

Corollary 2.4. *Assume that we have* (1.4) *and that* $\mathrm{tr}_E(\widehat{\rho}_E(0)\widehat{E}_j\widehat{E}_{j'}) = \delta_{j,j'}d_j$, $1 \leqslant j, j' \leqslant N$, *then we have*

$$\ddot{\mathcal{P}}_S(0) = -4 \sum_{1\leqslant j\leqslant N} \left(\|\widehat{S}_j\psi_S\|^2 - \langle\psi_S, \widehat{S}_j\psi_S\rangle^2\right) d_j, \tag{2.13}$$

where $\rho_S(0)$ *is the projection to* ψ_S. *In particular, if there exists* j_0 *such that* $d_{j_0} > 0$ *and* ψ_S *is not an eigenfunction of* $\widehat{S}_{j_0}$, *then* $\ddot{\mathcal{P}}_S(0) < 0$.

We apply this result to the Quantum Brownian Motion (1.2), (1.3). Denote $\pi_S(z) := 2\pi^{-d}\rho_S(z)\,dz$ and $\pi_E(u) := (2\pi)^{-N}\rho_E(u)du$ (they are quasiprobabilities in $\mathbb{R}^{2d}$, respectively $\mathbb{R}^{2N}$). Here we assume that $\widehat{\rho}_S(0)$ is a pure state $\psi_S \in \mathcal{S}(\mathbb{R}^d)$. We introduce the commutators:

$$s_{j'j} = [\widehat{S}_{j'}, \widehat{S}_j], \quad e_{j'j} = [\widehat{E}_{j'}, \widehat{E}_j],$$

and the classical (symmetric) covariance matrices:

$$\Sigma^{(S)}_{jj'} = \int\limits_{\mathbb{R}^{2d}} \pi_S(z)S_{j'}(z)S_j(z)\,dz - \Big(\int\limits_{\mathbb{R}^{2d}} \pi_S(z)S_j(z)\,dz\Big)\Big(\int\limits_{\mathbb{R}^{2d}} \pi_S(z)S_{j'}(z)\,dz\Big)$$

and

$$\Sigma^{(E)}_{jj'} = \int\limits_{\mathbb{R}^{2N}} \pi_E(u)E_{j'}(u)E_j(u)\,du.$$

So we get the following statement.

Corollary 2.5.

$$\ddot{\mathcal{P}}_S(0) = -4\mathrm{tr}_{\mathbb{R}^{2m}}(\Sigma^{(S)}\Sigma^{(E)}) + \sum_{1\leqslant j,j'\leqslant m} s_{j'j}e_{j'j}. \tag{2.14}$$

We remark that on the right-hand side in formula (2.14), the first term is classical and the second term is a quantum correction, which vanishes if the coupling of the system and its environment is only in position (or momentum) variables (as it is usually in the physics literature). Assume now that

$$S_j(z) = z_j \quad \text{and} \quad E_j(u) = \sum_{1\leqslant \ell\leqslant 2N} G_{j,\ell}u_\ell\,,$$

where $1 \leqslant j \leqslant 2d$. Then $G_{j,\ell}$ is a $(2d\times 2N)$-matrix with real coefficients. With these notation, for the quantum correction we have

$$q_c = \sum_{1\leqslant j,j'\leqslant 2d} s_{j'j}e_{j'j} = \mathrm{tr}_{\mathbb{R}^{2d}}(J_S G J_E G^\top), \tag{2.15}$$

where J_S, J_E are, respectively, the matrix of the canonical symplectic form in $\mathbb{R}^{2d}$ and in $\mathbb{R}^{2N}$: $\sigma_S(z,z') = z \cdot J_S z'$, $\sigma_E(u,u') = u \cdot J_E u'$ (the scalar products are denoted by a dot).

For the "classical part" we have

$$-4\mathrm{tr}_{\mathbb{R}^{2m}}\big(\Sigma^{(S)}\Sigma^{(E)}\big) = -4\mathrm{tr}\big(G^\top \mathrm{Cov}_{\rho_S} G \mathrm{Cov}_{\rho_E}\big). \tag{2.16}$$

Corollary 2.6.

$$\boxed{\ddot{\mathcal{P}}_S(0) = -4\mathrm{tr}_{\mathbb{R}^{2d}}\big(\mathrm{Cov}_{\pi_S} G \mathrm{Cov}_{\pi_E} G^\top\big) + \mathrm{tr}_{\mathbb{R}^{2d}}\big(J_S G J_E G^\top\big)} \tag{2.17}$$

where Cov_π *is the covariance matrix for the quasiprobability* π.

Recall here that the Wigner function of a pure state ψ is nonnegative if and only if ψ is a Gaussian by the Hudson theorem (see [8]).

We get a more explicit formula for the quantum Brownian motion or a variant of the quantum Brownian motion. Let us assume that

$$V(x,\xi;y,\eta) = x \cdot \left(\sum_{1\leqslant j\leqslant N} c_j y_j + \sum_{1\leqslant j\leqslant N} c_{j+N}\eta_j \right) + \xi \cdot \left(\sum_{1\leqslant j\leqslant N} d_j y_j + \sum_{1\leqslant j\leqslant N} d_{j+N}\eta_j \right).$$

Then the quantum correction q_c is obtained by the formula

$$q_c = \big(2(d_1 c_{N+1} + \cdots + d_N c_{2N}) - 2(c_1 d_{N+1} + \cdots + c_N d_{2N})\big).$$

In the quantum Brownian motion, it is assumed that the initial data for the environment is a thermal state:

$$\rho_{\tau,E}(y,\eta) = (2\tau)^N \exp\left(-\tau \sum_{1\leqslant j\leqslant N} (y_j^2 + \eta_j^2) \right), \quad 0 < \tau < 1.$$

Corollary 2.7. *Assume that* $d = 1$, $c_j = 0$ *for* $j \geqslant N+2$, *and* $d_j = 0$ *for* $j \geqslant 2$, $\psi_S \in \mathcal{S}(\mathbb{R})$, *and that* $\rho_E(0) = \rho_{\tau,E}$ *is a thermal state. Then we have*

$$\begin{aligned} \ddot{\mathcal{P}}_S(0) &= \frac{2}{\tau}\big((c_1^2 + \cdots + c_N^2 + c_{N+1}^2)\mathrm{Cov}_{x,x}(\psi_0) \\ &\quad + \big(2c_1 d_1 \mathrm{Cov}_{x,\xi}(\psi_0) + d_1^2 \mathrm{Cov}_{\xi,\xi}(\psi_0)\big) + \underbrace{c_{N+1}d_1}_{\text{quantum correction}} \end{aligned} \tag{2.18}$$

where $\mathrm{Cov}(\psi_S)$ *is the* (2×2) *covariance matrix of the Wigner function of* ψ_S *and*

$$\mathrm{Cov}(\psi_S) = \begin{pmatrix} \mathrm{Cov}_{x,x}(\psi_S) & \mathrm{Cov}_{x,\xi}(\psi_S) \\ \mathrm{Cov}_{x,\xi}(\psi_S) & \mathrm{Cov}_{\xi,\xi}(\psi_S) \end{pmatrix}.$$

So we see a new quantum correction term appearing when the coupling mixes positions and momenta variables. When $d_1 = 0$, we recover a known formula for the quantum Brownian motion.

2.2. Proofs of the statements of Section 2.1.

2.2.1. *Proof of Theorem* 2.3. It is easier here to consider the interaction formulation of quantum mechanics to "eliminate" the "free" (noninteracting) evolution: $U_0(t) = \mathrm{e}^{-it\widehat{H}_0}$. We introduce the inter-acting evolution

$$\widehat{\rho}^{(I)}(t) = U_0(t)^*\widehat{\rho}(t)U_0(t),$$

We easily see that

$$\widehat{\rho}_S^{(I)}(t) := \mathrm{tr}_E(\widehat{\rho}^{(I)}(t)) = \mathrm{e}^{it\widehat{H}_S}\widehat{\rho}_S(t)\mathrm{e}^{-it\widehat{H}_S},$$

and $\mathcal{P}_S(t) = \mathrm{tr}_S(\widehat{\rho}_S^I(t)^2)$. We shall use the simpler notation $\widehat{r}(t) = \widehat{\rho}_S^{(I)}(t)$. Using cyclicity of the trace, we obtain

$$\dot{\mathcal{P}}_S(t) = 2\mathrm{tr}_S(\widehat{r}(t)\dot{\widehat{r}}(t)), \tag{2.19}$$

$$\ddot{\mathcal{P}}_S(t) = 2\left(\mathrm{tr}_S(\widehat{r}(t)\ddot{\widehat{r}}(t)) + \mathrm{tr}_S(\dot{\widehat{r}}(t))^2\right). \tag{2.20}$$

We have, at time $t = 0$, where $V = V(0)$,

$$\dot{\widehat{r}}(0) = i^{-1}\mathrm{tr}_E[\widehat{V}, \widehat{\rho}_S \otimes \widehat{\rho}_E], \tag{2.21}$$

$$\ddot{\widehat{r}}(0) = i^{-1}\mathrm{tr}_E[\dot{\widehat{V}}, \widehat{\rho}_S \otimes \widehat{\rho}_E] - \mathrm{tr}_E[\widehat{V}, [\widehat{V}, \widehat{\rho}_S \otimes \widehat{\rho}_E]]. \tag{2.22}$$

Notice that

$$\mathrm{tr}_S\left(\mathrm{tr}_E[\dot{\widehat{V}}, \widehat{\rho}_S \otimes \widehat{\rho}_E]\widehat{\rho}_S\right) = 0. \tag{2.23}$$

This follows from the definition of the relative trace tr_E and the cyclicity of the trace. Hence we get

$$\mathrm{tr}_S\left(\mathrm{tr}_E[\dot{\widehat{V}}, \widehat{\rho}_S \otimes \widehat{\rho}_E]\widehat{\rho}_S\right) = \mathrm{tr}\left([\dot{\widehat{V}}, \widehat{\rho}_S \otimes \widehat{\rho}_E]\widehat{\rho}_S \otimes 1\right) = 0.$$

Finally we get formula (2.12) using the identity

$$[\widehat{V}, [\widehat{V}, \widehat{\rho}]] = \widehat{V}^2\widehat{\rho} + \widehat{\rho}\widehat{V}^2 - 2\widehat{V}\widehat{\rho}\widehat{V}. \qquad \square$$

2.2.2. *Proof of the corollaries.* They are easily obtained after standard computations for traces of operators starting with formula (2.12).

§3. Studying separability

3.1. Statements. We assume in this section that

$$\mathcal{H}_S = L^2(\mathbb{R}^d) \quad \text{and} \quad \mathcal{H}_E = L^2(\mathbb{R}^N),$$

and we use here properties of Weyl quantization (see, for example, [8, 15] for the proofs of properties used here). We have to consider partial transposition.

In the complex Hilbert space $L^2(\mathbb{R}^m)$, we define the bilinear form

$$u \cdot v = \int_{\mathbb{R}^m} u(x)v(x)\,dx.$$

If $\widehat{A}$ is a bounded operator on $L^2(\mathbb{R}^m)$, its transpose $\widehat{A}^\top$ is defined by the formula

$$\widehat{A}u \cdot v = u \cdot \widehat{A}^\top v, \quad u,\, v \in L^2(\mathbb{R}^m).$$

We easily see that the Weyl symbol $A^\top$ of $\widehat{A}^\top$ is given by $A^\top(x,\xi) = A(x,-\xi)$ and if $\widehat{A}$ is a quantum state (i.e., a density matrix), then $\widehat{A}^\top$ is also a quantum state.

Now we define the partial transpose in the environment space. Let $\psi_S^{(j)} \in \mathcal{H}_S$ and $\psi_E^{(j)} \in \mathcal{H}_E$, $j = 1, 2$. There exists a unique bounded operator $\widehat{A}_{\psi_S^{(1)},\psi_S^{(2)}}$ in $\mathcal{H}_E$ such that

$$(\psi_S^{(2)} \otimes \psi_E^{(2)}) \cdot \widehat{A}(\psi_S^{(1)} \otimes \psi_E^{(1)}) = \psi_E^{(2)} \cdot \widehat{A}_{\psi_S^{(1)},\psi_S^{(2)}} \psi_E^{(1)}.$$

Definition 3.1. The partial transposition of $\widehat{A}$ is a unique bounded operator $\widehat{A}^{\top E}$ in $\mathcal{H}_S \widehat{\otimes} \mathcal{H}_E$ satisfying

$$\begin{gathered}\left(\psi_S^{(2)} \otimes \psi_E^{(2)}\right) \cdot \widehat{A}^{\top E}\left(\psi_S^{(1)} \otimes \psi_E^{(1)}\right) = \psi_E^{(1)} \cdot \widehat{A}_{\psi_S^{(1)},\psi_S^{(2)}} \psi_E^{(2)}, \\ \psi_S^{(j)} \in \mathcal{H}_S, \quad \psi_E^{(j)} \in \mathcal{H}_E.\end{gathered} \tag{3.24}$$

Proposition 3.2 ([23]). *Let be $\widehat{\rho}$ a separable density matrix in $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. Then the partial transpose $\widehat{\rho}^{\top E}$ is again a density matrix in $\mathcal{H}$.*

Using anti-Wick quantization (see [3]), we get a sufficient condition for separability.

Proposition 3.3. *Assume that $\mathcal{H}_S = L^2(\mathbb{R}^d)$ and $\mathcal{H}_E = L^2(\mathbb{R}^N)$. Let $\widehat{\rho}$ be a mixed state in $L^2(\mathbb{R}^{d+N})$ such that $\widehat{\rho}$ admits an anti-Wick symbol defining a Radon probability measure in $\mathbb{R}^{2(d+N)}$. Then $\widehat{\rho}$ is separable. In particular, if $\widehat{\rho} = \rho^\Gamma$ is a Gaussian mixed state with covariance matrix Γ, mean m, and such that $\Gamma \geqslant \frac{1}{2}$, then $\rho^{(\Gamma,m)}$ is separable.*

A remarquable result is the following reverse statement for Proposition 3.2 in [33, 23].

Theorem 3.4. *Assume that* $\mathcal{H}_S = L^2(\mathbb{R})$, $\mathcal{H}_E = L^2(\mathbb{R}^N)$. *Let be* $\widehat{\rho}$ *a density matrix with a Gaussian Weyl symbol* $\rho = G^{(\Gamma,m)}$. *Then* $\widehat{\rho}$ *is separable if and only if its partial transpose* $\widehat{\rho}^{\top E}$ *is a density matrix.*

Theorem 3.4 was used in [12] to prove separability results for propagation of Gaussian states in the quantum Brownian motion (1.2), (1.3). We shall give later the details for a mathematical proof of these results.

Recall that a thermal state at temperature $\frac{1}{\beta}$ for the Hamiltonian H_E is the mixed state defined as

$$\widehat{\mathcal{T}}_{\beta,E} = \frac{\mathrm{e}^{-\beta H_E}}{\mathrm{tr}(\mathrm{e}^{-\beta H_E})}. \tag{3.25}$$

We denote $\widehat{\rho}_{g,\beta}(t) = \mathcal{U}_g^*(t,0)\widehat{\rho}(0)\mathcal{U}_g(t,0)$, the time evolution of the initial density matrix $\widehat{\rho}(0) = \widehat{\rho}_S(0) \otimes \mathcal{T}_\beta$, by the Hamiltonian (1.2), (1.3).

Theorem 3.5. *For any quantum Brownian motion* (1.2), (1.3) *with* $\omega_S > 0$, $\omega_j > 0$, $1 \leqslant j \leqslant N$, *we have the following.*

(A) *Assume here that the coupling* g *is time independent. Then for any quantum Brownian motion model with* $\omega_j > 0$, $1 \leqslant j \leqslant N+1$, *sufficiently small* (*see* (3.29)), *there exists a Gaussian initial density matrix* $\widehat{\rho}_S(0)$ *and a temperature* $\frac{1}{\beta} > 0$ *such that* $\widehat{\rho}_{g,\beta}(t)$ *is separable for any* $t \in \mathbb{R}$.

(B) *If furthermore* $g(0) \neq 0$ *then, for any pure state* $\widehat{\rho}_S(0)$ *and for any temperature* $\frac{1}{\beta} > 0$ *there exists* $\varepsilon > 0$ *such that* $\widehat{\rho}_g, \beta$ *is not separable for any* $t \in]0, \varepsilon[$.

Remark 3.6. The results (A) and (B) of Theorem 3.5 were stated in [12]. We shall revisit here the proofs by supplying mathematical details, in particular, concerning the proof of (B) where the computations of [12] were not correct.

3.2. Proofs of the separability results. First we recall some properties concerning Gaussian density matrices. We recall the definition.

Definition 3.7. An operator $\widehat{G}$ in the Hilbert space $L^2(\mathbb{R}^n)$ is said to be Gaussian if its Weyl symbol G is a Gaussian in the phase space $\mathbb{R}^{2n}$, denoted by $G^{\Gamma,m}$ where Γ is the covariance matrix (a positive definite $(2n\times 2n)$-matrix) and $m \in \mathbb{R}^{2d}$ is the mean of G. So we have

$$G^{(\Gamma,m)}(z) = c_\Gamma \mathrm{e}^{-\frac{1}{2}(z-m)\cdot\Gamma^{-1}(z-m)}, \quad z = (x,\xi) \in \mathbb{R}^{2n}, \tag{3.26}$$

where $c_\Gamma = \det(\Gamma)^{-1/2}$.

Some condition is needed on the covariance matrix Γ such that (3.26) defines a nonnegative operator in $L^2(\mathbb{R}^n)$ (see Remark 3.9).

Here J is the matrix of the symplectic form on $\mathbb{R}^n \times \mathbb{R}^n$ and $X = (x, \xi) \in \mathbb{R}^{2n}$.

Proposition 3.8. *$G^{\Gamma,m}(X)$ defines a density matrix if and only if $\Gamma + i\frac{J}{2} \geqslant 0$, or equivalently, if and only if all the symplectic eigenvalues of Γ are greater than $\frac{1}{2}$. Moreover, up to conjugation by a unitary metaplectic transform in $L^2(\mathbb{R}^n)$, $\rho^{\Gamma,0}$ is a product of one degree of freedom thermal states $\mathcal{T}_\beta$ (see Remark 3.9). Next, $\rho^{\Gamma,m}(X)$ determines a pure state if and only if 2Γ is positive and symplectic or equivalently $2\Gamma = FF^\top$, where F is a linear symplectic transformation.*

For completeness, a proof of Proposition 3.8 is sketched in Appendix B. From these results we can compute the purity (hence the linear entropy):

$$\mathcal{P}_{\widehat{G}^{\Gamma,m}} = (2\pi)^{-n} \int\limits_{\mathbb{R}^{2d}} G^{\Gamma,m}(z)^2\, dz = 2^{-n}(\det\Gamma)^{-1/2}. \qquad (3.27)$$

Remark 3.9. From Proposition 3.8 we claim that the environment state $\widehat{\rho}_{\tau,E}$ is nonnegative if and only if $\tau \leqslant 1$. We can give a direct prove of this. It suffices to prove the claim for $N = 1$. By a holomorphic continuation argument in τ, we can see that, for $\tau > 1$, $\widehat{\rho}_{\tau,E}$ is negative on the subspace of $L^2(\mathbb{R})$ spanned by the odd Hermite functions.

3.2.1. *Proof of Propositions* 3.2 *and* 3.3. To prove Proposition 3.2 (and the necessity part of Theorem 3.4), we remark that $(\widehat{\rho}_S \otimes \widehat{\rho}_E)^{\top E} = \widehat{\rho}_S \otimes (\widehat{\rho}_E)^\top$ and that for any $\psi_E \in \mathcal{H}_E$ we have $\langle \psi_E, \widehat{\rho}_E^\top \psi_E\rangle = \langle \bar{\psi}_E, \widehat{\rho}_E \bar{\psi}_E\rangle$. So we see that $\widehat{\rho}^{\top E}$ is a nonnegative operator. It is easy to check that it is in trace class so it is a density matrix. □

The proof of Proposition 3.3 results from properties of coherent states. For convenience, we use the notation of [8] for the coherent states φ_z. Here we denote $z = (z_S, z_E)$, $z_S \in \mathbb{R}^{2d}$, $z_E \in \mathbb{R}^{2N}$. So from the definition of coherent states we have $\varphi_z = \varphi_{z_S} \otimes \varphi_{z_E}$ and $\Pi_z = \Pi_{z_S} \otimes \Pi_{z_E}$, where Π_z is the orthogonal projection to φ_z. If ρ^{aw} is the anti-Wick symbol of $\widehat{\rho}$, then we have

$$\widehat{\rho} = \int\limits_{\mathbb{R}^{2(d+N)}} (\Pi_{z_S} \otimes \Pi_{z_E})\rho^{aw}(dz_S, dz_E).$$

Usually it is assumed that an anti-Wick symbol is L^∞. But the definition can be extended to finite Radon measures on the phase space.

Assume now that $\rho = \rho^\Gamma$. The Fourier transform $\widetilde{\rho}$ of ρ satisfies

$$\widetilde{\rho}(Y) = \mathrm{e}^{-\frac{\Gamma}{2}Y\cdot Y} = \widetilde{\rho}^{aw}(Y)\mathrm{e}^{-\frac{1}{2}Y\cdot Y}.$$

So ρ^{aw} defines a Schwartz distribution if and only if $\Gamma \geqslant \frac{1}{2}$. If this condition is satisfied, ρ^{aw} is a finite Radon measure.

Hence we have proved Proposition 3.3. □

3.2.2. *Proof of Theorem* 3.4. Here $\rho = G^{(\Gamma,m)}$. It suffices to assume that $m = 0$ and denote $G^{(\Gamma)} = G^{(\Gamma,0)}$. If $G^{(\Gamma)}$ is separable, we saw in Proposition 3.2 that $G^{(\Gamma),\top E}$ is a density matrix.

The reverse property is more difficult to prove. For simplicity, we give the details only for $N = 1$ following [33]. The general case is proved by induction on N (see [35])

The coordinates in the phase space for $X \in \mathbb{R}^4$ are denoted as follows:

$$X = (x_1, \xi_1, x_2, \xi_2),$$

and the matrices are written as 4 blocks of (2×2)-matrices:

$$\Gamma = \begin{pmatrix} A & C \\ C^\top & B \end{pmatrix}, \quad J = \begin{pmatrix} J_1 & 0 \\ 0 & J_1 \end{pmatrix},$$

where A, B are symmetric, $J_1 = \begin{pmatrix} 0 & 1 \\ -1, & 0 \end{pmatrix}$.

We know that $\Gamma + \frac{i}{2}J \geqslant 0$ (Proposition 3.8) so we have $A \geqslant \frac{1}{2}$ and $B \geqslant \frac{1}{2}$. To prove that $G^{(\Gamma)}$ is separable, we have to prove that $\Gamma \geqslant \frac{1}{2}$ (Proposition 3.3). From the assumption we know that $G^{(\Gamma),\top E}$ is a mixed Gaussian state with the covariance matrix

$$\Gamma^{\top E} = \begin{pmatrix} A & C\sigma \\ \sigma C^\top & \sigma B \sigma \end{pmatrix}; \quad \sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

So we also have $\Gamma^{\top E} + \frac{i}{2}J \geqslant \frac{1}{2}$.

We remark here that separability for states defined in $L^2(\mathbb{R}^2)$ is preserved by the metaplectic transformations associated with the symplectic transformations of the form $S = \begin{pmatrix} S_1 & 0 \\ 0 & S_2 \end{pmatrix}$, where S_1, S_2 are (2×2)-symplectic matrices. Matrices like these constitute a subgroup, denoted by $Sp_{1,1}(\mathbb{R})$, of the symplectic group $Sp_2(\mathbb{R})$ of $\mathbb{R}^2_{x_1,\xi_1} \times \mathbb{R}^2_{x_2,\xi_2}$. So it suffices to prove that there exists $S \in Sp_{1,1}(\mathbb{R})$ such that $S^\top \Gamma S \geqslant \frac{1}{2}$. This is proved in two steps. A, B being real and symmetric, they can be diagonalized by rotations R_1, R_2. So there exits $S_1 = \begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}$ such that

$$S_1^\top \Gamma S_1 = \Gamma_1 := \begin{pmatrix} a\mathbf{1_2} & C' \\ C'^{,\top} & b\mathbf{1_2} \end{pmatrix}.$$

But we have $C' = ER_3$, where E is symmetric and R_3 is a rotation. Then there exist rotations R_1', R_2' such that if $S_2 = \begin{pmatrix} R_1' & 0 \\ 0 & R_2' \end{pmatrix}$, we have

$$S_2^\top \Gamma S_2 = \Gamma_1 := \begin{pmatrix} a & 0 & c_1 & 0 \\ 0 & a & 0 & c_2 \\ c_1 & 0 & b & 0 \\ 0 & c_2 & 0 & b \end{pmatrix}$$

with $a, b \geqslant \frac{1}{2}$, $c_1, c_2 \in \mathbb{R}$.

Assume that $\det C > 0$. We may assume that $c_1 > 0$, $c_2 > 0$.

At the second step we conjugate Γ_1 by a family of squeezing symplectic transformations $\Sigma(r,s) = \Sigma(r) \otimes \Sigma(s)$, where $\Sigma(r) = \begin{pmatrix} r & 0 \\ 0, & \frac{1}{r} \end{pmatrix}$, $r, s \in]0, \infty[$. Choosing $\frac{s}{r} = \theta := \left(\frac{ac_2+bc_2}{ac_1+bc_2}\right)^{1/2}$, we can find a symplectic rotation R in $\mathbb{R}^4$ such that $\Gamma_2 := \Sigma(\theta s, s)^\top \Gamma_1 \Sigma(\theta s, s)$ can be diagonalized. Then we can choose s such that the smallest eigenvalue of Γ_2 is greater than $\frac{1}{2}$. So we get Theorem 3.4 if $\det C > 0$. A slight modification is needed if $\det C = 0$. Now if $\det C < 0$, we have $\det(C^{\top E}) > 0$, then $G^{(\Gamma)\top E}$ is separable so $G^{(\Gamma)}$ is separable. □

3.3. Proof of Theorem 3.5. (A) Assuming the coupling constants g and β sufficiently small, we have to find an initial Gaussian density matrix G_S such that the time evolution $\widehat{\rho}_{\gamma,\beta}(t)$ of the initial state $G_S \otimes \mathcal{T}_{\beta,E}$ stays separable at any time. It is well known that $\widehat{\rho}_{V,\beta}(t)$ is a Gaussian state (for computations see Section 4). Denote by $\Gamma_{g,\beta}(t)$ the covariance matrix of $\widehat{\rho}_{g,\beta}(t)$ and by $\Gamma_{g,\beta}^{\top E}(t)$ the covariance matrix of $\widehat{\rho}_{g,\beta}^{\top E}(t)$.

If Λ_E denotes the $(2N+2) \times (2N+2)$-matrix defined by the reflection

$$(y_1, y', \eta_1, \eta') \mapsto (y_1, y', \eta_1, -\eta'),$$

for $y_1, \eta_1 \in \mathbb{R}$, $y', \eta' \in \mathbb{R}^N$, denote

$$M^{\top E} = \Lambda_E M \Lambda_E,$$

where M is any $(2N+2) \times (2N+2)$-matrix. According to Theorem 3.4 and Proposition 3.8, we have to prove that

$$\Gamma_{g,\beta}^{\top E}(t) + \frac{i}{2} J \geqslant 0, \quad \text{or} \quad \Gamma_{g,\beta}(t) + \frac{i}{2} J^{\top E} \geqslant 0. \tag{3.28}$$

Let us introduce the full potential, where $y_1 = x$ and $y' = (y_2, y_3, \ldots, y_{N+1})$,

$$W_g(y_1, y') = \frac{1}{2}\left(\sum_{1 \leqslant j \leqslant N+1} \omega_j^2 y_j^2\right) + y_1 \sum_{2 \leqslant j \leqslant N+1} g_j y_j.$$

W_γ is a quadratic form on $\mathbb{R}^{N+1}$. Its matrix is denoted by M_g. It is positive definite if the following condition is satisfied:

$$\max_{2\leqslant j\leqslant N+1} \frac{|g_j|}{2\omega_1\omega_j} < 1. \tag{3.29}$$

Hence there exists a rotation R in $\mathbb{R}^{1+N}$ such that $RM_gR^\top := D_g$ is a diagonal matrix with eigenvalues $\widetilde{\omega}_j^2$, $1 \leqslant j \leqslant N+1$.

So if $\mathbf{R} := \begin{pmatrix} R & 0 \\ 0 & R \end{pmatrix}$, the quadratic form H_V is transformed in a sum of independent oscillators:

$$\widetilde{H}(x,\xi) := H(\mathbf{R}(x,\xi)) = \frac{1}{2}\Bigg(\sum_{1\leqslant j\leqslant N+1} \xi_j^2 + \widetilde{\omega}_j^2 x_j^2\Bigg). \tag{3.30}$$

The thermal state at temperature $\frac{1}{\delta}$ of $\widetilde{H}_V$ ($V = V_g$) is denoted by $\mathcal{T}_{\delta\widetilde{H}}$ and can be computed by using Remark 3.9. Denote $\tau(u) = \tanh(u/2)$, $u \in \mathbb{R}$. We have

$$\mathcal{T}_{\delta\widetilde{H}}(x,\xi) = 2^{-1-N} \prod_{1\leqslant jk\leqslant N+1} \tau(\delta\widetilde{\omega}_j) \exp\Bigg(-\sum_{1\leqslant j\leqslant N+1} \tau(\delta\widetilde{\omega}_j)\left(\widetilde{\omega}_j x_j^2 + \frac{1}{\widetilde{\omega}_j}\xi_j^2\right)\Bigg). \tag{3.31}$$

If $\Gamma_{\delta\widetilde{H}}$ denotes the covariance matrix of the Gaussian state $\widehat{\mathcal{T}}_{\delta\widetilde{H}}$, elementary estimates show that we have

$$2\Gamma_{\delta\widetilde{H}} \geqslant \mathbf{1}_{2+2N} \quad \text{if} \quad 0 < \delta \leqslant \ell(\widetilde{\omega}_j), \quad \text{for} \quad 1 \leqslant j \leqslant 1+N, \tag{3.32}$$

where $\ell(u) = \frac{1}{u}\ln\left(\frac{1+u}{|1-u|}\right)$ if $u \neq 1$ and $\ell(1) = \infty$. Using the relation

$$\Gamma_{\delta H} = \mathbf{R}\Gamma_{\delta\widetilde{H}}\mathbf{R}^\top,$$

we get (3.32) for $\Gamma_{\delta H}$.

Denote by $\Phi_{H_V}^t$ the linear flow defined by the quadratic Hamiltonian H_V. Then we have $\Gamma_{g,\beta}(t) = \Phi_{H_V}^t \Gamma_{g,\beta}(0)\Phi_{H_V}^{t,\top}$, where

$$\Gamma_{g,\beta}(0) = \begin{pmatrix} \Gamma_0^S & 0 \\ 0 & \Gamma_{\beta H_E} \end{pmatrix}.$$

So we write

$$\Gamma_{g,\beta}(t) + \frac{i}{2}J^{\top E} = \Phi_{H_V}^t(\Gamma_{g,\beta}(0) - \Gamma_{\delta H_V})\Phi_{H_V}^{t,\top} + \Gamma_{\delta H_V} + \frac{i}{2}J^{\top E}. \tag{3.33}$$

To conclude, we see that it is possible to choose the (2×2)-symmetric matrix Γ_0^S and β such that the symmetric matrix

$$E_{g,\beta,\delta} := \Gamma_{g,\beta}(0) - \Gamma_{\delta H}$$

is diagonally dominant [4]. Hence, using the Gersgorin Theorem [4, 21] and (3.32), we see that $E_{g,\beta,\delta}$ is nonnegative hence we get (3.28). □

(B) Now we assume that $\widehat{\rho}_S(0)$ is a pure state. Then Γ_0^S is a symplectic symmetric matrix. Here it suffices to assume that $N = 1$. With the notation of part (A), let us denote $\Gamma_t := \Gamma_{g,\beta}(t)$, we have to prove that the Hermitian matrix $2\Gamma_t + iJ^{\top E}$ has at least one negative eigenvalue for $0 < t < \varepsilon$ if $g(0) \neq 0$. Equivalently, we have to prove that the smallest eigenvalue, $\lambda_{\min}(t)$, of $4|iJ^{\top E}\Gamma_t|^2$ is smaller than 1 for $t \in]0, \varepsilon[$.

Recall that $\Gamma_t = \begin{pmatrix} A_t & C_t \\ C_t^\top & B_t \end{pmatrix}$. The eigenvalues of $4|iJ^{\top E}\Gamma_t|^2$ satisfiy

$$\lambda^4 - 4\lambda^2(\det A_t + \det B_t - 2\det C_t) + 16 \det \Gamma_t = 0.$$

So we have

$$\lambda_{\min}(t)^2 = 2\left(d_t - \sqrt{d_t^2 - 4\gamma_t}\right) =: 2v(t), \tag{3.34}$$

where $d_t = a_t + b_t - 2c_c$, $a_t = \det A_t$, $b_t = \det B_t$, $c_t = \det C_t$, $\gamma_t = \det \Gamma_t$. In particular, $\lambda_{\min}(0) = 1$.
The initial data Γ_0 is chosen here as the diagonal matrix

$$\Gamma_0 = \mathrm{Diag}\left(\frac{r}{2}, \frac{1}{2r}, \frac{s}{\omega_2}, s\omega_2\right)$$

where $r > 0$, $s > 1$, $\omega_2 > 0$. The parameter s is related to the temperature of the thermal state: $s = \coth(\beta\omega_2/2)$.

We are going to prove that $\dot{v}(0) = 0$ and $\ddot{v}(0) < 0$. In [12] it was claimed that $\dot{v}(0) < 0$, which is not correct.

Recall here the Liouville formula to compute the derivative of the determinant for an invertible matrix $M(t)$, smooth in time t:

$$\frac{d}{dt}\det(M(t)) = \det(M(t))\mathrm{tr}\left(M(t)^{-1}\frac{d}{dt}(M(t))\right). \tag{3.35}$$

The time evolution of Γ_t is given by the classical flow determined by the quadratic classical Hamiltonian $H_V(X) = \frac{1}{2}X \cdot S(t)X$, where $S(t)$ is a symmetric matrix. Denote by Φ^t this flow. We have

$$\dot{\Phi}^t = JS(t)\Phi^t \quad \text{and} \quad \Gamma_t = (\Phi^t)^\top\Gamma_0\Phi^t. \tag{3.36}$$

As a consequence of (3.34) and (3.36), we can compute $\dot{v}(0)$ and $\ddot{v}(0)$. Denote $\check{S} := JS$, $\Gamma = \Gamma(0)$, $S = S(0)$. We compute

$$\dot{\Gamma} = -\check{S}\Gamma - \Gamma\check{S}^\top, \tag{3.37}$$

$$\ddot{\Gamma} = 2\check{S}\Gamma\check{S}^\top + \check{S}^2\Gamma + \Gamma(\check{S}^\top)^2. \tag{3.38}$$

For the first derivative we get

$$\dot{\Gamma} = \begin{pmatrix} 0 & \frac{r}{2}\omega_1^2 - \frac{1}{2r} & 0 & \kappa\frac{r}{2} \\ \frac{r}{2}\omega_1^2 - \frac{1}{2r} & 0 & \frac{\kappa s}{2\omega_2} & \\ 0 & \frac{\kappa s}{2\omega_2} & 0 & 0 \\ \kappa\frac{r}{2} & 0 & 0 & 0 \end{pmatrix}. \tag{3.39}$$

From (3.39) using (3.35) and (3.34), we deduce easily that $\dot{d} = \dot{\gamma} = 0$, hence $\dot{v} = 0$.

For the second derivatives similar computations give:

$$\ddot{a} = 2\kappa^2\frac{rs}{\omega_2}, \quad \ddot{b} = \kappa^2\frac{rs}{2\omega_2}, \quad \ddot{c} = \kappa^2\frac{rs}{2\omega_2}, \quad \ddot{\gamma} = -\kappa^2\frac{rs}{16\omega_2}(s^2 - 2s - 1). \tag{3.40}$$

We get finally

$$\ddot{v} = \kappa^2\frac{rs}{\omega_2}\left(\frac{3}{2} - \frac{4s^2 - 2s + 2}{s^2 - 1}\right) \leqslant -3.9\frac{rs}{\omega_2}\kappa^2. \tag{3.41}$$

Hence $t \mapsto \lambda_{\min}(t)$ is strictly concave at $t = 0$ (see the following figure). Morever, in this figure we see that $v(t)$ oscillates: above $1/2$ the state is separable, below $1/2$ the state is entangled. □

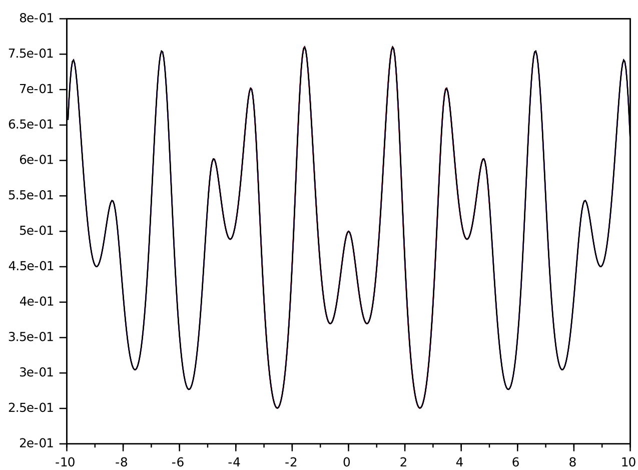

Fig. 1. Local maximum for $v(t)$ at t=0 and oscillations for the state $\widehat{\rho}_{g,\beta}(t)$ between separability and entanglement.

§4. The master equation in the Weyl-quadratic case

4.1. General quadratic Hamiltonians. In this section we find a time dependent partial differential equation (often called the master equation) satisfied by the reduced density matrix $\widehat{\rho}_S$ of the open system (S). Moreover, this equation can be solved explicitly using the well-known characteristics method. Several results proved in many places [24, 20, 18, 14] for the quantum Brownian motion model with bilinear position coupling will be extended here to any quadratic Hamiltonians with arbitrary bilinear coupling. Our results are inspired by the paper [14] but do not use the path integral methods as in the papers quoted above. In [10, 11] another presentation was given with the emphasis on a Fokker–Planck type equation.

There exist many papers in the physicist literature concerning exact or approximate master equation for the quantum Brownian motion model (see the Introduction and References in [14]). Our aim here is to give a different mathematical presentation, with straightforward general computations, for the time evolution of the reduced density matrix $\widehat{\rho}_S(t)$.

Here we assume that H_S and H_E are the quadratic Weyl symbols of $\widehat{H}_S$ and $\widehat{H}_E$, respectively. We denote by Φ_0^t the Hamiltonian flow generated by H_0, and by Φ^t the Hamiltonian flow generated by $H = H_0 + V(t)$. The symbol $V(t)$ stands for a C^1-time dependent bilinear coupling between the system and the environment:

$$V(z,u) = z \cdot G(t)u,$$

where $G(t)$ is a linear map from $\mathbb{R}^{2N}$ to $\mathbb{R}^{2d}$ (note that the coupling can mix positions and momenta variables).

Recall that $\mathbb{R}^{2d}$ (respectively, $\mathbb{R}^{2N}$) is the classical phase space of the system (respectively, the environment). Next, $\Psi^t = \Phi_0^{-t}\Phi^t$ is the interacting flow in the global phase space $\mathbb{R}^{2(d+N)}$. The phase space of the global system is identified with the direct sum $\mathbb{R}^{2d} \oplus \mathbb{R}^{2N}$ and in this decomposition the flows are represented by 4 matrix blocks

$$\Psi^t = \begin{pmatrix} \Psi_{ii}^t & \Psi_{ie}^t \\ \Psi_{ei}^t & \Psi_{ee}^t \end{pmatrix} \quad \text{and} \quad \Psi_0^t = \begin{pmatrix} \Phi_S^t & 0 \\ 0 & \Phi_E^t \end{pmatrix}, \quad \text{with} \quad \Psi_0^0 = \Psi^0 = \mathbf{1}_{\mathbb{R}^{2d+2N}}.$$

The interacting classical Hamiltonian is

$$H_I(t,z,u) = V(t,z,u) = z \cdot G^{(I)}(t)u, \quad \text{where} \quad G^{(I)}(t) = (\Phi_S^t)^\top \cdot G(t) \cdot \Phi_E^t.$$

The classical interacting evolution is given by the equation

$$\dot{\Psi}^t = J\nabla_{z,u}^2 V(t)\Psi^t, \quad \text{with } J = \begin{pmatrix} J_S & 0 \\ 0 & J_E \end{pmatrix},$$

where $\nabla^2_{z,u}V(t)$ is the Hessian matrix in variables $(z,u) \in \mathbb{R}^{2d} \times \mathbb{R}^{2N}$. So for the block components of the interacting dynamics we have

$$\dot{\Psi}^t_{ii} = J_S G(t)\Psi^t_{ei}, \qquad \dot{\Psi}^t_{ie} = J_S G(t)\Psi^t_{ee}, \tag{4.42}$$

$$\dot{\Psi}^t_{ei} = J_E G(t)^\top \Psi^t_{ii}, \quad \dot{\Psi}^t_{ee} = J_E G(t)^\top \Psi^t_{ie}. \tag{4.43}$$

Since all the Hamiltonians considered here are quadratic (eventually time dependent), they generate well-defined quantum dynamics in Hilbert spaces $L^2(\mathbb{R}^n)$ where $n = d$ for the system (S), $n = N$ for the environment (E)), and $n = d + N$ for the global system $(S) \cup (E)$.

Recall the notation

$$U(t) = \mathrm{e}^{-it\widehat{H}}, \quad U_0(t) = \mathrm{e}^{-it\widehat{H}_0}, \quad U_S(t) = \mathrm{e}^{-it\widehat{H}_S}, \quad U_E(t) = \mathrm{e}^{-it\widehat{H}_E}.$$

We have $U_0(t) = U_S(t) \otimes U_E(t)$ and the quantum interacting dynamics $U_I(t)$ is $U_0(t)^*U(t)$.

At time $t = 0$, we assume that $\widehat{\rho}(0) = \widehat{\rho}_S(0) \otimes \widehat{\rho}_E(0)$, where $\widehat{\rho}_S$ (respectively, $\widehat{\rho}_E$) is a density matrix in the Hilbert space $\mathcal{H}_S = L^2(\mathbb{R}^d)$ (respectively, in $\mathcal{H}_E = L^2(\mathbb{R}^N)$);
ρ, ρ_S, ρ_E are the Weyl symbols (i.e., the Weyl–Wigner functions, with $\hbar = 1$, of the corresponding density matrices).

The coefficients of the quadratic forms H_S, H_E, V may be time dependent. In this case $U(t)$ means $U(t,0)$, where $U(t,s)$ is the propagator solving

$$i\frac{\partial}{\partial t}U(t,s) = \widehat{H}U(t,s), \quad U(s,s) = \mathbf{1}_{\mathcal{H}}.$$

We denote $U(t) := U(t,0)$. It is well known that for quadratic Hamiltonians, every mixed state $\widehat{\rho}$ of $(S) \cup (E)$ propagates in accordance with the classical evolution (see [8] for details):

$$\widehat{\rho}(t) := U^*(t)\widehat{\rho}(0)U(t), \quad \rho(t,X) = \rho(0,\Phi^t X), \quad X \in \mathbb{R}^{2(d+N)}. \tag{4.44}$$

Our aim is to compute $\widehat{\rho}_S(t) = \mathrm{tr}_E(\widehat{\rho}(t))$. The Weyl symbol of $\widehat{\rho}_S(t)$ is given by the following integral:

$$\rho_S(t,z) = \int\limits_{\mathbb{R}^{2N}} \rho(t,z,u)\, du. \tag{4.45}$$

In particular, if $\rho(0)$ is Gaussian in all the variables,

$$X = (z,u) \in \mathbb{R}^{2d} \times \mathbb{R}^{2N},$$

then $\rho_S(t,z)$ is Gaussian in z. Nevertheless, a direct computation on the formula (4.45) seems not easy to perform, so a different strategy will be used.

4.2. Time evolution of reduced mixed states. Here we state and prove the main results of this section. It is convenient to work in the interacting setting. Recall that we have

$$\widehat{\rho}_S^{(I)}(t) = U_S^*(t)\widehat{\rho}_S(0)U_S(t)), \text{hence } \rho_S^{(I)}(t,z) = \rho_S(t,\Phi_S^t z). \tag{4.46}$$

Theorem 4.1. *Let $t_c > 0$ be the largest time t_c such that Ψ_{ii}^t is invertible for every $t \in [0, t_c[$. Assume that the environment density matrix $\widehat{\rho}_E(0)$ is Gaussian with mean m_E. Then there exist two time-dependent $(2d \times 2d)$-matrices $A^{(I)}(t)$ and $B^{(I)}(t)$, and a time dependent vector $v^{(I)}(t) \in \mathbb{R}^{2d}$ such that for $t \in [0, t_c[$ and for every $\rho_S(0)$ in $\mathcal{S}(\mathbb{R}^{2d})$, the Weyl symbol $\rho_S^{(I)}(t,z)$ of the interacting evolution $\widehat{\rho}_S^{(I)}(t)$ of the system (S) satisfies the following master equation (a Fokker–Planck type equation):*

$$\begin{aligned}\frac{\partial}{\partial t}\rho_S^{(I)}(t,z) = (A^{(I)}(t)\nabla_z)\cdot z\rho_S^{(I)}(t,z) + (B^{(I)}(t)\nabla_z)\cdot\nabla_z\rho_S^{(I)}(t,z)\\ + v^{(I)}(t)\cdot\nabla_z\rho_S^{(I)}(t,z).\end{aligned} \tag{4.47}$$

Moreover, we have the following formula to compute $A^{(I)}(t)$ and $B^{(I)}(t)$:

$$A^{(I)}(t)^\top = -J_S G(t)\Psi_{ei}^t(\Psi_{ii}^t)^{-1}, \quad B^{(I)}(t) = \frac{L(t)+L(t)^\top}{2}, \tag{4.48}$$

where

$$L(t) = J_S \cdot G(t)\left(\Psi_{ee}^t - \Psi_{ei}^t(\Psi_{ii}^t)^{-1}\Psi_{ie}^t\right)\mathrm{Cov}_{\rho_E}(\Psi_{ie}^t)^\top, \tag{4.49}$$

$$v^{(I)}(t) = -J_S G(t)\Psi_{ee}^t m_E. \tag{4.50}$$

Proof. In this proof (and only here) we shall erase the upper index (I) for the interacting dynamics. Taking the partial trace in equation (1.5), we have

$$\dot{\rho}_S(t,z) = \int_{\mathbb{R}^{2N}} \{V(t),\rho(t)\}(z,u)\,du$$

For simplicity we shall assume that $m_E = 0$. It is not difficult to take this term into account.

The Poisson bracket is in the variables (z,u) but due to integration in u we have only to consider the Poisson bracket in z. Hence we get

$$\dot{\rho}_S(t,z) = -\int_{\mathbb{R}^{2N}} J_S G(t)u\cdot\nabla_z\rho(0,\Psi^t(z,u))\,du. \tag{4.51}$$

Denote by $\widetilde{f}(\zeta)$ the Fourier transform of f in the variable z. Then we have

$$\widetilde{\dot{\rho}}_S(t,\zeta) = i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} J_S G(t) u \rho(0, \Psi^t(z,u) \mathrm{e}^{-iz\cdot\zeta}\, dz\, du.$$

Now we perform the symplectic change of variables $(z', u') = \Psi^t(z,u)$,

$$\widetilde{\dot{\rho}}_S(t,\zeta) = i\zeta \times \int_{\mathbb{R}^{2(d+N)}} dz'\, du' J_S G(t) (\Psi^t_{ei} z' + \Psi^t_{ee} u') \rho_S(z') \rho_E(u') \mathrm{e}^{-i\zeta\cdot(\Psi^t_{ii} z' + \Psi^t_{ie} u')}. \tag{4.52}$$

Denoting $\varphi = \Psi^t_{ii} z' + \Psi^t_{ie} u'$ and using the identity

$$i(\Psi^t_{ii})^{-1} \nabla_\zeta \mathrm{e}^{-i\zeta\cdot\varphi} = (z' + (\Psi^t_{ii})^{-1} \Psi^t_{ie} u') \mathrm{e}^{-i\zeta\cdot\varphi},$$

we get

$$\begin{aligned} \widetilde{\dot{\rho}}_S(t,\zeta) = &-\zeta \cdot J_S G(t) \Psi^t_{ei} (\Psi^t_{ii})^{-1} \nabla_\zeta \widetilde{\rho}_S(t,\zeta) \\ &- i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} dz'\, du' J_S G(t) \Psi^t_{ei} (\Psi^t_{ii})^{-1} \Psi^t_{ie}(u') \rho_E(u') \rho_S(z') \mathrm{e}^{-i\zeta\cdot\varphi} \\ &+ i\zeta \cdot \int_{\mathbb{R}^{2(d+N)}} dz'\, du' J_S G(t) (\Psi^t_{ee} u') \rho_E(u') \rho_S(z') \mathrm{e}^{-i\zeta\cdot\varphi}. \end{aligned} \tag{4.53}$$

To absorb the linear terms in u', we use the fact that ρ_E is Gaussian, $\rho_E = c_\Lambda \mathrm{e}^{-1/2 u\cdot\Lambda u}$, where Λ is a positive definite $(2N \times 2N)$-matrix and c_Λ a normalization constant. So we have $\Lambda^{-1} \nabla_u \rho_E(u) = u\rho_E(u)$, and integrating by parts we have

$$\widetilde{\dot{\rho}}_S(t,\zeta) = -\zeta \cdot A^{(I)}(t)^\top \nabla_\zeta \widetilde{\rho}_S(t,\zeta) - (\zeta \cdot L(t)\zeta) \widetilde{\rho}_S(t,\zeta). \tag{4.54}$$

We get (4.47) by taking inverse Fourier transforms. □

Corollary 4.2. *In the notation of Theorem* 4.1, *the reduced density matrix for the system satisfies the following master equation*:

$$\begin{aligned} \frac{\partial}{\partial t} \rho_S(t,z) = &\{H_S, \rho_S(t)\}(z) \\ &+ (A(t)\nabla_z) \cdot z\rho_S(t,z) + (B(t)\nabla_z) \cdot \nabla_z \rho_S(t,z) \\ &+ v(t) \cdot \nabla_z \rho_S(t,z), \quad \textit{for} \quad t \in [0, t_c[. \end{aligned} \tag{4.55}$$

Remark 4.3. The function $\rho_S(t,z)$ is of course well defined for every time $t \in \mathbb{R}$ but the coefficients of the master equation (4.47) may have singularity at $t = t_c$, as we shall see later.

Denote $\gamma = \sup_{t\geqslant 0} \|G(t)\|$ and $\varphi(t) = \|\Phi^t_S\| + \|\Phi^t_E\|$.

Proposition 4.4. *If*

$$\sup_{t \geqslant 0} \varphi(t) < +\infty,$$

then there exists $c > 0$ such that $t_c \geqslant \frac{c}{\gamma}$. If there exist $C, \delta > 0$ such that $\varphi(t) \leqslant C\mathrm{e}^{\delta t}$ for every $t > 0$, then there exists $C_1 \in \mathbb{R}$ such that

$$t_c \geqslant \frac{1}{\delta} \log(\frac{1}{\gamma}) + C_1.$$

The constants δ and C_1 are independant of γ.

Proof. It suffices to work in the interaction representation. Using interacting time evolution Ψ^t for the total classical system $(S) \cup (E)$, we get

$$\|\Psi^t - \mathbf{1}\| \leqslant \gamma \int_{\mathbf{0}}^{\mathbf{t}} \varphi(\mathbf{s})\mathbf{ds} + \gamma \int_{\mathbf{0}}^{\mathbf{t}} \varphi(\mathbf{s})\|\mathbf{\Psi^s} - \mathbf{1}\|\mathbf{ds}.$$

Denote $\phi(t) = \int_0^t \varphi(t)ds$. Using the Gronwall lemma and integrating by parts, we get

$$\|\Psi^t - \mathbf{1}\| \leqslant \gamma\phi(\mathbf{t}) + \frac{\gamma^{\mathbf{3}}}{\mathbf{6}}\phi(\mathbf{t})^{\mathbf{3}}\mathrm{e}^{\gamma\phi(\mathbf{t})}. \tag{4.56}$$

From inequality (4.56), we easily get the proposition. □

Remark 4.5. Explicite computations on the model of coupled harmonic oscillators (see the Appendix for details) show that we may have $t_c < +\infty$ or $t_c = \infty$. Assume that $d = N = 1$, $V(x, y) = gxy$, $\widehat{H} = \widehat{H}_S + \widehat{H}_E + V$,

$$\widehat{H}_S = \frac{1}{2}(-\partial^2_{x^2} + {\omega_1}^2 x^2), \quad \widehat{H}_E = \frac{1}{2}(-\partial^2_{y^2} + {\omega_E}^2 y^2).$$

If $\omega_S^2 = 1$, $\omega_E^2 = -1$ and $g \neq 0$, then $0 < t_c < +\infty$. If $\omega_S^2 = 1 = \omega_E^2$ and $0 \leqslant g \leqslant \frac{1}{\sqrt{2}}$, then $t_c = +\infty$.

Remark 4.6. The coefficients of equation (4.47) are related to the first and second moments of the reduced density matrix $\rho_S(t)$. We denote

$$m_j^{(I)}(t) = \int_{\mathbb{R}^{2d}} z_j \rho_S^{(I)}(t, z)\, dz, \quad \mu_{jk}^{(I)}(t) = \int_{\mathbb{R}^{2d}} z_j z_k \rho_S^{(I)}(t, z)\, dz.$$

From (4.47), after computations using (4.43), we get

$$m^{(I)}(t) = \Psi^t_{ii} m^{(I)}(0). \tag{4.57}$$

Computations of the second moments, by using (4.51), (4.43), and (4.47), give

$$\mu^{(I)}(t) = \frac{1}{2}\Big(\Psi_{ii}^{t\top}\mu^{(I)}(0)\Psi^t_{ii} + \Psi_{ie}^{t\top}\mu_E(0)\Psi^t_{ie}\Big), \tag{4.58}$$

where $\mu_E(0)$ is the second moments matrix of $\rho_E(0)$.

Remark 4.7. Suppose that the initial state of the total system $(S) \cup (E)$ is Gaussian:

$$\rho(0, z, u) = c_\Gamma \mathrm{e}^{-(1/2)\Gamma^{-1}(z,u)\cdot(z,u)}, \quad c_\gamma > 0$$

is a normalization constant. Then we have the following direct computation for $\rho_S(t, z)$. We get first the Fourier transform:

$$\widetilde{\rho}_S(t, \zeta) = \mathrm{e}^{-(1/2)\Gamma(t)(\zeta,0)\cdot(\zeta,0)},$$

where $\Gamma(t) = (\Phi^t)^\top \Gamma(\Phi^t)$. Using inverse Fourier transforms, we obtain

$$\rho_S(t, z) = c_{\gamma,t} \mathrm{e}^{-(1/2)\Gamma_S^{-1}(t) z\cdot z} \tag{4.59}$$

where $\Gamma_S(t)$ is the matrix of the positive definite quadratic form

$$\mathcal{Q}_t(\zeta, \zeta) := \Gamma(t)(\zeta, 0) \cdot (\zeta, 0)$$

on $\mathbb{R}^{2d}$ and $c_{\Gamma,t} = (2\pi)^{-d} \det^{1/2} \Gamma_t$.

We can see on this example what is the meaning of critical times t_c. Assume that $\Gamma = \Gamma_S \oplus \Gamma_E$, where the $\Gamma_{S,E}$ are positive definite quadratic forms on $\mathbb{R}^{2d}$, respectively, on $\mathbb{R}^{2N}$. We have easily: $\mathcal{Q}_0(\zeta, \zeta) = \Gamma_S \zeta \cdot \zeta$ and

$$\mathcal{Q}_t(\zeta, \zeta) = \Gamma_S(\Phi^t_{ii})\zeta \cdot (\Phi^t_{ii})\zeta + \Gamma_E(\Phi^t_{ei})\zeta \cdot (\Phi^t_{ei})\zeta. \tag{4.60}$$

We see from (4.60) that the initial state $\widehat{\rho}_S(0)$ cannot be recovered by its evolution at time t_c: only the restriction of $\mathcal{Q}_0$ to $(\ker \Phi_{ii})^\perp$ is recovered by $\mathcal{Q}_{t_c}$. The physical interpretation is that a part of information contained in $\widehat{\rho}_S(t_c)$ has escaped in the environment represented here by Γ_E.

Now we consider more general initial $\rho_S \in \mathcal{S}(\mathbb{R}^d)$ for the system (S). The master equation (4.47) can easily be solved by the characteristics method after a Fourier transform. As in the proof of Theorem 4.1, $\widetilde{\rho}^{(I)}_S(t, \zeta)$ denotes the Fourier transform of $\rho^{(I)}_S(t)$.

Theorem 4.8. *Assume (for simplicity) that the mean of the environment state is* 0. *With the notation of Theorem* 4.1, *we have*:

$$\widetilde{\rho}^{(I)}_S(t, \zeta) = \widetilde{\rho}_S(0, (\Psi^t_{ii})\zeta) \exp\Big(-\frac{1}{2}\zeta \cdot \Theta^{(I)}(t)\zeta\Big), \quad t \in \mathbb{R}, \tag{4.61}$$

where $\Theta^{(I)}(t) = \Psi^{t\top}_{ie} \mathrm{Cov}_{\rho_E(0)}(\Psi^t_{ie})$.

Remark 4.9. The interpretation of the right-hand side in formula (4.61) is the following: the first factor is a transport term. The second term is a dissipation term due to the influence of the environment which is controlled by the nonnegative matrix $\Theta^{(I)}(t)$. Formula (4.8) is an extension of a formula obtained in [14] for the Brownian quantum motion model where $\Theta^{(I)}(t)$ is named the "thermal covariance" when the environment is in a thermal equilibrium state.

As far as Φ_{ii}^t is invertible, from (4.61) we see that the time evolution of $\widehat{\rho}_S$ is reversible but this is no longer true for $t \geqslant t_c$. From (4.61) we get an explicit representation formula for the reduced density of the system as a convolution integral.

Corollary 4.10. *With the notation of Theorem* 4.8, *we have*

$$\begin{aligned} \rho_S^{(I)}(t,z) &= c_S^{(I)}(t)\int_{\mathbb{R}^{2d}} \rho_S\left(0, \Psi_{ii}^{(t,0)} z'\right) \exp\left(-\frac{1}{2}(z-z') \cdot \Theta^{(I)}(t)^{-1}(z-z')\right) dz', \\ \rho_S(t,z) &= c_S(t)\int_{\mathbb{R}^{2d}} \rho_S\left(0, \Phi_{ii}^{(t,0)} z'\right) \exp\left(-\frac{1}{2}(z-z') \cdot \Theta(t)^{-1}(z-z')\right) dz', \end{aligned} \tag{4.62}$$

where

$$c_S^{(I)}(t) = (2\pi)^{-d/2} \det(\Psi_{ii}^t)^{-1} \det\left(\Theta^{(I)}(t)\ \right)^{-1/2}$$

and

$$c_S(t) = (2\pi)^{-d/2} \det(\Phi_{ii}^t)^{-1} \det\left(\Theta(t)\right)^{-1/2}.$$

If $\det(\Phi_{ii}^t) = 0$ *or* $\det((\Phi_{ie}^t(\Phi_{ie}^t)^\top) = 0$, *the integrals in* (4.62) *are defined as convolutions of distributions.*

Formula (4.62) shows clearly the damping influence of the environment on the system because $\Theta(t)$ is a positive matrix under our assumptions. If $\Theta(t)$ is singular, then the Fourier transform of $\exp\left(-\frac{1}{2}\zeta \cdot \Theta(t)\zeta\right)$ is a distribution supported in some linear subspace of $\mathbb{R}^{2d}$ where the damping occurs.

Appendix §A. Coupled harmonic oscillators

More explicit computations can be done for systems with two coupled one-dimensional harmonic oscillators:

$$\widehat{H}_S = \frac{1}{2}(-\partial_{x^2}^2 + {\omega_S}^2 x^2), \quad \widehat{H}_E = \frac{1}{2}(-\partial_{y^2}^2 + {\omega_E}^2 y^2).$$

We assume that $\omega_S > 0$ and ω_E can be real positive or pure imaginary ($\omega_E^2 < 0$). The inequality $\omega_E^2 > 0$ means a stable environment, and $\omega_E^2 < 0$ means an unstable environment. Unstable environment like this was considered in the paper [6].

The first step is to compute the classical flow of the total Hamiltonian depending on the coupling constant g:

$$H(x,\xi,y,\eta) = \frac{1}{2}(\xi^2 + \eta^2 + {\omega_S}^2 x^2 + {\omega_E}^2 y^2) + gxy.$$

Let $M = \begin{pmatrix} \omega_S^2 & g \\ g & \omega_E^2 \end{pmatrix}$ be the matrix of the quadratic potential for the total system:

$$V(x, y) = \frac{1}{2}({\omega_S}^2 x^2 + {\omega_E}^2 y^2) + gxy.$$

The eigenvalues $\lambda_\pm$ of M are

$$\lambda_\pm = \frac{1}{2}\Big(\omega_S^2 + \omega_E^2 \pm \sqrt{(\omega_S^2 - \omega_E^2)^2 + 4g^2}\Big).$$

So we can diagonalize M and next the Hamiltonian H. From that we compute the flow defined by H. We get in particular

$$\det\big(\Phi_{ii}^t\big) = 1 + 2\frac{g^2}{(\omega_S^2 - \omega_E^2)^2 + 4g^2} \Big(\cos(t\lambda_+^{1/2})\cos(t\lambda_-^{1/2}) + \frac{\omega_S^2 + \omega_E^2}{2\sqrt{\omega_S^2\omega_E^2 - g^2}}\sin(t\lambda_+^{1/2})\sin(t\lambda_-^{1/2}) - 1\Big). \tag{A.63}$$

From equation (A.63) we can compute the critical time t_c. We see here that we may have t_c finite or infinite, depending on the coupling constant g and on the sign of ω_E^2.

1. Assume that $\omega_S^2\omega_E^2 > g^2$ and $\omega_S^2 \neq \omega_E^2$. We have $\lambda_+ > \lambda_- > 0$. We see easily that, for some constant C depending only on ω_S, ω_E, we have

$$\big|\det\big(\Phi_{ii}^t\big) - 1\big| \leqslant Cg^2, \quad t \in \mathbb{R}.$$

Then if $\kappa < \frac{1}{C}$, (Φ_{ii}^t) is invertible for every $t \in \mathbb{R}$.

2. If $\omega_S^2 = \omega_E^2$ and $\omega_S^2 > g^2$, we deduce from (A.63) that there exists $C > 0$ such that Φ_{ii}^t is invertible for $0 \leqslant t \leqslant \frac{C}{\kappa}$.

3. If $\omega_S^2\omega_E^2 < g^2$, then $\lambda_+ > 0 > \lambda_-$. We can find constants C_1, C_2 such that if $ge^{C_2 t} \leqslant C_1$, then Φ_{ii}^t is invertible.

Appendix §B. Gaussian density matrices

We shall give here a proof of Proposition 3.8. This is a consequence of a particular case of the following Williamson theorem (see [36] and [2, Appendix 6]).

Theorem B.1. *Let Γ be a positive nondegenerate linear transformation in $\mathbb{R}^{2N}$. Then there exists a linear symplectic transformation S and positive real numbers $\lambda_1, \dots, \lambda_N$ such that*

$$S^\top \Gamma S e_j = \lambda_j e_j \quad \textit{and} \quad S^\top \Gamma S e_{j+N} = \lambda_j e_{j+N} \tag{B.64}$$

for $1 \leqslant j \leqslant N$, where $\{e_1, \dots, e_N, \dots, e_{2N}\}$ is the canonical basis of $\mathbb{R}^{2N}$.

In [31] the authors gave a simple proof that we recall here. Recall the following known lemma

Lemma B.2. *Let A be a nondegenerate antisymmetric linear mapping in $\mathbb{R}^{2N}$. Then there exists an orthonormal basis $\{v_1, v_1^*, \dots, v_N, v_N^*\}$ of $\mathbb{R}^{2N}$ and positive real numbers $\{\nu_1, \dots, \nu_N\}$ such that*

$$Av_j = \nu_j v_j^* \quad \textit{and} \quad Av_j^* = -\nu_j v_j.$$

Proof of Lemma B.2. We proceed by induction on N. This is obvious for $N = 1$.

Assume that $N \geqslant 2$. Let ν_1 be an eigenvalue of the symmetric matrix A^2, $A^2 v_1 = \nu_1 v_1$, $\|v_1\| = 1$. We can choose a vector v_1^* and $a \in \mathbb{R}$ such that $Av_1 = -av_1^*$ and $\|v_1^*\| = 1$. Then we easily see that $v_1 \cdot v_1^* = 0$ and if P is the plane spanned by $\{v_1, v_1^*\}$, then P and $P^\perp$ are invariant under A. So we can apply the inductive assumption to A acting in $P^\perp$, and the lemma is proved. □

Proof of Theorem B.1. Consider the antisymmetric matrix

$$A = \Gamma^{-1/2} J \Gamma^{-1/2}.$$

Using Lemma B.2, we can find an orthogonal matrix R and a diagonal matrix $\Omega = \mathrm{diag}\{\nu_1, \nu_2, \dots, \nu_N\}$, $\nu_j > 0$, $1 \leqslant j \leqslant N$, such that

$$R^\top \Gamma^{-1/2} J \Gamma^{-1/2} R = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}.$$

Denote $B = \begin{pmatrix} \Omega^{-1/2} & 0 \\ 0 & \Omega^{-1/2} \end{pmatrix}$ and $S = \Gamma^{-1/2} R B$. We easily see that $S^\top \Gamma S = B^2$ and $S^\top J S = J$, so the proof of Theorem B.1 follows. □

The N real numbers λ_j in Theorem B.1 are the symplectic eigenvalues of Γ. Using the ralation $S^\top = -JS^{-1}J$, we see that $J\Gamma$ is diagonalizable with eigenvalues $\{\pm\lambda_j,\ 1 \leqslant j \leqslant N\}$ and that $\{\lambda_1, \dots, \lambda_N\}$ are the eigenvalues (with multiplicities) of $|J\Gamma| = (-J\Gamma^2 J)^{1/2}$.

Proof of Proposition 3.8. We can assume that $m = 0$ and we denote $\rho_\Gamma = \rho^{\Gamma,0}$. We use the symplectic normal form for Γ given by Theorem B.1. Let $\widehat{R}(S)$ be the metaplectic unitary operator associated with S (see, for example, [8]). Hence we have

$$\widehat{R}(S)^* \widehat{\rho}_\Gamma \widehat{R}(S) = \widehat{\rho}_{S^\top \Gamma S} = \widehat{\rho}_{\tau_1} \otimes \widehat{\rho}_{\tau_1} \cdots \otimes \widehat{\rho}_{\tau_N},$$

where the τ_j are the symplectic eigenvalues of $\frac{\Gamma^{-1}}{2}$. So $\widehat{\rho}_\Gamma$ is a density matrix if and only if we have $0 \leqslant \tau_j \leqslant 1$ for $1 \leqslant j \leqslant d$ (Remark 3.9). This condition means that the symplectic eigenvalues of 2Γ are greater than 1 or, equivalently, $2\Gamma + iJ \geqslant 0$.

If $\widehat{\rho}_\Gamma$ is a Gaussian pure state, by computing its Wigner (see, for example, [8]), function we see that Γ is a symplectic matrix. Conversely, if $2\Gamma = F^\top F$ with F symplectic, then $\widehat{\rho}_\Gamma$ is the Wigner function of a squeezed state $\widehat{R}(F)\varphi_0$, φ_0 being the standard Gaussian.

Gaussian states are thermal states for positive nondegenerate quadratic Hamiltonians and conversely. This can be proved as follows. Let $H(u) = \frac{1}{2}u\cdot\Lambda$, where Λ is a positive nonsingular linear transformation in $\mathbb{R}^{2N}$. We consider symplectic coordinates for u: $y_j = u \cdot e_j$ and $\eta_j = u \cdot e_{j+N}$, $1 \leqslant j \leqslant N$. Using Theorem B.1, we have $H(u) = H_\Delta(Su)$, where S is a symplectic linear transformation and

$$H_\Delta(u) = \sum_{1\leqslant j\leqslant N} \lambda_j u_j^2, \quad u_j = (x_j, \xi_j) \in \mathbb{R}^2.$$

Applying the metaplectic transformation, we have $\widehat{H} = \widehat{R}(S)\widehat{H}_\Delta\widehat{R}(S)^*$ and

$$\mathrm{e}^{-\beta\widehat{H}} = \widehat{R}(S)\mathrm{e}^{-\beta\widehat{H}_\Delta}\widehat{R}(S)^*.$$

From the Melher formula for the harmonic oscillator, the Weyl symbol W_Δ of $\mathrm{e}^{-\beta\widehat{H}_\Delta}$ is

$$W_\Delta(y,\eta) = \prod_{1\leqslant j\leqslant N} \frac{\exp\Big(-\tanh(\beta\lambda_j)(y_j^2+\eta_j^2)\Big)}{\cosh(\beta\lambda_j)},$$

so the Weyl symbol W of $\mathrm{e}^{-\beta\widehat{H}}$ is given by

$$W(y,\eta) = W_\Delta(S^{-1}(y,\eta)).$$

This proves that $\frac{\mathrm{e}^{-\beta\widehat{H}}}{\mathrm{tr}\mathrm{e}^{-\beta\widehat{H}}}$ is a Gaussian state. □

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