

ANNALES DE L'I. H. P., SECTION A

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Annales de l'I. H. P., section A, tome 67, n° 4 (1997), p. 425-445

<http://www.numdam.org/item?id=AIHPA_1997__67_4_425_0>

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From resonances to master equations

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ABSTRACT. — We study the long-time behavior of the dynamics of a 2-level atom coupled to a scalar radiation field at positive temperature. We discuss the deep relations between results proven recently in [JP1], [JP2], and the Davies master equation technique [D1], [D2].

Key words: Quantum friction, master equations, open systems, Markov approximation, spin-boson model.

RÉSUMÉ. — Dans la limite des grands temps, nous étudions la dynamique d'un atome à deux niveaux couplé à un champ de radiation scalaire à température positive. Nous discutons en particulier la relation entre les résultats récemment obtenus dans [JP1], [JP2], et les équations maîtresses étudiées par Davies [D1], [D2].

1. INTRODUCTION

This paper is a note on the results we recently proved in [JP1]-[JP3]. There we studied the dynamics of an open quantum system \mathcal{A} , characterized

by a discrete set of energy levels $\{e_i\}$, allowed to interact with a large reservoir \mathcal{B} . The reservoir is an infinite free Bose gas at inverse temperature β without Bose-Einstein condensate. Using algebraic and spectral techniques we have shown that in the weak-coupling/high-temperature regime the interacting system $\mathcal{A} + \mathcal{B}$ has strong ergodic properties. In particular, it approaches thermal equilibrium exponentially fast. The techniques we employed shed a new light on the origin and derivation of master equations for this class of models, and it is this aspect that we would like to discuss here.

The basic idea of our approach is to reduce ergodic properties of the system to spectral problems for a distinguished self-adjoint operator: the Liouvillean. This operator is defined in abstract terms. We use Tomita-Takesaki theory to compute the Liouvillean, and complex deformation techniques to study its spectrum. It turns out that complex resonances of the Liouvillean carry critical information concerning physical mechanism of thermal relaxation. For instance, it is well-known that the time evolution of an open system is Markovian if the time variable is suitably rescaled (the Van Hove weak-coupling limit). We show that the generator of this Markov approximation arises as Fermi's Golden Rule for the resonances of the Liouvillean. Our technique is not restricted to second order perturbation theory, and gives an exact transport equation with convergent expansion in the powers of the coupling constant. The first non-trivial contribution to this expansion is the generator of the Markov approximation.

Although our results can be presented in an abstract form, as in [D1], we prefer to be concrete, and develop the theory on a specific, physically important model. Thus, in this paper we will study the dissipative dynamics of a 2-level atom (or spin 1/2) interacting with a free Bose gas. In the physics literature, this model is known as the spin-boson system. The master equation which governs the spin relaxation is the well-known Bloch equation. The literature on the subject is enormous and is partially listed in [JP2]. We remark that the results of this paper have a straightforward extension to models in which the spin is replaced by an N -level atom. An extension of our results to a variety of related models, including non-relativistic QED, will be presented in [JP3].

Originally, this paper was meant to be a part of [JP3]. The mathematical analysis of the models in non-relativistic QED is, however, very technical. It has been suggested that results discussed here might be of interest to a wider audience, and we decided to present them separately.

2. THE MODEL

We recall that a W^* -dynamical system is a pair (\mathcal{M}, τ) , where \mathcal{M} is a von Neumann algebra (weakly closed $*$ -algebra of bounded operators on some separable Hilbert space) and $\mathbf{R} \ni t \mapsto \tau^t$ a weakly continuous group of $*$ -automorphisms of \mathcal{M} . The elements of \mathcal{M} are associated with *observables* of the quantum mechanical system under consideration. The group τ^t specifies their time evolution. The physical states of the system are represented by normalized continuous positive linear functionals, *i.e.* *states*, over \mathcal{M} . A state \mathcal{S} is normal if there is a density matrix ρ (a positive trace class operator of unit trace) such that $\mathcal{S}(A) = \text{Tr}(\rho A)$. A state \mathcal{S} is faithful if $\mathcal{S}(A^*A) = 0$ implies $A = 0$. A quantum dynamical system is a triple $(\mathcal{M}, \mathcal{S}, \tau)$, where \mathcal{S} is a faithful, normal, τ -invariant state.

Thermal equilibrium states of quantum systems are characterized by the KMS condition.

DEFINITION 2.1. – Let (\mathcal{M}, τ) be a W^* -dynamical system and $\beta > 0$. A state \mathcal{S} on \mathcal{M} is a (τ, β) -KMS state if it satisfies:

1. \mathcal{S} is normal.
2. For any $A, B \in \mathcal{M}$ there exist a function $F_{A,B}(z)$, analytic in the strip $0 < \text{Im}(z) < \beta$, continuous and bounded on its closure, and satisfying the KMS boundary conditions

$$\begin{aligned} F_{A,B}(t) &= \mathcal{S}(A\tau^t(B)), \\ F_{A,B}(t+i\beta) &= \mathcal{S}(\tau^t(B)A), \end{aligned}$$

for $t \in \mathbf{R}$.

Remark. – A KMS-state is τ -invariant, and a unique KMS state is automatically faithful.

In the sequel we restrict ourselves to quantum dynamical systems of the form $(\mathcal{M}, \mathcal{S}^\beta, \tau)$, where \mathcal{S}^β is a unique (τ, β) -KMS state. To characterize the ergodic properties of such systems, Robinson [RO1], [RO2] introduced the following notion:

DEFINITION 2.2. – A quantum dynamical system $(\mathcal{M}, \mathcal{S}^\beta, \tau)$ has the property of return to equilibrium if, for any $A \in \mathcal{M}$ and any normal state \mathcal{S} , one has

$$\lim_{|t| \rightarrow \infty} \mathcal{S}(\tau^t(A)) = \mathcal{S}^\beta(A).$$

For a detailed discussion of this definition and its various reformulations we refer the reader to [RO1].

We now describe the spin-boson system. We introduce first the isolated spin and the reservoir. The Hilbert space of the isolated spin is \mathbf{C}^2 . Its algebra of observables is M_2 , the algebra of all 2×2 matrices on \mathbf{C}^2 . We denote by $\sigma_x, \sigma_y, \sigma_z$ the usual Pauli matrices. The Hamiltonian of this system is chosen to be $H_s \equiv \sigma_z$. This Hamiltonian induces a flow

$$\tau_s^t : A \mapsto e^{itH_s} A e^{-itH_s}.$$

The eigenenergies of the spin are $e_{\pm} = \pm 1$, and we denote the corresponding eigenstates by χ_{\pm} . At inverse temperature β , the equilibrium state of the spin is defined by the Gibbs Ansatz

$$\mathcal{S}_s^\beta(A) \equiv \frac{1}{Z_s^\beta} \operatorname{Tr}(e^{-\beta H_s} A),$$

where Z_s^β is a normalization factor. It is well-known that \mathcal{S}_s^β is a unique (τ_s, β) -KMS state on M_2 .

The heat reservoir is an infinite gas of free massless bosons at positive temperature without Bose-Einstein condensate. The detailed mathematical description of this system is presented in [JP2]. Thus, here we will just introduce the necessary notation, referring the reader to [JP2] for details and additional information.

The reservoir is described by a triple $\{\mathcal{H}_B, \Omega_B, H_B\}$ where \mathcal{H}_B is a Hilbert space, Ω_B a unit vector in \mathcal{H}_B , and H_B a self-adjoint operator on \mathcal{H}_B . We denote by $\omega(\mathbf{k})$ the energy of a boson with momentum $\mathbf{k} \in \mathbf{R}^3$. We are interested in the physically realistic case:

$$\omega(\mathbf{k}) = |\mathbf{k}|.$$

Our method easily accommodates other dispersion laws, as long as the bosons remain massless. The equilibrium momentum distribution of the bosons is given by the Planck law

$$\varrho(\mathbf{k}) = \frac{1}{e^{\beta\omega(\mathbf{k})} - 1}. \quad (2.1)$$

The space \mathcal{H}_B carries a regular, cyclic representation of Weyl's algebra (CCR) over the space of test functions

$$\mathcal{D} = \{f : (1 + \omega(\mathbf{k})^{-1/2})f \in L^2(\mathbf{R}^3)\},$$

such that

$$(\Omega_B, W_B(f)\Omega_B) = \exp \left[-\frac{\|f\|^2}{4} - \frac{1}{2} \int_{\mathbf{R}^3} |f(\mathbf{k})|^2 \varrho(\mathbf{k}) d^3k \right] \quad (2.2)$$

for $f \in \mathcal{D}$. We denote by $\varphi_B(f)$ the field operators, $W_B(f) \equiv e^{i\varphi_B(f)}$. The operator H_B is uniquely specified by the requirements

$$e^{itH_B} W_B(f) e^{-itH_B} = W_B(e^{it\omega} f), \quad (2.3)$$

$$H_B \Omega_B = 0. \quad (2.4)$$

We denote by \mathcal{M}_B the von Neumann algebra generated by $\{W_B(f) : f \in \mathcal{D}\}$. The triple $\{\mathcal{H}_B, \Omega_B, H_B\}$ and \mathcal{M}_B are, up to unitary equivalence, uniquely determined by (2.1)-(2.4). We remark that these structures can be explicitly identified, see e.g. [AW] or [JP2]. Let

$$\mathcal{S}_B^\beta(A) = (\Omega_B, A\Omega_B),$$

and

$$\tau_B^t : A \mapsto e^{itH_B} A e^{-itH_B}.$$

Then \mathcal{S}_B^β is a unique (τ_B, β) -KMS state on \mathcal{M}_B . The quantum dynamical system $(\mathcal{M}_B, \mathcal{S}_B^\beta, \tau_B)$ defines the heat reservoir.

The spin-boson system is defined as follows. The Hilbert space of the combined system is $\mathbf{C}^2 \otimes \mathcal{H}_B$, and its algebra of observables is $\mathcal{M} \equiv M_2 \otimes \mathcal{M}_B$. The Hamiltonian of the system is

$$H_\lambda = H_s \otimes I + I \otimes H_B + \lambda Q \otimes \varphi_B(\alpha), \quad (2.5)$$

where λ is a real constant, $Q \equiv \sigma_x$, and $\alpha \in \mathcal{D}$. In the sequel, we will refer to α as the form factor. In [JP1] we have shown that H_λ is essentially self-adjoint on $\mathbf{C}^2 \otimes D(H_B)$ for each $\lambda \in \mathbf{R}$, provided

$$(\omega(\mathbf{k}) + \omega(\mathbf{k})^{-1})\alpha \in L^2(\mathbf{R}^3).$$

Thus, under this assumption

$$\tau_\lambda^t : A \mapsto e^{itH_\lambda} A e^{-itH_\lambda}$$

is a weakly continuous group of $*$ -automorphisms of \mathcal{M} , and the spin-boson model defines a W^* -dynamical system $(\mathcal{M}, \tau_\lambda)$.

The following result was proven for the first time in [FNV] (see also Theorem 6.1 in [JP2]).

PROPOSITION 2.3. – *For any $\lambda \in \mathbf{R}$ and $\beta > 0$, there exists a unique (τ_λ, β) -KMS state S_λ^β on \mathcal{M} .*

In [JP2] we investigated the ergodic properties of the quantum dynamical system $(\mathcal{M}, \mathcal{S}_\lambda^\beta, \tau_\lambda)$. To state the result, we need some additional notation. Let S^2 be the unit sphere in \mathbf{R}^3 and $d\sigma$ its surface measure. Let $H^2(\delta, L^2(S^2))$ be the Hardy class of $L^2(S^2)$ -valued functions in the strip $\{z : |\text{Im}(z)| < \delta\}$. For a given function f on \mathbf{R}^3 , we define a new function \tilde{f} on $\mathbf{R} \times S^2$ by the formula

$$\tilde{f}(s, \hat{k}) = \begin{cases} s^{1/2} \cdot f(s\hat{k}) & \text{if } s \geq 0 \\ -|s|^{1/2} \cdot \overline{f}(|s|\hat{k}) & \text{if } s < 0. \end{cases}$$

We set the Hypothesis:

(H1) The form-factor α in Equation (2.5) satisfies

$$(\omega(\mathbf{k}) + \omega(\mathbf{k})^{-1})\alpha \in L^2(\mathbf{R}^3).$$

(H2) There exists $\delta > 0$ such that

$$\tilde{\alpha} \in H^2(\delta, L^2(S^2)).$$

(H3) $\int_{S^2} |\alpha(2\hat{k})|^2 d\sigma(\hat{k}) > 0$.

The Hypothesis (H2) is a technical condition related to the use of the complex deformation technique. The Hypothesis (H3) ensures that the spin effectively couples to the reservoir at Bohr's frequency $e_+ - e_- = 2$.

We have proven the following two theorems in [JP2].

THEOREM 2.4. – Suppose that Hypotheses (H1)-(H3) hold. Then, for $\beta > 0$, there exists a constant $l(\beta) > 0$, depending only on the form-factor α , such that the spin-boson system has property of return to equilibrium for any real λ satisfying $0 < |\lambda| < l(\beta)$.

The return to equilibrium is exponentially fast in the following sense:

THEOREM 2.5. – Suppose that Hypotheses (H1)-(H3) hold, and let $l(\beta)$ be as in Theorem 2.4. There exists a norm dense set of normal states \mathcal{N}_0 and a strongly dense $*$ -algebra $\mathcal{M}_0 \subset \mathcal{M}$, both independent of β , and such that for $0 < |\lambda| < l(\beta)$, $\mathcal{S} \in \mathcal{N}_0$ and $A \in \mathcal{M}_0$, one has

$$|S(\tau_\lambda^t(A)) - S_\lambda^\beta(A)| \leq C(S, A) e^{-\eta(\lambda)|t|}, \quad (2.6)$$

for some $C(S, A)$ independent of λ and β . The function $\eta(\lambda)$ is positive for $0 < |\lambda| < l(\beta)$, and satisfies

$$\eta(\lambda) = \lambda^2 \frac{4\pi}{\tanh \beta} \int_{S^2} |\alpha(2\hat{k})|^2 d\sigma(\hat{k}) + O(\lambda^4),$$

as $\lambda \rightarrow 0$.

Remark. – By the best estimate we have, $l(\beta) = O(\beta^{-1})$ as $\beta \rightarrow \infty$. Thus, the above results do not yield any information concerning the zero-temperature model.

The traditional approach to the dynamics of open quantum systems is based on the use of master equations. In this paper we would like to discuss the relation between the master equation technique, and the techniques we introduced in [JP1], [JP2] to prove Theorems 2.4 and 2.5. Although the quantum mechanical master equations are extensively studied in the physics literature [HA], [KTH], the rigorous results on the subject are scarce. We will discuss here only the mathematically rigorous results of Davies [D1], [D2]. These results played an important role in our understanding of the subject.

3. DAVIES' THEORY

Davies' theory is most conveniently developed in the Schrödinger picture. We introduce first the necessary notation. Let \mathcal{M}_* be the predual of \mathcal{M} , i.e. the Banach space of all normal linear functionals over \mathcal{M} . Every such linear functional is represented by a trace class operator over $\mathbf{C}^2 \otimes \mathcal{H}_B$. Let M_{2*} and \mathcal{M}_{B*} be the preduals of M_2 and \mathcal{M}_B . Clearly,

$$\mathcal{M}_* = M_{2*} \otimes \mathcal{M}_{B*}.$$

Throughout this section we will assume that Hypothesis (H1) holds. Let L_λ be an operator on \mathcal{M}_* defined by

$$(L_\lambda \mathcal{S})(A) = \mathcal{S}([H_\lambda, A]). \quad (3.7)$$

For each real λ , L_λ is a closed, densely defined operator. It generates a strongly continuous group of isometries

$$T_\lambda^t \equiv e^{tL_\lambda},$$

of \mathcal{M}_* such that

$$(T_\lambda^t \mathcal{S})(A) = \mathcal{S}(\tau_\lambda^t(A)).$$

Let

$$(L_I \mathcal{S})(A) = \mathcal{S}([Q \otimes \varphi_B(\alpha), A]).$$

Then L_I is a closed, densely defined operator, and

$$L_\lambda = L_0 + \lambda L_I.$$

We introduce the partial trace

$$P : \mathcal{M}_* \mapsto M_{2*},$$

by the formula

$$(P\mathcal{S})(X) = \mathcal{S}(X \otimes I), \quad X \in M_2.$$

Identifying M_{2*} with a subspace of \mathcal{M}_* by the injection $\zeta \mapsto \zeta \otimes \mathcal{S}_B^\beta$, P becomes a projection. The reduced dynamics of the system is obtained by projecting out the reservoir variables,

$$U_\lambda(t) = PT_t^\lambda P.$$

Let $Q = 1 - P$. Defining

$$V_\lambda(t) = e^{t(L_0 + \lambda Q L_I Q)},$$

we derive the integral form of NPRZ (Nakajima-Prigogine-Resibois-Zwanzig) equation as follows. First, since PL_I is a bounded operator, we have a well-defined equation

$$U_\lambda(t) = V_\lambda(t) + \lambda \int_0^t V_\lambda(t-s) PL_I Q T_t^\lambda P ds,$$

see e.g. Theorem 9.1 in [D3]. We have used that $PL_I P = 0$. Since $L_I P$ is also bounded, we have

$$Q T_t^\lambda P = \lambda \int_0^t V_\lambda(t-s) Q L_I P U_\lambda(s) ds.$$

Combining the above equations and using that $V_\lambda(t)P = U_0(t)$, we obtain the NPRZ equation:

$$U_\lambda(t) = U_0(t) + \lambda^2 \int_0^t ds \int_0^s ds' U_0(t-s) PL_I Q V_\lambda(s-s') Q L_I P U_\lambda(s').$$

This equation is also known as the generalized master equation. Introducing the new variables $\bar{t} = \lambda^2 t$ and $u = \lambda^2 s'$ we get

$$U_\lambda(\bar{t}/\lambda^2) = U_0(\bar{t}/\lambda^2) + \int_0^{\bar{t}} U_0((\bar{t}-u)/\lambda^2) K(\lambda, \bar{t}-u) U_\lambda(u/\lambda^2) du,$$

where

$$K(\lambda, \bar{t}) = \int_0^{\bar{t}/\lambda^2} U_0(-s) PL_I Q V_\lambda(s) Q L_I P ds.$$

This operator acts on M_{2*} . One can immediately conjecture that the van Hove limit $\lambda \rightarrow 0$, $t \rightarrow \infty$, $\bar{t} = \lambda^2 t$, will yield the generator

$$K = \int_0^\infty U_0(-s) PL_I Q U_0(s) Q L_I P ds.$$

The matter is, however, more complicated. Let L_s be defined on M_{2*} according to

$$(L_s \mathcal{S})(X) = \mathcal{S}([H_s, A]), \quad X \in M_2,$$

and let

$$K^\# = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T e^{tL_s} K e^{-tL_s} dt.$$

We now state Davies results [D1], [D2] specialized to the spin-boson system. Note that M_{2*} can be identified with the vector space of 2×2 matrices equipped with the trace norm $\|\cdot\|_1$.

THEOREM 3.1. – For any $a > 0$,

$$\lim_{\lambda \rightarrow 0} \sup_{\lambda^2 t \in (0, a)} \|e^{tL_s + \lambda^2 t K} - e^{tL_s + \lambda^2 t K^\#}\|_1 = 0. \quad (3.8)$$

THEOREM 3.2. – Suppose that for some $\delta > 0$ the form-factor α satisfies

$$\int_0^\infty (1+t)^\delta \left[\int_{\mathbf{R}^3} e^{it\omega(\mathbf{k})} |\alpha(\mathbf{k})|^2 d^3 k \right] dt < \infty. \quad (3.9)$$

Then for any $a > 0$

$$\lim_{\lambda \rightarrow 0} \sup_{\lambda^2 t \in (0, a)} \|U_\lambda(t) - e^{tL_s + \lambda^2 t K}\|_1 = 0, \quad (3.10)$$

$$\lim_{\lambda \rightarrow 0} \sup_{\bar{t} \in (0, a)} \|U_0(-\bar{t}/\lambda^2) U_\lambda(\bar{t}/\lambda^2) - e^{\bar{t} K^\#}\|_1 = 0. \quad (3.11)$$

Furthermore, for $\bar{t} \geq 0$, the semi-group $e^{\bar{t} K^\#}$ is positivity and trace preserving on M_{2*} . It also leaves the Gibbs state S_s^β invariant,

$$e^{\bar{t} K^\#} S_s^\beta = S_s^\beta. \quad (3.12)$$

Remark. – Since in general $K \neq K^\#$ [SD], Relations (3.8), (3.10) and (3.11) imply that the Markov approximation is unambiguously defined only

in the interaction picture. This ambiguity is clearly related to the fact that the master equation technique does not provide sufficiently sharp estimates which can distinguish between K and $K^\#$. The matter is aggravated by the fact that the Markov generator commonly used in the physics literature differs from both K and $K^\#$. For a detailed discussion we refer the reader to [SD]. We will return to this point in the next section.

Notation. – In the sequel, all the matrices are written in the basis (χ_+, χ_-) . The generator $K^\#$ can be explicitly computed. Let

$$\Gamma_\pm^\beta = 2\pi \frac{e^{\pm\beta}}{\sinh(\beta)} \int_{S^2} |\alpha(2\hat{k})|^2 d\sigma(\hat{k}), \quad (3.13)$$

$$\Pi_\pm^\beta = \pm \frac{1}{2} \text{PV} \int_{\mathbf{R} \times S^2} \frac{e^{\pm\beta s/2}}{|\sinh(\beta s/2)|} \frac{|\tilde{\alpha}(s, \hat{k})|^2}{2-s} ds d\sigma(\hat{k}), \quad (3.14)$$

and

$$\begin{aligned} \Gamma^\beta &= \Gamma_-^\beta + \Gamma_+^\beta, \\ \Pi^\beta &= \Pi_+^\beta - \Pi_-^\beta. \end{aligned}$$

If

$$\zeta = \begin{pmatrix} \zeta_{11} & \zeta_{12} \\ \zeta_{21} & \zeta_{22} \end{pmatrix},$$

then

$$K^\# \zeta = \begin{pmatrix} 2\Gamma_-^\beta \zeta_{22} - 2\Gamma_+^\beta \zeta_{11} & -\zeta_{12}(\Gamma^\beta + i\Pi^\beta) \\ -\zeta_{21}(\Gamma^\beta - i\Pi^\beta) & 2\Gamma_+^\beta \zeta_{11} - 2\Gamma_-^\beta \zeta_{22} \end{pmatrix}. \quad (3.15)$$

Note that to second order, the coefficient $2\Gamma_\pm^\beta$ is the probability per unit time that the spin will make a transition $\pm \rightarrow \mp$ by emitting or absorbing one quantum respectively. This probability is different from zero iff the Hypothesis (H3) holds. The coefficient Π_\pm^β is the Lamb shift of the energy level ± 1 . These coefficients differ from the usual physics textbook values by a factor λ^2 , which has been absorbed in \bar{t} . Note also that $\eta(\lambda)$ in Equation (2.6) satisfies $\eta(\lambda) = \lambda^2 \Gamma^\beta + O(\lambda^4)$. We refer the reader to [JP1], [JP2] for a detailed discussion of the coefficients Γ_\pm^β .

It is instructive to reformulate Relation (3.11) in the Heisenberg picture. Assume that the initial state of the system is given by the density matrix

$$\rho = \zeta \otimes |\Omega_B\rangle\langle\Omega_B|.$$

If (3.9) holds, then for any $X \in M_2$,

$$\lim_{\lambda \rightarrow 0} \text{Tr}(\rho \tau_0^{-\bar{t}/\lambda^2} \circ \tau_\lambda^{\bar{t}/\lambda^2}(X \otimes I)) = \text{Tr}\left(e^{\bar{t}K^\#} \zeta X\right). \quad (3.16)$$

We denote the right hand side of (3.16) by $\langle X(\bar{t}) \rangle$. The spin-boson model is completely analogous to the following nuclear magnetic resonance problem: A spin 1/2 particle in a constant magnetic field pointing in the z -direction interacts with scalar radiation field in the x -direction only [LCD]. For such a problem, the phenomenological Bloch equations are commonly used in the physics literature to describe the evolution of the expectation values $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$, $\langle \sigma_z \rangle$ [BL], [BLW], [KTH], [PU]. The Bloch equations for the spin-boson system follow immediately from (3.15):

$$\begin{aligned} \frac{d\langle \sigma_x(\bar{t}) \rangle}{d\bar{t}} &= \Pi^\beta \langle \sigma_y(\bar{t}) \rangle - \frac{\langle \sigma_x(\bar{t}) \rangle}{T_2}, \\ \frac{d\langle \sigma_y(\bar{t}) \rangle}{d\bar{t}} &= -\Pi^\beta \langle \sigma_x(\bar{t}) \rangle - \frac{\langle \sigma_y(\bar{t}) \rangle}{T_2}, \\ \frac{d\langle \sigma_z(\bar{t}) \rangle}{d\bar{t}} &= -\frac{\langle \sigma_z(\bar{t}) \rangle}{T_1} \end{aligned}$$

Note that these equations and (3.12) uniquely specify $K^\#$. The constants T_1 and T_2 are the longitudinal and transversal relaxation times respectively, and

$$\frac{1}{T_1} = 2\Gamma^\beta, \quad \frac{1}{T_2} = \Gamma^\beta.$$

If the initial state of the spin system is diagonal ($\zeta_{12} = \zeta_{21} = 0$) then

$$\frac{d\zeta(\bar{t})}{d\bar{t}} = K^\# \zeta(\bar{t})$$

reduces to Pauli's master equation [P1], [P2]

$$\dot{p}_-(\bar{t}) = 2\Gamma_+ p_+(\bar{t}) - 2\Gamma_- p_-(\bar{t}),$$

$$\dot{p}_+(\bar{t}) = 2\Gamma_- p_-(\bar{t}) - 2\Gamma_+ p_+(\bar{t}).$$

Here $p_\pm(\bar{t})$ is the probability that, at the rescaled time \bar{t} , the spin is in the state $|\chi_\pm\rangle\langle\chi_\pm|$.

The original derivations of Pauli and Bloch equation were based on the statistical assumption of “random phases at all times”, which is similar in spirit to Boltzmann Stosszahlansatz, and subject to similar objections [VH3]. The first derivation not using this assumption was given by van

Hove [VH1], [VH2], see also [PR], [M], [Z1], [Z2]. Mathematically rigorous derivations were given for the first time by Pule [PU] and Davies [D1].

We finish this section with a number of remarks concerning the results of Davies. The matrix $e^{\bar{t}K^\#}$ can be computed. If $\zeta \in \mathcal{M}_{2*}$ is a state, then

$$e^{\bar{t}K^\#}\zeta = S_s^\beta + \frac{1}{2\Gamma^\beta} D(\bar{t})\zeta,$$

where

$$D(\bar{t})\zeta = \begin{pmatrix} e^{-2\bar{t}\Gamma^\beta} \left(2\Gamma_+^\beta \zeta_{11} - 2\Gamma_-^\beta \zeta_{22} \right) & e^{-\bar{t}(\Gamma^\beta + i\Pi^\beta)} 2\Gamma^\beta \zeta_{12} \\ e^{-\bar{t}(\Gamma^\beta - i\Pi^\beta)} 2\Gamma^\beta \zeta_{21} & e^{-2\bar{t}\Gamma^\beta} \left(2\Gamma_-^\beta \zeta_{22} - 2\Gamma_+^\beta \zeta_{11} \right) \end{pmatrix}.$$

We conclude that if Hypothesis (H3) holds, then *at the time scale \bar{t}* the spin system approaches thermal equilibrium exponentially fast. The linear transport equation of thermal relaxation is the Bloch equation, as expected. The technical assumption (3.9) is very mild and the method works equally well at zero-temperature ($\beta = \infty$). Clearly, Theorem 3.2 is a powerful result. On the other hand, the final conclusions of the theory yield only a crude understanding of the problem of thermal relaxation. It has been realized quite early [VH3] that a natural next step is to abandon the simplifying assumption $\lambda \rightarrow \infty$, $t \rightarrow \infty$, $\lambda^2 t$ finite, and to study the expectation values $\text{Tr}(\rho\tau_\lambda^t(A))$ for both λ and t finite. This problem cannot be treated by the old techniques, and the following two questions were open for some years:

1. Does the quantum dynamical system $(\mathcal{M}, \mathcal{S}_\lambda^\beta, \tau_\lambda)$ returns to equilibrium for sufficiently small nonzero λ ?

2. What are the higher order corrections to the linear transport equation? Is it possible to derive an exact transport equation with convergent expansion in powers of λ , such that its first non-trivial term is the Bloch equation?

We remark that Theorems 2.4 and 2.5 answered the Question 1. In the sequel we will discuss how our techniques resolve the Question 2.

4. SPECTRAL THEORY OF THERMAL RELAXATION

The spectral approach to dynamics of infinite quantum systems is based on the non-commutative analog of Koopman's lemma. We briefly recall some basic facts concerning this approach. For details we refer the reader to Section 4 in [JP2].

Let $(\mathcal{M}, \mathcal{S}^\beta, \tau)$ be a quantum dynamical system. We denote by $(\mathcal{H}, \pi, \Omega)$ the GNS representation of \mathcal{M} associated to \mathcal{S} . There is a unique self-adjoint operator \mathcal{L} on \mathcal{H} such that

$$\begin{aligned}\pi(\tau^t(A)) &= e^{it\mathcal{L}}\pi(A)e^{-it\mathcal{L}}, \\ \mathcal{L}\Omega &= 0,\end{aligned}$$

see e.g. Corollary 2.3.17 in [BR1]. We call \mathcal{L} the Liouvillean of the system. It is a simple exercise to show that if \mathcal{M} is abelian, then \mathcal{L} reduces to the familiar Koopman operator. In [JP2] we proved (Theorem 4.2):

THEOREM 4.1. – *A quantum dynamical system $(\mathcal{M}, \mathcal{S}^\beta, \tau)$ returns to equilibrium if and only if*

$$w - \lim_{|t| \rightarrow \infty} e^{-it\mathcal{L}} = P_\Omega,$$

where P_Ω is the orthogonal projection of \mathcal{H} along the cyclic vector Ω . In particular, if the Liouvillean has absolutely continuous spectrum except for a simple eigenvalue 0, then the system returns to equilibrium.

Tomita-Takesaki's theory relates the Liouvillean of the system to its modular structure. Since the vector Ω is cyclic and separating for $\pi(\mathcal{M})$, the basic construction of modular theory applies (see e.g. [BR1], Section 2.5). Let Δ and J be the modular operator and modular conjugation associated to the pair $(\pi(\mathcal{M}), \Omega)$. The Liouvillean \mathcal{L} is related to the modular operator Δ by the formula

$$\Delta = e^{-\beta\mathcal{L}}.$$

The modular conjugation plays a critical role in the perturbation theory of the Liouvillean [A1].

Since the reservoir is given in the cyclic representation, it follows from (2.3) and (2.4) that its Liouvillean is

$$\mathcal{L}_B \equiv H_B.$$

The explicit construction of the triple $(\mathcal{H}_B, \Omega_B, H_B)$ is given in [AW], see also [JP1], [JP2], [BR2]. From this construction it follows that \mathcal{L}_B has purely absolutely continuous spectrum filling the real axis, except for a simple eigenvalue 0. Thus, the isolated free reservoir is an ergodic system. We denote by J_B the modular conjugation of the pair $(\mathcal{M}_B, \Omega_B)$.

The cyclic representation $(\mathcal{H}_s, \pi_s, \Omega_s)$ of the spin system associated to the Gibbs state \mathcal{S}_s^β can be explicitly constructed (for the details, see [JP2], or the Section V.1.4 in [H]). Let

$$\mathcal{H}_s \equiv M_2,$$

with the inner product $(\Phi, \Psi) = \text{Tr}(\Phi^* \Psi)$,

$$\pi_s(X) : \Phi \mapsto X\Phi,$$

$$\Omega_s \equiv \frac{1}{\sqrt{Z_s^\beta}} e^{-\beta H_s/2}.$$

The modular conjugation of the pair $(\pi_s(M_2), \Omega_s)$ is $J_s : \Phi \mapsto \Phi^*$, and the Liouvillean of the spin system is

$$\mathcal{L}_s : \Phi \mapsto [H_s, \Phi].$$

In the absence of the interaction, the state $\mathcal{S}_0^\beta = \mathcal{S}_s^\beta \otimes \mathcal{S}_B^\beta$ is a unique (τ_0, β) -KMS state on \mathcal{M} . The corresponding cyclic representation is given by $(\mathcal{H}, \pi, \Omega_0^\beta)$, where

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_s \otimes \mathcal{H}_B, \\ \pi(X \otimes W_B(f)) &= \pi_s(X) \otimes W_B(f), \\ \Omega_0^\beta &= \Omega_s^\beta \otimes \Omega_B. \end{aligned}$$

In the absence of the interaction, the Liouvillean of the combined system is

$$\mathcal{L}_0 = \mathcal{L}_s \otimes I + I \otimes \mathcal{L}_B.$$

In [JP2] we have computed the Liouvillean of the interacting system by invoking Araki's perturbation theory of W^* -dynamical systems [A1], see also [BR2], Theorem 5.4.4, and [A2]. We quote the final result (Theorem 6.1 in [JP2]).

THEOREM 4.2. – *Let $(\mathcal{H}, \pi, \Omega_0^\beta)$ be the cyclic representation of the non-interacting spin-boson system $(\mathcal{M}, \mathcal{S}_0^\beta, \tau_0)$. For any $\lambda \in \mathbf{R}$ there is a cyclic and separating vector $\Omega_\lambda^\beta \in \mathcal{H}$ such that*

$$\mathcal{S}_\lambda^\beta(A) \equiv (\Omega_\lambda^\beta, \pi(A)\Omega_\lambda^\beta),$$

is the unique (τ_λ, β) -KMS state on \mathcal{M} . The Liouvillean of the interacting spin-boson system is given by

$$\mathcal{L}_\lambda = \mathcal{L}_0 + \lambda \mathcal{L}_I,$$

where

$$\mathcal{L}_I = \pi_s(Q) \otimes \varphi_B(\alpha) - J_s \pi_s(Q) J_s \otimes J_B \varphi_B(\alpha) J_B.$$

Remark. – The Liouvillean can be written in a completely explicit form, see Section 6 in [JP2].

The basic idea of our approach is to deduce thermodynamic properties of the combined system *spin + reservoir* from the spectral properties of \mathcal{L}_λ . The resulting picture can be roughly summarized as follows. The spectrum of \mathcal{L}_0 is

$$\begin{aligned}\sigma_{ac}(\mathcal{L}_0) &= \mathbf{R}, \\ \sigma_{sc}(\mathcal{L}_0) &= \emptyset, \\ \sigma_{pp}(\mathcal{L}_0) &= \{-2, 0, 2\},\end{aligned}$$

where ± 2 are simple eigenvalues while 0 is two-fold degenerate eigenvalue. These eigenvalues are embedded in the continuous spectrum. After the perturbation term is “switched on”, all these eigenvalues turn into complex resonances except for 0 which remains a simple eigenvalue. Thus, for small non-zero λ the spectrum of \mathcal{L}_λ is absolutely continuous except for a simple eigenvalue zero. Theorem 4.1 then implies that the spin-boson system has the property of return to equilibrium. The complex resonances of \mathcal{L}_λ determine the transport equation of thermal relaxation. In particular, the Fermi’s Golden Rule for the complete set of resonances yields the Bloch equations, while the Fermi’s Golden Rule for the degenerate eigenvalue 0 yields Pauli’s equation.

To prove these results we have developed, in [JP1], a field-theoretic version of the spectral deformation technique. The general strategy of this argument is well-known [AC], [BC], [S]. One tries to construct a one-parameter group of unitary operators $U(\theta) : \mathcal{H} \mapsto \mathcal{H}$, such that the operators

$$\mathcal{L}_\lambda(\theta) = U(\theta) \mathcal{L}_\lambda U(-\theta),$$

can be extended to an analytic family for θ and λ complex. The construction should be such that for complex θ the essential spectrum of $\mathcal{L}_\lambda(\theta)$ moves away from the real axis, unveiling the resonances which can then be computed by the usual Rayleigh-Schrödinger expansion. The formula

$$(\Phi, (\mathcal{L}_\lambda - z)^{-1} \Psi) = (U(\theta) \Phi, (\mathcal{L}_\lambda(\theta) - z)^{-1} U(\theta) \Psi),$$

relates these resonances to the poles of the analytic continuation of matrix elements of the resolvent into the unphysical Riemann sheet. The

construction of $U(\theta)$ and other details of this analysis are technically involved. They are presented in [JP1], [JP2]. We quote the final result, Theorem 6.2 in [JP2]. Recall that Γ_{\pm}^{β} , Π_{\pm}^{β} are given by (3.13)-(3.14).

THEOREM 4.3. – Suppose that Hypotheses (H1)-(H2) are satisfied. Then there exists a dense subspace $\mathcal{E} \subset \mathcal{H}$ and, for each $\eta \in]0, \delta[$, a constant $\Lambda(\eta) > 0$ such that for $\lambda \in]-\Lambda(\eta), \Lambda(\eta)[$ and $\Phi, \Psi \in \mathcal{E}$, the functions

$$z \mapsto (\Phi, (\mathcal{L}_{\lambda} - z)^{-1}\Psi), \quad (4.17)$$

have a meromorphic continuation from the upper half-plane onto the region

$$\mathcal{O} \equiv \{z : \text{Im}(z) > -\eta\}.$$

The poles of matrix elements (4.17) in \mathcal{O} are independent of Φ and Ψ . They are identical to the eigenvalues of a quasi-energy operator Σ_{λ} on \mathcal{H}_s . This operator is analytic for $|\lambda| < \Lambda(\eta)$, with a power expansion of the form

$$\Sigma_{\lambda} = \mathcal{L}_s + \sum_{n=1}^{\infty} \lambda^{2n} \Sigma^{(2n)}. \quad (4.18)$$

The matrix $\Sigma^{(2)}$ can be explicitly computed. Denoting by P_E the eigenprojections of \mathcal{L}_s , we have $P_E \Sigma^{(2)} = \Sigma^{(2)} P_E$, and

$$P_{\pm 2} \Sigma^{(2)} P_{\pm 2} = (\pm \Pi^{\beta} - i \Gamma^{\beta}), \quad (4.19)$$

for simple eigenvalues, and

$$P_0 \Sigma^{(2)} P_0 = \begin{pmatrix} -2i\Gamma_+^{\beta} & 2i\Gamma_+ e^{-\beta} \\ 2i\Gamma_- e^{\beta} & -2\Gamma_+^{\beta} \end{pmatrix}, \quad (4.20)$$

for the degenerate one.

Remark. – The formula for the matrix (4.20) in [JP2] (Relation 6.7) has a typographical error - the factors $e^{\pm\beta}$ in the off-diagonal elements are interchanged.

Hypothesis (H3) ensures that zero is the only real eigenvalue of $\Sigma^{(2)}$. An immediate consequence is that if (H1)-(H3) hold, then for $\lambda \neq 0$ sufficiently small the spectrum of \mathcal{L}_{λ} is purely absolutely continuous except for the simple eigenvalue 0. Thus, invoking Theorem 4.1 we derive Theorem 2.4.

We remark that, in principle, all terms in the expansion (4.18) can be computed. The formulas from which these terms are generated are given

in the proof of Proposition 4.7 in [JP1]. These formulas are cumbersome and we will not reproduce them here.

It should be clear by now that $\Sigma^{(2)}$ and $K^\#$ are closely related. The road from resonances to master equations starts with the following set of observations (see also the proof of Theorem 4.2 in [JP2]). Since Ω_λ^β is a separating vector for $\pi(\mathcal{M})$, $\pi(\mathcal{M})'\Omega_\lambda^\beta$ is dense in \mathcal{H} . One can further show that there is a * sub-algebra $\mathcal{Z} \subset \pi(\mathcal{M})'$ such that $\mathcal{Z}\Omega_\lambda^\beta$ is dense and $\mathcal{Z}\Omega_\lambda^\beta \subset \mathcal{E}$, see Relation (6.9) in [JP1]. The set \mathcal{N}_0 of vector states associated to $\mathcal{Z}\Omega_\lambda^\beta$ is total (in the norm topology) in the set of all normal states over \mathcal{M} . Let \mathcal{S} be a state associated to a normalized vector $\Psi = C\Omega_\lambda^\beta$, $C \in \mathcal{Z}$. We then have

$$\mathcal{S}(\tau_\lambda^t(A)) = (\Psi, e^{it\mathcal{L}_\lambda} \pi(A) e^{-it\mathcal{L}_\lambda} \Psi) \quad (4.21)$$

$$= (\pi(A^*)\Omega_\lambda^\beta, e^{-it\mathcal{L}_\lambda} C^* C \Omega_\lambda^\beta) \quad (4.22)$$

Furthermore, one can show that if $\pi(A) \in J\mathcal{Z}J$ then $\pi(A^*)\Omega_\lambda^\beta \in \mathcal{E}$. In particular, this will be true for $A = X \otimes I$, $X \in M_2$. By construction, $C^* C \Omega_\lambda^\beta \in \mathcal{E}$ as well. We now invoke the dynamical consequence of Theorem 4.3 (Theorem 2.5 in [JP1] and Theorem 6.3 in [JP2]):

THEOREM 4.4. – Suppose that Hypothesis (H1)-(H2) hold, and let \mathcal{E} be as in Theorem 4.3. Then for each $\eta \in]0, \delta[$ there is a constant $\Lambda(\eta) > 0$ with the following property: For $|\lambda| < \Lambda(\eta)$ there are two maps $W_\lambda^\pm : \mathcal{E} \mapsto \mathcal{H}_s$ such that for any $\Phi, \Psi \in \mathcal{E}$, one has $(W_\lambda^- \Phi, W_\lambda^+ \Psi) = (\Phi, \Psi)$ and

$$(\Phi, e^{-it\mathcal{L}_\lambda} \Psi) = (W_\lambda^- \Phi, e^{-it\Sigma_\lambda} W_\lambda^+ \Psi) + O(e^{-\eta t})$$

as $t \rightarrow +\infty$.

Remark. – We will comment on the case $t \rightarrow -\infty$ shortly.

Combining Relations (4.21)-(4.22) and Theorem 4.4, we derive that for the dense set of states \mathcal{N}_0 and the dense set of observables $\mathcal{M}_0 \equiv \pi^{-1}(J\mathcal{Z}J)$ the following fundamental relation holds:

$$\mathcal{S}(\tau_\lambda^t(A)) = \left(W_\lambda^- \pi(X^*) \Omega_\lambda^\beta, e^{-it\Sigma_\lambda} W_\lambda^+ C^* C \Omega_\lambda^\beta \right) + O(e^{-\eta t}). \quad (4.23)$$

Note that Theorem 2.5 follows immediately from (4.23). We proceed to simplify the quantity

$$\left(W_\lambda^- \pi(X^*) \Omega_\lambda^\beta, e^{-it\Sigma_\lambda} W_\lambda^+ C^* C \Omega_\lambda^\beta \right).$$

From the construction of W_λ^\pm we know that $W_\lambda^\pm = 1 + O(\lambda^2)$ in the strong topology. Similarly, from the construction of Ω_λ^β we know that

$\Omega_\lambda^\beta = \Omega_0^\beta + O(\lambda)$. Finally, any vector $\Psi \in \mathcal{H}_s$ can be written as $C_s \Omega_s^\beta$ for some $C_s \in \pi_s(M_2)'$. Thus, if the initial state \mathcal{S} is of the form $\zeta \otimes \mathcal{S}_B^\beta$, we have the following estimate:

$$\mathcal{S}(\tau_\lambda^t(X \otimes I)) = (\Omega_s^\beta, \pi_s(X) e^{-it\Sigma_\lambda} C_s^* C_s \Omega_s^\beta) + O(\lambda)$$

for some C_s which depends on ζ . Since Ω_s^β is a separating vector for $\pi_s(M_2)$,

$$M_2 \ni Y \mapsto \pi_s(Y) \Omega_s^\beta \in \mathcal{H}_s,$$

is an isomorphism. Thus, the relation

$$e^{it\Sigma_\lambda^*} \pi_s(Y) \Omega_s^\beta = \pi_s(\hat{\gamma}_\lambda^t(Y)) \Omega_s^\beta, \quad Y \in M_2, \quad (4.24)$$

defines a semi-group of automorphisms $\hat{\gamma}_\lambda^t$ of M_2 . Defining

$$\gamma_\lambda^t(Y) = (\hat{\gamma}_\lambda^t(Y^*))^*, \quad (4.25)$$

we can write

$$\begin{aligned} (\Omega_s^\beta, \pi_s(X) e^{-it\Sigma_\lambda} C_s^* C_s \Omega_s^\beta) &= (\pi_s(\hat{\gamma}_\lambda^t(X^*))) \Omega_s^\beta, C_s^* C_s \Omega_s^\beta \\ &= (C_s \Omega_s^\beta, \pi_s(\gamma_\lambda^t(X)) C_s \Omega_s^\beta) \\ &= \text{Tr}(\zeta \gamma_\lambda^t(X)). \end{aligned}$$

Let $\gamma_\lambda^{t*} : \mathcal{M}_{2*} \mapsto \mathcal{M}_{2*}$ be the dual semi-group to γ_λ^t , and let \mathcal{K}_λ be its generator,

$$\gamma_\lambda^{t*}(\zeta) = e^{t\mathcal{K}_\lambda} \zeta. \quad (4.26)$$

Since Σ_λ is analytic for small λ , it is a simple exercise to show that \mathcal{K}_λ is also analytic:

$$\mathcal{K}_\lambda = L_s + \sum_{n=1}^{\infty} \lambda^{2n} \mathcal{K}^{(2n)}. \quad (4.27)$$

Any term in the expansion (4.27) can be computed from the corresponding term of the series (4.18). The calculations are easier in the tensor product realizations

$$\begin{aligned} \mathcal{H}_s &= \mathbf{C}^2 \otimes \mathbf{C}^2, \\ \pi_s(X) &= X \otimes I, \\ \Omega_s^\beta &= \frac{1}{Z_s^\beta} \left(e^{\beta/2} \chi_- \otimes \chi_- + e^{-\beta/2} \chi_+ \otimes \chi_+ \right). \end{aligned}$$

Following the steps (4.24)-(4.26) (with $i\Sigma^{(2)*}$ in (4.24) instead of $e^{it\Sigma_\lambda^*}$) one computes $\mathcal{K}^{(2)}$ from (4.19)-(4.20). As expected,

$$\mathcal{K}^{(2)} = K^\#.$$

We summarize these results in

THEOREM 4.5. – *Suppose that Hypotheses (H1)-(H2) hold and that the initial state is of the form $\rho = \zeta \otimes |\Omega_B\rangle\langle\Omega_B|$. If \mathcal{K}_λ is given by (4.26), then for any $X \in M_2$*

$$\lim_{\lambda \rightarrow 0} \sup_{t > 0} |\text{Tr}(\rho \tau_\lambda^t(X \otimes I)) - \text{Tr}(e^{t\mathcal{K}_\lambda} \zeta X)| = 0. \quad (4.28)$$

In particular, we recover Davies' result,

$$\lim_{\lambda \rightarrow 0} \text{Tr}(\rho \tau_0^{-\bar{t}/\lambda^2} \circ \tau_\lambda^{\bar{t}/\lambda^2}(X \otimes I)) = \text{Tr}(e^{\bar{t}K^\#} \zeta X).$$

The Relations (4.23) and (4.28) improve Davies' result. They provide sharper estimates and a generator \mathcal{K}_λ defined to all orders in λ . This generator is completely determined by the resonances of the Liouvillean. The Markovian generator $K^\#$ arises as the first non-trivial contribution to the expansion of \mathcal{K}_λ in powers of λ . These results also clarify the ambiguities concerning the choice of the Markovian generator which are inherent in the traditional theory of master equations [SD]. Finally, they give a complete justification for regarding the equation

$$\frac{d\zeta(t)}{dt} = \mathcal{K}_\lambda \zeta(t),$$

as the exact transport equation of thermal relaxation.

We would like to add, however, that our central technical condition (H2) is more stringent than Davies condition (3.9). The master equation technique is more robust, and applies to the situation as zero-temperature or positive mass models, for which our technique fails.

We finish with a few remarks concerning a choice of the time-direction. Theorem 2.4 asserts that the combined system relaxes to equilibrium as $t \rightarrow \pm\infty$. We have derived the transport equation when $t \rightarrow \infty$, but a similar argument applies when $t \rightarrow -\infty$. Then we study the analytic continuation of the matrix resolvent elements (4.17) from the *lower half-plane* onto the region

$$\mathcal{O} \equiv \{z : \text{Im}(z) < \eta\},$$

for $\eta \in]0, \delta[$. The poles of the matrix elements are again independent of $\Phi, \Psi \in \mathcal{E}$, and are identical to the eigenvalues of a quasi-energy operator Σ_λ^- with a power expansion

$$\Sigma_\lambda^- = \mathcal{L}_s + \sum_{n=1}^{\infty} \lambda^{2n} \Sigma_-^{(2n)}.$$

The matrix $\Sigma_-^{(2)}$ can be explicitly computed (in fact $\Sigma_-^{(2)} = \Sigma_-^{(2)*}$), and one derives equations analogous to (4.23) and (4.28) arguing as before.

ACKNOWLEDGMENTS

We are grateful to H. Spohn for useful discussions. The first author was supported in part by the NSERC, the second by the Fonds National Suisse. This paper was completed while the first author was a visitor at California Institute of Technology. V. J. is grateful to B. Simon and C. Peck for their hospitality.

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(Manuscript received January 12th, 1996.)