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Markovian Master Equations

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Abstract. We give a rigorous proof that under certain technical conditions the memory effects in a quantum-mechanical master equation become negligible in the weak coupling limit. This is sufficient to show that a number of open systems obey an exponential decay law in the weak coupling limit for a rescaled time variable. The theory is applied to a fairly general finite dimensional system weakly coupled to an infinite free heat bath.

§ 1. Introduction

In the last fifteen years there has been a growing realisation by physicists of the importance of master equations for the study of the time evolution of open quantum-mechanical systems. As well as providing a suitable framework for the consideration of the fundamental property of irreversibility [1], they have proved an important technique in the analysis of a variety of models, such as harmonic oscillators and lasers. It becomes clear in the excellent survey article of Haake [2] that one of the main reasons for the usefulness of master equations is the radical simplification obtained when memory effects are neglected.

It is rather surprising, therefore, that in the recent rigorous studies of these models, the use of master equations has been avoided. This appears to be because, although it is possible to give a rigorous proof of the master equation itself, conditions under which the memory effects can be neglected have not been found.

In this paper we give a rigorous proof that the time evolution of an open system is Markovian in the weak coupling limit. As the coupling constant converges to zero we rescale the time variable to compensate for the slower decay of the system. The theory is developed in a general form and its application to a variety of models is outlined. The case of a general finite-dimensional system weakly coupled to an infinite free heat bath is investigated in some detail and relaxation to the Gibbs state is proved.

§ 2. The Abstract Theory of the Weak Coupling Limit

In order to establish our notation we start with the derivation of the master equation. For motivation and a historical discussion we refer the reader to [1, 2]. We let P_0 be a projection on a Banach space $\mathscr{B}$ and put $P_1 = 1 - P_0$. We refer to $\mathscr{B}_0 = P_0 \mathscr{B}$ as the system and to $\mathscr{B}_1 = P_1 \mathscr{B}$ as the bath. We suppose that the free evolution of both is determined by a strongly continuous one-parameter group U_t of isometries on $\mathscr{B}$ which leaves each of $\mathscr{B}_0$, $\mathscr{B}_1$ invariant. The infinitesimal generator Z is then closed and densely defined and

$$[Z, P_0] = 0 . \tag{2.1}$$

We define $Z_i = P_i Z$ for later use.

We introduce a perturbation A which is supposed to be a bounded operator on $\mathscr{B}$. Writing $A_{ij} = P_i A P_j$, we suppose from here onwards that

$$A_{00} = 0 . \tag{2.2}$$

We let U_t^λ be the one-parameter group generated by $Z + \lambda A_{11}$ so that for all t

$$[U_t^\lambda, P_0] = 0 . \tag{2.3}$$

We also let V_t^λ be the one-parameter group generated by $Z + \lambda A$, so that by a well-known formula [3]

$$V_t^\lambda = U_t^\lambda + \lambda \int_{s=0}^{t} U_{t-s}^\lambda (A_{01} + A_{10}) V_s^\lambda \, ds . \tag{2.4}$$

In this and all subsequent integrals, the integrand is everywhere bounded and strongly continuous, so no difficulties of interpretation occur. From Eq. (2.4) we can obtain

$$P_0 V_t^\lambda P_0 = U_t^\lambda P_0 + \lambda \int_{s=0}^{t} U_{t-s}^\lambda A_{01} P_1 V_s^\lambda P_0 \, ds \tag{2.5}$$

and

$$P_1 V_t^\lambda P_0 = \lambda \int_{s=0}^{t} U_{t-s}^\lambda A_{10} P_0 V_s^\lambda P_0 \, ds . \tag{2.6}$$

Putting $W_t^\lambda = P_0 V_t^\lambda P_0$ we obtain by substitution

$$W_t^\lambda = U_t^\lambda P_0 + \lambda^2 \int_{s=0}^{t} \int_{u=0}^{s} U_{t-s}^\lambda A_{01} U_{s-u}^\lambda A_{10} W_u^\lambda \, du \, ds . \tag{2.7}$$

Using Eq. (2.2) we finally obtain

$$W_t^\lambda = U_t + \lambda^2 \int_{s=0}^{t} \int_{u=0}^{s} U_{t-s} A_{01} U_{s-u}^\lambda A_{10} W_u^\lambda \, du \, ds \tag{2.8}$$

where we have dropped reference to P_0 since we shall from now on work entirely within $\mathscr{B}_0$.

This is an integrated form of the master equation constructed by Nakajima, Prigogine, Resibois, and Zwanzig. To see this we put $\varphi_t = W_t^\lambda \varphi$ where $\varphi \in \mathscr{B}_0$ to get

$$\varphi_t = U_t \left(\varphi_0 + \lambda^2 \int_{s=0}^{t} \int_{u=0}^{s} U_{-s} A_{01} U_{s-u}^\lambda A_{10} \varphi_u \, du \, ds \right) \tag{2.9}$$

so that formally

$$\frac{\partial \varphi_t}{\partial t} = Z_0 \varphi_t + \lambda^2 \int_{u=0}^{t} A_{01} U_{t-u}^\lambda A_{10} \varphi_u \, du \,. \tag{2.10}$$

However we prefer not to work with this equation because it necessitates consideration of domain questions. It does indicate that in Eq. (2.8) the integral contains memory terms. We now come to the problem of going to the weak coupling limit.

Since the memory term is small compared with the free term we change to the interaction representation before letting $\lambda \to 0$. Putting

$$Y_\tau^\lambda = U_{-t} W_t^\lambda \tag{2.11}$$

where $\tau = \lambda^2 t$ we obtain

$$Y_\tau^\lambda = 1 + \int_{\sigma=0}^{\tau} H(\lambda, \tau - \sigma, \sigma) \, Y_\sigma^\lambda \, d\sigma \tag{2.12}$$

where

$$H(\lambda, \tau, \sigma) = U_{-\lambda^{-2}\sigma} K(\lambda, \tau) \, U_{\lambda^{-2}\sigma} \tag{2.13}$$

and

$$K(\lambda, \tau) = \int_{x=0}^{\lambda^{-2}\tau} U_{-x} A_{01} U_x^\lambda A_{10} \, dx \,. \tag{2.14}$$

If the kernel $H(\lambda, \tau, \sigma)$ converges as $\lambda \to 0$ to an operator H on $\mathscr{B}_0$ which is independent of τ and σ then the convergence of V_τ^λ to a limit operator Y_τ as $\lambda \to 0$ may easily be proved. However upon examining the dependence of $H(\lambda, \tau, \sigma)$ on σ it becomes apparent that such limiting behaviour is unlikely, and that a more sophisticated approach is necessary.

We now restrict attention to the case where $\mathscr{B}_0$ is finite dimensional. If $\{Q_\alpha\}$ are the spectral projections of Z_0 on $\mathscr{B}_0$ then we can write

$$P_0 U_t = e^{Z_0 t} = \sum_\alpha Q_\alpha e^{i\omega_\alpha t} \tag{2.15}$$

where the ω_α are distinct and real. If X is any operator on $\mathscr{B}_0$ we define

$$X^\natural = \sum_\alpha Q_\alpha X Q_\alpha \tag{2.16}$$

or, equivalently

$$X^\natural = \lim_{t\to\infty} \frac{1}{2t} \int_{-t}^{t} U_x X U_{-x}\, dx \tag{2.17}$$

which makes no reference to the spectral projections of Z_0.

Theorem 2.1. *Suppose that for all $\tau_1 > 0$ there is a constant c such that*

$$\|K(\lambda, \tau)\| \leqq c \tag{2.18}$$

provided $|\lambda| \leqq 1$ and $0 \leqq \tau \leqq \tau_1$. Suppose also that there is a bounded operator K on $\mathscr{B}_0$ such that if $0 < \tau_0 \leqq \tau_1 < \infty$ then

$$\lim_{\lambda\to 0} \|K(\lambda, \tau) - K\| = 0 \tag{2.19}$$

uniformly with respect to τ if $\tau_0 \leqq \tau \leqq \tau_1$. Then if $\mathscr{B}_0$ is finite-dimensional and $b \in \mathscr{B}_0$

$$\lim_{\lambda\to 0} \|Y_\tau^\lambda b - Y_\tau b\| = 0 \tag{2.20}$$

uniformly on each interval $0 \leqq \tau \leqq \tau_1$, where

$$Y_\tau = \exp\{K^\natural \tau\} \tag{2.21}$$

where

$$K^\natural U_t = U_t K^\natural \tag{2.22}$$

as operators on $\mathscr{B}_0$ for all $t \in \mathbb{R}$.

Proof. We let $\mathscr{V}$ be the Banach space of continuous $\mathscr{B}_0$-valued functions on $[0, \tau_1]$. If $\mathscr{H}_\lambda : \mathscr{V} \to \mathscr{V}$ is defined by

$$(\mathscr{H}_\lambda f)(\tau) = \int_{\sigma=0}^{\tau} H(\lambda, \tau - \sigma, \tau)\, f(\sigma)\, d\sigma \tag{2.23}$$

then $f_\lambda = Y_\tau^\lambda b$ is the solution of

$$f_\lambda = g + \mathscr{H}_\lambda f_\lambda \tag{2.24}$$

where $g(\tau)=b$ for $0 \leqq \tau \leqq \tau_1$. We now define $\tilde{\mathscr{H}}_\lambda : \mathscr{V} \to \mathscr{V}$ by

$$(\tilde{\mathscr{H}}_\lambda f)(\tau) = \int_{\sigma=0}^{\tau} U_{-\lambda^{-2}\sigma} K U_{\lambda^{-2}\sigma} f(\sigma)\, d\sigma \tag{2.25}$$

By Eqs. (2.13) and (2.19) it is easy to show that $(\mathscr{H}_\lambda - \tilde{\mathscr{H}}_\lambda)$ converges strongly to zero as $\lambda \to 0$.

Using Eq. (2.15) we can put

$$(\tilde{\mathscr{H}}_\lambda f)(\tau) = \sum_{\alpha,\beta} Q_\beta K Q_\alpha \int_{\sigma=0}^{\tau} e^{i(\omega_\alpha - \omega_\beta)\lambda^{-2}\sigma} f(\sigma)\, d\sigma\,. \tag{2.26}$$

As $\lambda \to 0$ this converges uniformly for $0 \leqq \tau \leqq \tau_1$ to

$$h(\tau) = \sum_{\alpha,\beta} Q_\beta K Q_\alpha \delta_{\alpha\beta} \int_{\sigma=0}^{\tau} f(\sigma)\, d\sigma\,. \tag{2.27}$$

Therefore $\tilde{\mathscr{K}}_\lambda$, and hence $\mathscr{K}_\lambda$, converges strongly to $\mathscr{K} : \mathscr{V} \to \mathscr{V}$ where

$$(\mathscr{K} f)(\tau) = \int_{\sigma=0}^{\tau} K^{\natural} f(\sigma)\, d\sigma\,. \tag{2.28}$$

Now $f(\tau) = Y_\tau b$ is the solution of

$$f = g + \mathscr{K} f \tag{2.29}$$

so

$$f = g + \mathscr{K} g + \mathscr{K}^2 g + \cdots \tag{2.30}$$

and a similar equation holds for f_λ. Therefore

$$\|f_\lambda - f\| \leqq \sum_{n=1}^{\infty} \|\mathscr{K}_\lambda^n g - \mathscr{K}^n g\|\,. \tag{2.31}$$

Since $\mathscr{K}_\lambda$ converges strongly to $\mathscr{K}$ each term of this series converges to zero. Also since $\mathscr{K}_\lambda$ and $\mathscr{K}$ are Volterra integral operators

$$\|\mathscr{K}_\lambda^n g - \mathscr{K}^n g\| \leqq 2\,\|g\|\, c^n \tau_1^n / n! \tag{2.32}$$

Therefore f_λ converges in norm to f as $\lambda \to 0$.

A simple condition for the existence of the limit operator is given below.

Theorem 2.2. *If* $A_{11} = 0$ *and*

$$\int_0^\infty \|A_{01} U_x A_{10}\|\, dx < \infty \tag{2.33}$$

then the conditions of Theorem 2.1 are satisfied with

$$K = \int_0^\infty U_{-x} A_{01} U_x A_{10}\, dx\,. \tag{2.34}$$

Proof. This is immediate once it is realized that when $A_{00} = A_{11} = 0$, the operator U_t^λ is independent of λ.

In order to deal with the more physically interesting case where $A_{11} \neq 0$ we introduce the notation

$$A_r = U_{-t_r} A U_{t_r} . \tag{2.35}$$

Theorem 2.3. *Suppose that*

$$\int_0^\infty \|P_0 A_0 A P_0\| \, dt < \infty . \tag{2.36}$$

Defining

$$a_n(t) = \int_{t_0=0}^{t} \cdots \int_{t_n=0}^{t_{n-1}} P_0 A_0 P_1 A_1 P_1 \ldots P_1 A_n P_1 A P_0 \, dt_n \ldots dt_0 \tag{2.37}$$

suppose that for $n \geqq 1$

$$\|a_n(t)\| \leqq c_n t^{n/2} \tag{2.38}$$

where the series $\sum_{n=1}^{\infty} c_n z^n$ *has infinite radius of convergence. Suppose also that for some* $\varepsilon > 0$, d_n *and all* $t \geqq 0$

$$\|a_n(t)\| \leqq d_n t^{n/2-\varepsilon} . \tag{2.39}$$

Then the conditions of Theorem 2.1 are satisfied with

$$K = \int_0^\infty P_0 A_0 A P_0 \, dt_0 . \tag{2.40}$$

Proof. Expanding U_t^λ as a power series in λ we obtain

$$\|K(\lambda, \tau) - K\| \leqq \int_{\lambda^{-2}\tau}^{\infty} \|P_0 A_0 A P_0\| \, dt_0 + \sum_{n=1}^{\infty} \lambda^n \|a_n(t)\| . \tag{2.41}$$

By Eq. (2.36) the integral vanishes as $\lambda \to 0$ uniformly for τ in any compact subset of the open interval $(0, \infty)$. By Eq. (2.38) if $0 \leqq \tau \leqq \tau_0$ the series is dominated by the convergent series $\sum_{n=1}^{\infty} c_n \tau_0^{n/2}$. But by Eq. (2.39) the nth term of the series is also dominated by

$$\lambda^{2\varepsilon} d_n \tau_0^{n/2-\varepsilon} \tag{2.42}$$

which converges to zero as $\lambda \to 0$. Therefore the series converges to zero uniformly if $0 \leqq \tau \leqq \tau_0$.

The above theorems complete the abstract theory and we give some remarks and applications.

(1) *The Wigner-Weisskopf Atom.* The solution in [4, 5] of the evolution equations for a harmonic oscillator weakly coupled to an infinite free heat bath reduces to a single-particle problem for the Wigner-Weisskopf atom. This and its multi-dimensional version [6], can be solved in a few lines using the above formalism. We remark, however, that the results obtained in [4, 6] are stronger than those given here in that the convergence was shown to be uniform in time. This is very important when discussing the interchange of the limits $\lambda \to 0$ and $t \to \infty$.

(2) *Stochastic Differential Equations.* There is a strong formal similarity of this work to a problem on stochastic differential equations on a Banach space $\mathscr{B}_0$. See [7]. If $(\Omega, d\omega)$ is a probability space then one can define

$$\mathscr{B} = L^1(\Omega, \mathscr{B}_0, d\omega) \tag{2.43}$$

and let the projection P_0 be

$$P_0 f = \int_\Omega f(\omega)\, d\omega\,. \tag{2.44}$$

The interaction is then

$$(Af)(\omega) = A(\omega)\, f(\omega) \tag{2.45}$$

where $A(\omega)$ is a "random" operator-valued function, and the free evolution is

$$(U_t f)(\omega) = f(t\omega) \tag{2.46}$$

where $t\omega \in \Omega$ for all $t \in \mathbb{R}$ and $\omega \in \Omega$.

(3) *On the Condition* $\|P_1\| = 1$. If the condition $\|P_1\| = 1$ were satisfied than a lot of the technical trouble involved in verifying the conditions of Theorem 2.1 could be avoided. However in the example of the next section it may be seen that $\|P_1\| = 2$. This difficulty also arose in [8] and was the reason for the condition on the spectrum of $(1-P)\,L(1-P)$ in Theorem 3.3 of that paper.

(4) *Extensions of the Theorems.* The theorems can be extended to certain cases where $\mathscr{B}_0$ is infinite dimensional and the operators involved are unbounded. However, a necessary restriction is that Z_0 has discrete spectrum, since otherwise the operation $\natural$ is not defined.

(5) *The Origin of Irreversibility.* We started with an evolution equation on $\mathscr{B}$ which is fully reversible and ended up with a semigroup on $\mathscr{B}_0$, which represents an irreversible dissipative process. The origin of the irreversibility in this case clearly lies in the initial conditions rather than in any dubious procedure such as coarse-graining.

§ 3. System in an Infinite Free Heat Bath

We show that an N-level atom weakly coupled to an infinite free heat bath relaxes to equilibrium in a Markovian fashion and that the equilibrium state is its Gibbs state at the temperature of the heat bath. This behaviour has already been proved in two particular cases [4, 9]. Our contribution is therefore to show that the result is of a very general type, being essentially independent of the nature of the system, and of whether the coupling to the bath is linear in the field operators (at least in the fermion cases). The problem could, as in [9], be solved without the use of master equations, but we believe they form a useful device for extracting the terms which contribute to the limiting behaviour. We make comments on possible variations of the model at the end of the section.

The atom is described by an N-dimensional Hilbert space $\mathscr{K}_A$ with a free Hamiltonian H_A. The heat bath is described by a quasi-free representation of the canonical anticommutation relations (CAR's) with an infinite number of degrees of freedom [10]. To be specific we let the complex Hilbert space $\mathscr{V}$ be the test function space and S the single particle Hamiltonian on $\mathscr{V}$. For each $f \in \mathscr{V}$ we have a bounded operator φ_f on a space $\mathscr{K}_B$ satisfying the CAR's

$$\varphi_f \varphi_g + \varphi_g \varphi_f = 2\,\mathrm{Re}\langle f, g\rangle\, 1\,. \tag{3.1}$$

There is given a cyclic vector Ω in $\mathscr{K}_B$ and a Hamiltonian H_B on $\mathscr{K}_B$ such that

$$H_B \Omega = 0 \tag{3.2}$$

and

$$e^{iH_B t}\, \varphi(f)\, e^{-iH_B t} = \varphi(e^{iSt} f)\,. \tag{3.3}$$

The representation is determined by its correlation functions as follows. For any integer n we define the set $\mathscr{P}_n$ of pairings as the set of all permutations p of $(1, \ldots, 2n)$ such that

$$p(2r-1) < p(2r) \quad \text{and} \quad p(2r-1) < p(2r+1) \tag{3.4}$$

for all r. Then writing $\langle \ldots \rangle$ for the expectation with respect to Ω,

$$\langle \varphi(f_1) \ldots \varphi(f_{2n}) \rangle = \sum_{p \in \mathscr{P}_n} \operatorname{sign} p \prod_{r=1}^{n} \langle \varphi(f_{p(2r-1)})\, \varphi(f_{p(2r)}) \rangle \tag{3.5}$$

while

$$\langle \varphi(f_1) \ldots \varphi(f_{2n+1}) \rangle = 0\,. \tag{3.6}$$

The formula for the two-point functions at the inverse temperature β is

$$\begin{aligned}\langle \varphi(f)\,\varphi(g)\rangle_\beta = \langle f, g\rangle + \langle (1+e^{-\beta S})^{-1}\, g, f\rangle \\ - \langle (1+e^{-\beta S})^{-1}\, f, g\rangle\,.\end{aligned} \tag{3.7}$$

The Hilbert space for the composite system is $\mathscr{K} = \mathscr{K}_A \otimes \mathscr{K}_B$ and the Hamiltonian is

$$H_\lambda = H_A \otimes 1 + 1 \otimes H_B + \lambda H_I \tag{3.8}$$

where the interaction term is

$$H_I = Q \otimes \Phi\,. \tag{3.9}$$

Here Q is an arbitrary self-adjoint operator on $\mathscr{K}_A$ and the self-adjoint operator Φ is given by

$$\Phi = i\,\varphi(f_1)\,\varphi(f_{-1}) \tag{3.10}$$

where the test functions f_1 and f_{-1} are supposed to have disjoint energy spectra, that is

$$\langle e^{iSt} f_1, f_{-1}\rangle = 0 \tag{3.11}$$

for all $t \in \mathbb{R}$.

We now state the problem in the terminology of Section 2. Let the Banach space $\mathscr{B}$ be the space of trace class operators on $\mathscr{K}$ and let $\mathscr{B}_0$ be the space of trace class operators on $\mathscr{K}_A$. The projection $P_0 : \mathscr{B} \to \mathscr{B}_0$ is the partial trace, which is determined by

$$\operatorname{tr}[P_0(\varrho)\, X] = \operatorname{tr}[\varrho(X \otimes 1)] \tag{3.12}$$

if ϱ is an arbitrary trace class operator on $\mathscr{K}$ and X is an arbitrary bounded operator on $\mathscr{K}_A$. For this to be a projection we have to identify $\mathscr{B}_0$ as a subspace of $\mathscr{B}$, and we do this by the injection $\varrho \to \varrho \otimes \sigma$ where σ is the state $|\Omega\rangle\langle\Omega|$ on $\mathscr{K}_B$.

The free evolution is the one parameter group of isometries on $\mathscr{B}$ given by

$$U_t(\varrho) = e^{-iH_0 t}\, \varrho\, e^{iH_0 t} \tag{3.13}$$

whose infinitesimal generator is formally

$$Z(\varrho) = -\,i[H_0, \varrho]\,. \tag{3.14}$$

The necessary and sufficient condition for U_t to leave $\mathscr{B}_0$ and $\mathscr{B}_1 = (1 - P_0)\,\mathscr{B}$ invariant is that $H_B \Omega = 0$, which we have assumed. The perturbation introduced is the derivation A on $\mathscr{B}$ given by

$$A(\varrho) = -\,i[Q \otimes \Phi, \varrho]\,. \tag{3.15}$$

The evolution group of the total system is therefore

$$V_t^\lambda(\varrho) = e^{-iH_\lambda t}\,\varrho\, e^{iH_\lambda t}\,. \tag{3.16}$$

The condition $A_{00}=0$ is satisfied provided

$$\langle \Phi\,\Omega, \Omega\rangle = 0 \tag{3.17}$$

and this is a consequence of Eqs. (3.10) and (3.11).

We have now set up the problem in the notation of Section 2 and have to check that the conditions of Theorem 2.3 are satisfied. We first introduce the following abbreviated notation.

$$\begin{aligned} A_r &= U_{-t_r} A\, U_{t_r}, \qquad Q_r = e^{iH_A t_r} Q\, e^{-iH_A t_r} \\ \Phi_r &= e^{iH_B t_r}\,\Phi\, e^{-iH_B t_r} \\ \varphi_r(f) &= e^{iH_B t_r}\,\varphi(f)\, e^{-iH_B t_r} = \varphi(e^{iSt_r} f) \end{aligned} \tag{3.18}$$

and define

$$\begin{aligned} h(t) &= \langle e^{iH_B t}\,\Phi\, e^{-iH_B t}\Phi\,\Omega, \Omega\rangle \\ h_i(t) &= \langle e^{iH_B t}\,\varphi(f_i)\, e^{-iH_B t}\,\varphi(f_i)\,\Omega, \Omega\rangle\,. \end{aligned} \tag{3.19}$$

It may easily be proved from Eqs. (3.5) and (3.11) that

$$h(t) = h_1(t)\, h_{-1}(t)\,. \tag{3.20}$$

Theorem 3.1. *If* $\int_0^\infty |h_1(t)|\, dt < \infty$ *then*

$$\int_0^\infty \|P_0 A_0 A P_0\|\, dt_0 < \infty\,. \tag{3.21}$$

Proof. If $\varrho \in \mathscr{B}_0$ then

$$\begin{aligned} P_0 A_0 A P_0 \varrho &= -P_0[Q_0 \otimes \Phi_0, [Q \otimes \Phi, \varrho \otimes \sigma]] \\ &= -Q_0 Q \varrho\, \mathrm{tr}[\Phi_0 \Phi \sigma] + Q_0 \varrho Q\, \mathrm{tr}[\Phi_0 \sigma \Phi] \\ &\quad + Q \varrho Q_0\, \mathrm{tr}[\Phi \sigma \Phi_0] - \varrho Q Q_0\, \mathrm{tr}[\sigma \Phi \Phi_0]\,. \end{aligned} \tag{3.22}$$

Therefore

$$\begin{aligned} \|P_0 A_0 A P_0\| &\leqq 4\, \|Q\|^2\, |h(t_0)| \\ &\leqq 4\, \|Q\|^2\, \|f_{-1}\|^2\, |h_1(t_0)| \end{aligned} \tag{3.23}$$

which immediately yields the result.

Lemma 3.2. $a_{2n+1}(t) = 0$ *for all* $t \geqq 0$ *and*

$$a_{2n}(t) = \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} P_0 A_0 A_1 P_1 A_2 A_3 P_1 \ldots P_1 A_{2n} A P_0\, dt_{2n} \ldots dt_0\,. \tag{3.24}$$

Proof. Let N be the operator counting the number of particles whose energy lies in the energy spectrum of f_1, so that $[N, \varphi(f_{-1})] = 0$, and define $\mathscr{E} : \mathscr{B} \to \mathscr{B}$ by

$$\mathscr{E}(\varrho) = (1 \otimes e^{\pi i N})\, \varrho\, (1 \otimes e^{-\pi i N}).$$

Then for all $\varrho \in \mathscr{B}_0$ and all $t \geqq 0$

$$\begin{aligned} \mathscr{E}\, U_t &= U_t \mathscr{E}, \qquad \mathscr{E}\, P_0 = P_0 \mathscr{E} \\ \mathscr{E}\, A &= -A \mathscr{E}, \qquad \mathscr{E}\, \varrho = \varrho\,. \end{aligned} \tag{3.25}$$

The statements of the lemma follow by applying the symmetry $\mathscr{E}$ to the integrand.

In the following we shall occasionally write A_{2n+1} for A; this is equivalent to introducing a dummy variable $t_{2n+1} \equiv 0$.

Lemma 3.3. *Let h_1 be integrable on $[0, \infty]$. Then if π is any permutation of $(0, \ldots, 2n+1)$*

$$\begin{aligned} &\left| \sum_p \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} \prod_{r=0}^{n} h_1(t_{\pi p\,(2r)} - t_{\pi p(2r+1)})\, dt_{2n} \ldots dt_0 \right| \\ &\qquad \leqq t^n \|h_1\|_1^{n+1} / 2^{n+1} (n+1)! \end{aligned} \tag{3.26}$$

Proof. For every permutation σ of $(0, \ldots, 2n+1)$ we obtain a pairing by associating $\sigma(2r)$ with $\sigma(2r+1)$ and then reordering appropriately. After counting repetitions this shows that the integral is dominated by

$$\begin{aligned} &\sum_{\sigma \in S_{2n+2}} \frac{1}{2^{n+1}(n+1)!} \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} \prod_{r=0}^{n} |h_1(t_{\sigma(r)} - t_{\sigma(2r+1)}|\, dt_{2n} \ldots dt_0 \\ &= \frac{1}{2^{n+1}(n+1)!} \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t} \prod_{r=0}^{n} |h_1(t_{2r} - t_{2r+1})|\, dt_{2n} \ldots dt_0 \end{aligned} \tag{3.27}$$

since $|h_1|$ is an even function. Integrating with respect to the even variables and remembering that $t_{2n+1} \equiv 0$, the result follows.

Theorem 3.4. *If $\|h_1\|_1 < \infty$ then Eq. (2.38) of Theorem 2.3 is satisfied for constants c_n of the required type.*

Proof. We put

$$\Phi_r^L(\varrho) = \Phi_r \varrho, \qquad \Phi_r^R(\varrho) = \varrho\, \Phi_r \tag{3.28}$$

and similarly for Q and A, so that

$$A_r(\varrho) = (A_r^L + A_r^R)(\varrho) = (-i Q_r^L \Phi_r^L + i Q_r^R \Phi_r^R)(\varrho)\,. \tag{3.29}$$

We now expand

$$a_{2n}(t)\,\varrho = \int_{t_0=0}^{t} \dots \int_{t_{2n}=0}^{t_{2n-1}} P_0(A_0^L + A_0^R)(A_1^L + A_1^R)(1-P_0)\dots \\ \dots(1-P_0)(A_{2n}^L + A_{2n}^R)(A^L + A^R)\,P_0\,\varrho\,dt_{2n}\dots dt_0 \tag{3.30}$$

to obtain

$$a_{2n}(t)\,\varrho = \sum_{\alpha,\beta} \operatorname{sign}\alpha \int_{t_0=0}^{t} \dots \int_{t_{2n}=0}^{t_{2n-1}} P_0\,A_0^{\beta(0)}\,A_1^{\beta(1)}\,A_2^{\beta(2)}\dots \\ A_{\alpha_1-1}^{\beta(\alpha_1-1)}\,P_0\,A_{\alpha_1}^{\beta(\alpha_1)}\dots A_{\alpha_j-1}^{\beta(\alpha_j-1)}\,P_0\,A_{\alpha_j}^{\beta(\alpha_j)}\dots \\ \dots A_{2n}^{\beta(2n)}\,A_{2n+1}^{\beta(2n+1)})\,P_0\,\varrho\,dt_{2n}\dots dt_0 \tag{3.31}$$

In this equation we sum over all functions $\beta:\{0,\dots,2n+1\}\to\{L,R\}$. We sum over all sequences $\alpha(0),\dots,\alpha(k+1)$ of even integers such that

$$0=\alpha(0)<\alpha(1)<\dots<\alpha(k)<\alpha(k+1)=2n+2\,. \tag{3.32}$$

We have put $\operatorname{sign}\alpha=(-1)^k$ and have introduced the dummy variable $t_{2n+1}\equiv 0$.

It may be observed that the operators in the above integral are tensor products and that P_0 acts only on the second component. This leads immediately to the estimate

$$\|a_{2n}(t)\,\varrho\| \leqq \sum_{\alpha,\beta} \|Q\|^{2n+2}\,\|\varrho\| \int_{t_0=0}^{t} \dots \int_{t_{2n}=0}^{t_{2n-1}} dt_{2n}\dots dt_0\,. \\ \prod_{j=0}^{k} |\operatorname{tr}[\Phi_{\alpha_j}^{\beta(\alpha_j)}\,\Phi_{\alpha_j+1}^{\beta(\alpha_j+1)}\dots\Phi_{\alpha_{j+1}-1}^{\beta(\alpha_{j+1}-1)}\,\sigma]| \tag{3.33}$$

$$= \sum_{\alpha,\beta} \|Q\|^{2n+2}\,\|\varrho\| \int_{t_0=0}^{t} \dots \int_{t_{2n}=0}^{t_{2n-1}} I(\alpha,\pi,t_0\dots t_{2n})\,dt_{2n}\dots dt_0 \tag{3.34}$$

where

$$I(\alpha,\pi,t_0\dots t_{2n}) = \prod_{j=0}^{k} |\langle \Phi_{\pi(\alpha_j)}\dots\Phi_{\pi(\alpha_{j+1}-1)}\rangle| \tag{3.35}$$

and the permutation π of $\{0,\dots,2n+1\}$ depends on α and β.

We now use the quasi-free hypothesis (for the first time) and Eq. (3.11) to deduce that

$$|I(\alpha,\pi,t_0\dots t_{2n})| \leqq \|f_{-1}\|^{2n+2} \prod_{j=0}^{k} |\langle \varphi_{\pi(\alpha_j)}(f_1)\dots\varphi_{\pi(\alpha_{j+1}-1)}(f_1)\rangle| \tag{3.36}$$

$$\leqq \|f_{-1}\|^{2n+2} \sum_{p} \prod_{r=0}^{n} |\langle \varphi_{\pi p(2r)}(f_1)\,\varphi_{\pi p(2r+1)}(f_1)\rangle|\,. \tag{3.37}$$

The use of Lemma 3.3 now yields

$$\begin{aligned}\|a_{2n}(t)\| &\leqq \sum_{\alpha,\beta} \|Q\|^{2n+2}\, \|f_{-1}\|^{2n+2}\, t^n \|h_1\|_1^{n+1}/2^{n+1}(n+1)! \\ &\leqq 2^{2n+1}\, \|Q\|^{2n+2}\, \|f_{-1}\|^{2n+2}\, t^n \|h_1\|_1^{n+1}/(n+1)!\end{aligned} \tag{3.38}$$

which is the required estimate.

Theorem 3.5. *Suppose that for $i=1,2$ and some $\varepsilon>0$*

$$\int_0^\infty |h_i(t)|\,(1+|t|)^\varepsilon\, dt < \infty\,. \tag{3.39}$$

Then Eq. (2.39) of Theorem 2.3 is satisfied.

Proof. This is harder than Theorem 3.4 in that we must make use of some cancellations of the situation, but easier in that we do not need to control the dependence of d_n on n.

We replace Eq. (3.31) by

$$\begin{aligned}a_{2n}(t)\,\varrho = \sum_{\alpha,\beta} \operatorname{sign}\alpha \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} & P_0\, A_0^{\beta(0)} A_1^{\beta(1)} A_2^{\beta(2)} \cdots \\ & \cdots A_{\alpha_1-1}^{\beta(\alpha_1-1)}\, P_0\, A_{\alpha_1}^{\beta(\alpha_1)} \cdots A_{\alpha_k-1}^{\beta(\alpha_k-1)}\, P_0 \{ A_{\alpha_k}^{\beta(\alpha_k)} A_{\alpha_k+1}^{\beta(\alpha_k+1)} \cdots A_{2n+1}^{\beta(2n+1)}\, P_0\, \varrho \\ & - A_{\alpha_k}^{\beta(\alpha_k)} A_{\alpha_k+1}^{\beta(\alpha_k+1)} \cdots A_{2n-1}^{\beta(2n-1)}\, P_0\, A_{2n}^{\beta(2n)} A_{2n+1}^{\beta(2n+1)}\, P_0\, \varrho \} \\ & \cdot dt_{2n} \cdots dt_0\,.\end{aligned} \tag{3.40}$$

In this equation β is as before but we sum over all sequences $\alpha(0), \ldots, \alpha(k)$ of even integers such that

$$0 = \alpha(0) < \alpha(1) < \cdots < \alpha(k) < 2n\,. \tag{3.41}$$

As before this leads to the estimate

$$\begin{aligned}\|a_{2n}(t)\,\varrho\| \leqq \sum_{\alpha,\beta} \|Q\|^{2n+2}\, \|\varrho\| \int_{t_0=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} & dt_{2n} \cdots dt_0\,. \\ \prod_{j=0}^{k-1} |\operatorname{tr}[\Phi_{\alpha_j}^{\beta(\alpha_j)}\, \Phi_{\alpha_j+1}^{\beta(\alpha_j+1)} \cdots \Phi_{\alpha_{j+1}-1}^{\beta(\alpha_{j+1}-1)}\, \sigma]|\,. & \\ |\operatorname{tr}[\Phi_{\alpha_k}^{\beta(\alpha_k)}\, \Phi_{\alpha_k+1}^{\beta(\alpha_k+1)} \cdots \Phi_{2n+1}^{\beta(2n+1)}\, \sigma] & \\ - tr[\Phi_{\alpha_k}^{\beta(\alpha_k)}\, \Phi_{\alpha_k+1}^{\beta(\alpha_k+1)} \cdots \Phi_{2n-1}^{\beta(2n-1)}\, \sigma]\, \operatorname{tr}[\Phi_{2n}^{\beta(2n)}\, \Phi_{2n+1}^{\beta(2n+1)}\, \sigma]|\,. & \end{aligned} \tag{3.42}$$

Using the quasi-free hypothesis and Eq. (3.11) the last term of Eq. (3.42) can be written as

$$\begin{aligned} &J(\beta, t_k, t_{k+1}, \ldots, t_{2n}) \\ &= \Big| \prod_{i=\pm 1} \operatorname{tr}[\varphi_{\alpha_k}^{\beta(\alpha_k)}(f_i)\, \varphi_{\alpha_k+1}^{\beta(\alpha_k+1)}(f_i) \ldots \varphi_{2n+1}^{\beta(2n+1)}(f_i)\, \sigma] \\ &\quad - \prod_{i=\pm 1} \operatorname{tr}[\varphi_{\alpha_k}^{\beta(\alpha_k)}(f_i) \ldots \varphi_{2n-1}^{\beta(2n+1)}(f_i)\, \sigma] \operatorname{tr}[\varphi_{2n}^{\beta(2n)}(f_i)\, \varphi_{2n+1}^{\beta(2n+1)}(f_i)\, \sigma] \\ &= |a_1 a_{-1} - b_1 c_1 b_{-1} c_{-1}| \end{aligned} \tag{3.43}$$

in an obvious notation,

$$\leqq |a_1 - b_1 c_1|\, |a_{-1}| + |b_1 c_1|\, |a_{-1} - b_{-1} c_{-1}|\,. \tag{3.44}$$

Now again using the quasi-free hypothesis

$$\begin{aligned} J(\beta, t_k, \ldots, t_{2n}) \leqq \sum_{i=+1} \|f_{-i}\|^{2n+2-\alpha_k} \sum_p{}' \prod_{r=\frac{1}{2}\alpha_k}^{n} \\ \cdot |\langle \varphi_{p(2r)}(f_i)\, \varphi_{p(2r+1)}(f_i) \rangle| \end{aligned} \tag{3.45}$$

where Σ_p' indicates the sum over all pairings p of $\{\alpha_k, \alpha_k+1, \ldots, 2n+1\}$ such that $2n$ is *not* paired with $(2n+1)$. Therefore

$$\begin{aligned} \|a_{2n}(t)\| \leqq \sum_{\alpha,\beta} \sum_{i=+1} \sum_p{}'' \|Q\|^{2n+2}\, \|f_{-i}\|^{2n+2} \\ \int_{t_0=0}^{t} \ldots \int_{t_{2n}=0}^{t_{2n-1}} \prod_{r=0}^{n} |h_i(t_{p(2r)} - t_{p(2r+1)})|\, dt_{2n} \ldots dt_0 \end{aligned} \tag{3.46}$$

where Σ_p'' indicates the sum over all pairings of $\{0, \ldots, 2n+1\}$ such that $2n$ is not paired with $(2n+1)$. Carrying out one-half of the integrations we see that each integral is dominated by an expression of the form

$$\|h_i\|_1^n \int_{s_0=0}^{t} \ldots \int_{s_n=0}^{s_{n-1}} |h_i(s_k)|\, ds_n \ldots ds_0 \tag{3.47}$$

where $1 \leqq k \leqq n$,

$$\begin{aligned} &\leqq \text{const.} \int_{s=0}^{t} (t-s)^{n-k}\, |h_i(s)|\, s^k\, ds \\ &\leqq \text{const.}\, t^{n-\varepsilon} \int_{s=0}^{t} s^{\varepsilon} |h_i(s)|\, \mathrm{d}s\,. \end{aligned} \tag{3.48}$$

Together with Eq. (3.39) this proves the required estimate.

This completes the proof of all the estimates required for the application of Theorem 2.3 to this model. We conclude this section with some comments on possible variations of the model. The interaction can be changed by putting

$$H_I = Q \otimes \varphi(f_1) \dots \varphi(f_n)\, i^{n(n-1)/2} \tag{3.49}$$

provided the test functions $f_1, \dots, f_n \in \mathscr{V}$ satisfy

$$\langle e^{iSt} f_r, f_s \rangle = 0 \tag{3.50}$$

for all $r \neq s$ and all $t \neq 0$. In the more singular Boson case, however, one seems to be restricted to the case $n = 1$, or possibly $n = 2$, because of the difficulty of even proving the Hamiltonian is a self-adjoint operator. The proof can be extended to the case where the system is coupled to a finite number of heat baths at different temperatures. The space $\mathscr{K}_A$ need not be finite-dimensional provided Q is bounded and H_A has purely discrete spectrum. The theory can be developed in an algebraic form, as in [11], without any essential changes.

§ 4. Dynamics of the Limit System

We have shown that the model of the last section satisfies all the conditions of Theorem 2.3 provided Eq. (3.39) is satisfied. The operator $K^\natural$ on the space $\mathscr{B}_0$ of density matrices on $\mathscr{K}_A$ is given explicitly by

$$\begin{aligned} K^\natural(\varrho) = \lim_{a \to \infty} \frac{1}{2a} \int_{s=-a}^{a} \int_{t=0}^{\infty} \{ & -Q_{t+s} Q_s \varrho\, h(t) \\ & + Q_{t+s} \varrho\, Q_s \overline{h(t)} + Q_s \varrho\, Q_{t+s} h(t) - \varrho\, Q_s Q_{t+s} \overline{h(t)} \}\, dt\, ds \end{aligned} \tag{4.1}$$

where

$$Q_t = e^{iH_A t} Q\, e^{-iH_A t} \tag{4.2}$$

and $h(t)$ is defined by Eq. (3.19).

Lemma 4.1. *The function $h(t)$ is continuous and integrable, and its transform satisfies*

$$\hat{h}(-x) = e^{-\beta x} \hat{h}(x) \tag{4.3}$$

for all $x \in \mathbb{R}$, where β is the inverse temperature of the heat bath.

Proof. The integrability of $h(t)$ follows from Eqs. (3.20) and (3.39). By Eq. (3.7)

$$\begin{aligned} h_i(t) = \langle e^{iSt} f_i, f_i\rangle + \langle (1+e^{-\beta S})^{-1} f_i, e^{iSt} f_i\rangle \\ - \langle (1+e^{-\beta S})^{-1} e^{iSt} f_i, f_i\rangle \end{aligned} \tag{4.4}$$

so by the spectral theorem

$$\hat{h}_i(-x) = e^{-\beta x} h_i(x)\,. \tag{4.5}$$

Now by Eq. (3.20) and Fourier analysis

$$\hat{h}(x) = \int_{-\infty}^{\infty} \hat{h}_1(y)\, \hat{h}_{-1}(x-y)\, dy \tag{4.6}$$

which together with Eq. (4.5) yields Eq. (4.3).

We now expand

$$Q_t \equiv e^{iH_A t} Q e^{-iH_A t} = \sum_{\omega} A_\omega e^{-i\omega t} \tag{4.7}$$

so that the operator A_ω on $\mathscr{K}_A$ is zero unless ω is the difference of two eigenvalues of H_A.

Theorem 4.2. *There exist real constants $a(\omega)$, $e(\omega)$, and $s(\omega)$ satisfying*

$$a(\omega) = e^{-\beta\omega} e(\omega) \geqq 0 \tag{4.8}$$

such that

$$\begin{aligned} K^\natural(\varrho) = &\sum_{\omega \geq 0} e(\omega) \{-\tfrac{1}{2} A_{-\omega} A_\omega \varrho + A_\omega \varrho A_{-\omega} - \tfrac{1}{2} \varrho A_{-\omega} A_\omega\} \\ &+ \sum_{\omega > 0} a(\omega) \{-\tfrac{1}{2} A_\omega A_{-\omega} \varrho + A_{-\omega} \varrho A_\omega - \tfrac{1}{2} \varrho A_\omega A_{-\omega}\} \\ &+ \sum_{\omega \in \mathbb{R}} \mathrm{i} s(\omega) [A_{-\omega} A_\omega, \varrho]\,. \end{aligned} \tag{4.9}$$

Comment. In the standard description of atomic radiation the three terms are respectively the emission term, the absorption term and a term describing a shift of the free energy levels (of order λ^2).

Proof. Substituting the expression for Q_t in the definition of $K^\natural$ and evaluating the integral with respect to x leads to

$$\begin{aligned} K^\natural(\varrho) = \sum_{\omega} \int_{t=0}^{\infty} \{ &- A_\omega A_{-\omega} \varrho e^{-i\omega t} h(t) \\ &+ A_\omega \varrho A_{-\omega} e^{-i\omega t} \overline{h(t)} + A_{-\omega} \varrho A_\omega e^{-i\omega t} h(t) \\ &- \varrho A_{-\omega} A_\omega e^{-i\omega t} \overline{h(t)}\}\, dt\,. \end{aligned} \tag{4.10}$$

Now

$$\int_0^\infty h(t)\, e^{i\omega t}\, dt = \tfrac{1}{2} \hat{h}(\omega) + \mathrm{i} s(\omega) \tag{4.11}$$

where $\hat{h}(\omega)$ and $s(\omega)$ are real, so

$$\begin{aligned} K^{\mathfrak{h}}(\varrho) = \tfrac{1}{2} \sum_{\omega} \{ & - A_{-\omega} A_{\omega} \varrho (\hat{h}(\omega) + 2is(\omega)) \\ & + A_{\omega} \varrho A_{-\omega} (\hat{h}(\omega) - 2is(\omega)) \\ & + A_{\omega} \varrho A_{-\omega} (\hat{h}(\omega) + 2is(\omega)) \\ & - \varrho A_{-\omega} A_{\omega} (\hat{h}(\omega) - 2is(-\omega)) \} \end{aligned} \tag{4.12}$$

which is the required result if for $\omega \geqq 0$

$$e(\omega) = \hat{h}(\omega) \quad \text{and} \quad a(\omega) = \hat{h}(-\omega). \tag{4.13}$$

Theorem 4.3. *The operator* $\exp(K^{\mathfrak{h}} \tau)$ is *for* $\tau \geqq 0$ *a positivity and trace preserving semigroup on* $\mathscr{B}_0$.

Proof. This result is true because of the limiting procedure we used to obtain $K^{\mathfrak{h}}$, but we give an independent proof.

The formula

$$\operatorname{tr}[\exp(K^{\mathfrak{h}} \tau) \varrho] = \operatorname{tr}[\varrho] \tag{4.14}$$

for all $\tau \geqq 0$ is equivalent to

$$\operatorname{tr}[K^{\mathfrak{h}} \varrho] = 0 \tag{4.15}$$

for all ϱ, which is valid by inspection. The positivity will follow by the Trotter product formula [12] if we can write $K^{\mathfrak{h}}$ as a sum of generators of semigroups which preserve positivity. Now if $K_1(\varrho) = A \varrho A^*$ and $\varrho \geqq 0$ then

$$e^{K_1 \tau}(\varrho) = \Sigma \frac{\tau^n}{n!} A^n \varrho A^{*n} \geqq 0. \tag{4.16}$$

If $K_2(\varrho) = -A^* A \varrho - \varrho A^* A$ and $\varrho \geqq 0$ then

$$e^{K_2 \tau}(\varrho) = e^{-A^* A \tau} \varrho \, e^{-A^* A \tau} \geqq 0 \tag{4.17}$$

while if $H_3(\varrho) = i[A^* A, \varrho]$ and $\varrho \geqq 0$ then

$$e^{K_3 \tau}(\varrho) = e^{iA^* A \tau} \varrho^{-iA^* A \tau} \geqq 0. \tag{4.18}$$

This completes the proof.

The above results give a complete justification for regarding the equation

$$\frac{d\varrho}{d\tau} = K^{\mathfrak{h}} \varrho \tag{4.19}$$

as a quantum-mechanical Fokker-Planck equation. We draw the reader's attention to [13], where more general equations of this type have been studied from the point of view of quantum stochastic processes. In [14] it is shown that semigroups of this type can always be regarded as

arising from interactions with singular heat baths, instead of from regular heat baths in the weak coupling limit. This is the point of view taken by Hepp and Lieb in [15]. They however work in the Heisenberg picture, which has some advantages.

We finally use the above equations to investigate the question of convergence to equilibrium. For the sake of simplicity we let $u_1, \ldots, u_n$ be an orthonormal basis of $\mathscr{K}_A$ and suppose

$$H_A u_r = \omega_r u_r \tag{4.20}$$

where the ω_r are all different.

Theorem 4.4. *The semigroup* $\exp\{K^\natural \tau\}$ *on* $\mathscr{B}_0$ *leaves the subspace* $\mathscr{D}$ *of diagonal matrices invariant and defines a classical Markov process on the integers* $\{1, \ldots, n\}$.

Proof. We first observe that

$$\mathscr{D} = \{\varrho \in \mathscr{B}_0 : U_t \varrho = \varrho \text{ for all } t \in \mathbb{R}\}. \tag{4.21}$$

If $\varrho \in \mathscr{D}$ then by Eq. (2.22)

$$U_t(K^\natural \varrho) = K^\natural U_t \varrho = K^\natural \varrho \tag{4.22}$$

so $K^\natural \varrho \in \mathscr{D}$. Therefore

$$\exp\{K^\natural \tau\} \varrho = \sum_{n=0}^{\infty} K^{\natural\, n} \varrho \tau^n / n! \in \mathscr{D}. \tag{4.23}$$

Now put

$$A_{rs} = \langle A u_r, u_s \rangle \tag{4.24}$$

and define $v_r \in \mathscr{D}$ by

$$v_r(u_s) = \delta_{rs} u_s. \tag{4.25}$$

Then

$$\begin{aligned} K^\natural(v_r) = \int_{t=0}^{\infty} \Big\{ & -\sum_s e^{-i\omega_r t} A_{rs} e^{i\omega_s t} A_{sr} v_r h(t) \\ & + \sum_s e^{-i\omega_r t} A_{sr} e^{i\omega_r t} A_{rs} v_s h(-t) \\ & + \sum_s A_{sr} e^{-i\omega_r t} A_{rs} e^{i\omega_s t} v_s h(t) \\ & - \sum_s A_{rs} e^{-i\omega_s t} A_{sr} e^{i\omega_r t} v_r h(-t) \Big\} \, dt \end{aligned} \tag{4.26}$$

$$\begin{aligned} = & -\sum_s A_{rs} A_{sr} \hat{h}(m_r - \omega_s) v_r \\ & + \sum_s A_{sr} A_{rs} \hat{h}(m_r - \omega_s) v_s. \end{aligned} \tag{4.27}$$

Therefore

$$K^{\natural}(v_r) = \sum_s a_{rs} v_s - \left(\sum_s a_{rs}\right) v_r \tag{4.28}$$

where

$$a_{rs} = A_{rs} A_{sr} \hat{h}(m_r - \omega_s) \geqq 0 . \tag{4.29}$$

Identifying the diagonal matrices on $\mathscr{K}_A$ with the functions on $\{1, \ldots, n\}$ by

$$\{\lambda_1, \ldots, \lambda_n\} \leftrightarrow \sum_{r=1}^{n} \lambda_r v_r \tag{4.30}$$

the density matrices on $\mathscr{K}_A$ correspond to the probability measures on $\{1, \ldots, n\}$. $K^{\natural}$ is then the generator of a Markov semigroup on $\{1, \ldots, n\}$. If the process is ergodic (which certainly occurs if $a_{rs} > 0$ for all r, s) then there is a unique equilibrium state and every state converges to the equilibrium state as $\tau \to \infty$. However ergodicity is not necessary for the existence of an equilibrium state.

Theorem 4.5. *If the heat bath is at the inverse temperature β then*

$$\varrho_\beta = \sum_{r=1}^{n} e^{-\beta\omega_r} v_r \Big/ \sum_{r=1}^{n} e^{-\beta\omega_r} \tag{4.31}$$

is an equilibrium state for the Markov process on $\{1, \ldots, n\}$.

Proof. We have to show that

$$0 = K^{\natural} \varrho_\beta = \sum_{r,s} e^{-\beta\omega_r} a_{rs} v_s - \sum_{r,s} a_{rs} e^{-\beta\omega_r} v_r \tag{4.32}$$

which is equivalent to

$$\sum_r e^{-\beta\omega_r} a_{rs} = \sum_r a_{sr} e^{-\beta\omega_s} . \tag{4.33}$$

This follows from Eqs. (4.3) and (4.29).

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