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Master equation for strongly interacting systems

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Abstract. A dissipating system consisting of two strongly interacting subsystems, each coupled to its respective thermal reservoir is considered. The usual method for obtaining a master equation for the reduced density operator of such a system is to assume the factorization of this density operator in the derivation of the irreversible term, retaining the coupling in the reversible term alone. This approach has the serious limitation that it fails to preserve detailed balance in general and yields an incorrect canonical form for the stationary solution of the density operator. A general approach, based on the introduction of a new interaction picture, is presented. This method is illustrated by applying it to a coupled boson system and to a two-level atom interacting with a single mode of the electromagnetic field.

1. Introduction

The master equation approach and the related Fokker-Planck and Langevin equation approaches have proved to be powerful methods for the treatment of a single quantum system interacting with a thermal reservoir. However, the current application of the master equation technique to coupled systems involves an approximation which introduces a serious defect, especially for strong coupling. Such applications of the master equation to coupled systems include the laser, super-radiance and certain problems in nonlinear optics. The reader is referred to the articles of Haken (1969), Pike (1970) and Agarwal (1973) for a review and extensive bibliography.

In evaluating the irreversible part of the master equation, it has been the practice to assume that the reduced density operator ρ for the entire system factorizes into the product of the individual density operators ρ_A and ρ_B for the coupled subsystems A and B. The irreversible part of the master equation is then given by

$$\left(\frac{\partial\rho}{\partial t}\right)_{\rm irrev} = \left(\frac{\partial\rho_{\rm A}}{\partial t}\right)_{\rm irrev}\rho_{\rm B} + \rho_{\rm A}\left(\frac{\partial\rho_{\rm B}}{\partial t}\right)_{\rm irrev}.$$
(1.1)

Hence, retaining the coupling in the reversible term, the full master equation takes the form

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H_{\rm A} + H_{\rm B} + H_{\rm AB}, \rho] + \left(\frac{\partial \rho}{\partial t}\right)_{\rm irrev}.$$
(1.2)

This approximation has been considered valid under the assumption of weak coupling. However, the master equation derived from equation (1.1) has the serious deficiency that it fails to satisfy the basic symmetry of detailed balance in general.

[†] This paper is based on a thesis submitted by H J Carmichael to the University of Auckland in partial fulfilment of the requirements for the MSc degree.

Furthermore, it may be shown that it leads to the incorrect canonical form for the stationary solution of the density operator. For an interaction hamiltonian H_{AB} which commutes with the free hamiltonians H_A and H_B , the stationary form for the density operator derived from equations (1.1) and (1.2) is

$$\rho = \exp\left(-\frac{H_{\rm A} + H_{\rm B}}{kT}\right) \tag{1.3}$$

which is inconsistent with the system hamiltonian.

The limitations of the factorization ansatz were first recognized by Walls (1970), who illustrated them by considering coupled boson-field modes interacting with heat baths at the same temperature. In this case it was possible to include the coupling to all orders in the irreversible part of the master equation by a transformation to normal modes. The only other publication to date on this subject is that of Schwendimann (1972) who derived a condition for the validity of the approximate master equation for the case of N atoms interacting with a single-field mode.

In this paper we introduce a general approach to the problem, the basic concept of which involves the introduction of a new interaction picture for internally coupled systems. We illustrate this method by its application to (i) two coupled boson-field modes, and (ii) a two-level atom interacting with an electromagnetic field mode.

2. A new interaction picture for treating internally coupled systems

The techniques for treating a single quantum system S coupled to a thermal reservoir R are now well known (see eg Haken 1969, Louisell 1969, Senitzky 1960, 1961).

Writing the complete hamiltonian for S plus R as

$$H = H_{\rm S} + H_{\rm R} + H_{\rm SR} \tag{2.1}$$

the markoffian master equation in the Born approximation for the reduced density operator $\tilde{\rho}$ of the system in the interaction picture reads

$$\frac{\partial \tilde{\rho}}{\partial t} = -\frac{1}{\hbar^2} \int_0^t \operatorname{Tr}_{\mathbf{R}}([V(t), [V(t'), \tilde{\rho}(t)f_0(\mathbf{R})]]) \, \mathrm{d}t'$$
(2.2)

where $f_0(\mathbf{R})$ is the density operator for the reservoir and

$$\tilde{\rho}(t) = \exp\left(\frac{iH_{s}}{\hbar}t\right)\rho(t)\exp\left(-\frac{iH_{s}}{\hbar}t\right)$$

$$V(t) = \exp\left(\frac{i(H_{s}+H_{R})}{\hbar}t\right)H_{sR}\exp\left(-\frac{i(H_{s}+H_{R})}{\hbar}t\right).$$
(2.3)

We consider a system consisting of two subsystems A and B, with free hamiltonians H_A and H_B , which are coupled via the interaction hamiltonian H_{AB} . Each of these subsystems is coupled to its respective reservoir R_A or R_B via the interaction hamiltonians H_{AR_A} and H_{BR_B} respectively. Thus if we designate the free hamiltonians for these independent reservoirs by H_{R_A} and H_{R_B} , the total hamiltonian assumes the form

$$H = H_{\rm A} + H_{\rm B} + H_{\rm AB} + H_{\rm R_{\rm A}} + H_{\rm R_{\rm B}} + H_{\rm AR_{\rm A}} + H_{\rm BR_{\rm B}}.$$
 (2.4)

All operators from the subsystems A and B commute with all operators from R_A and R_B , and all operators from R_A commute with all those from R_B .

Now following the normal practice adopted in perturbation theory, we might group the hamiltonians in equation (2.4) so that the total hamiltonian reads

$$H = H_0 + H_1 \tag{2.5}$$

where

$$H_{0} = H_{A} + H_{B} + H_{R_{A}} + H_{R_{B}}$$

$$H_{1} = H_{AB} + H_{AR_{A}} + H_{BR_{B}}.$$
(2.6)

Then if we work in the normal interaction picture for the construction of the master equation for the reduced density operator $\rho_{AB}(t)$ of the system A plus B following standard methods we obtain

$$\frac{\partial \rho_{AB}(t)}{\partial t} = \frac{1}{i\hbar} [\tilde{H}_{AB}(0), \tilde{\rho}_{AB}(0)] - \frac{1}{\hbar^2} \int_0^t \mathrm{Tr}_{R}([\tilde{H}_{AB}(t) + \tilde{H}_{AR_A}(t) + \tilde{H}_{BR_B}(t), [\tilde{H}_{AB}(t') + \tilde{H}_{AR_A}(t') + \tilde{H}_{BR_B}(t'), \tilde{\chi}_{AB}(t')]]) dt'$$

$$(2.7)$$

where $\tilde{\chi}_{AB}(t)$ is the density operator for the system plus reservoir. The trace is taken over the complete reservoir consisting of R_A plus R_B and

$$\begin{split} \widetilde{H}_{AB}(t) &= \exp\left(\frac{\mathrm{i}H_{0}}{\hbar}t\right)H_{AB}\exp\left(-\frac{\mathrm{i}H_{0}}{\hbar}t\right)\\ \widetilde{H}_{AR_{A}}(t) &= \exp\left(\frac{\mathrm{i}H_{0}}{\hbar}t\right)H_{AR_{A}}\exp\left(-\frac{\mathrm{i}H_{0}}{\hbar}t\right)\\ \widetilde{H}_{BR_{B}}(t) &= \exp\left(\frac{\mathrm{i}H_{0}}{\hbar}t\right)H_{BR_{B}}\exp\left(-\frac{\mathrm{i}H_{0}}{\hbar}t\right)\\ \widetilde{\chi}_{AB}(t) &= \exp\left(\frac{\mathrm{i}H_{0}}{\hbar}t\right)\chi_{AB}(t)\exp\left(-\frac{\mathrm{i}H_{0}}{\hbar}t\right)\\ \widetilde{\rho}_{AB}(t) &= \exp\left(\frac{\mathrm{i}(H_{A}+H_{B})}{\hbar}t\right)\rho_{AB}(t)\exp\left(-\frac{\mathrm{i}(H_{A}+H_{B})}{\hbar}t\right). \end{split}$$
(2.8)

The usual master equation obtained using the factorization ansatz in the derivation of the irreversible term, when written in this interaction picture takes the form

$$\frac{\partial \tilde{\rho}_{AB}(t)}{\partial t} = \frac{1}{i\hbar} [\tilde{H}_{AB}(0), \tilde{\rho}_{AB}(0)] - \frac{1}{\hbar^2} \int_0^t \operatorname{Tr}_{\mathbf{R}_A}([\tilde{H}_{AR_A}(t), [\tilde{H}_{AR_A}(t'), \tilde{\rho}_{AB}(t)f_0(\mathbf{R}_A)]]) dt' - \frac{1}{\hbar^2} \int_0^t \operatorname{Tr}_{\mathbf{R}_B}([\tilde{H}_{BR_B}(t), [\tilde{H}_{BR_B}(t'), \tilde{\rho}_{AB}(t)f_0(\mathbf{R}_B)]]) dt'.$$
(2.9)

This may obviously be obtained from equation (2.7) by ignoring the internal interaction in the integral and proceeding to the Born and markoffian approximations in the usual manner.

Attempts to treat H_{AB} to higher orders by further iteration of the integrals may be made. However, it is of far greater advantage to find a technique which treats H_{AB} to all orders. This can be achieved quite simply by regrouping the hamiltonian (2.4) in a manner consistent with the formalism for single quantum systems. The derivation of equation (2.2) makes no assumptions about the explicit form of the hamiltonian (2.1). Consequently, if we abandon the grouping in equation (2.5) and for it substitute that of equation (2.1) with

$$H_{\rm S} = H_{\rm A} + H_{\rm B} + H_{\rm AB}$$

$$H_{\rm R} = H_{\rm R_A} + H_{\rm R_B}$$

$$H_{\rm SR} = H_{\rm AR_A} + H_{\rm BR_B}$$
(2.10)

we may apply the master equation (2.2) directly. This accomplishes our aim of treating H_{AB} to all orders as well as allowing us to treat both single and internally coupled systems under a consistent formalism. This technique obviously amounts to using an interaction picture with H_{AB} included as part of H_0 rather than H_1 . If we are able to find solutions to the Heisenberg equations of motion

$$\frac{\mathrm{d}H_{\mathrm{AR}_{\mathrm{A}}}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[H_{\mathrm{AR}_{\mathrm{A}}}(t), H_{\mathrm{S}} + H_{\mathrm{R}}]$$

$$\frac{\mathrm{d}H_{\mathrm{BR}_{\mathrm{B}}}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[H_{\mathrm{BR}_{\mathrm{B}}}(t), H_{\mathrm{S}} + H_{\mathrm{R}}]$$
(2.11)

we may obtain the master equation in operator form. If it is not possible to obtain solutions to the Heisenberg equations of motion, as for nonlinear problems, we may obtain the master equation for the matrix elements of the density operator.

3. The master equation for coupled boson-field modes

As an illustrative example of a problem to which the technique described above may be successfully applied to obtain the master equation in operator form, we consider independent boson-field modes a and b coupled at resonance. Both modes are damped by coupling to thermal reservoirs R_a and R_b respectively. Adopting the notation for the total hamiltonian in equations (2.1) and (2.10), the system hamiltonian reads

$$H_{\rm S} = H_{\rm a} + H_{\rm b} + H_{\rm ab} = \hbar\omega_0 a^{\dagger}a + \hbar\omega_0 b^{\dagger}b + \hbar\kappa(a^{\dagger}b + ab^{\dagger})$$
(3.1)

where ω_0 is the resonant frequency and κ the coupling constant for the internal interaction. (Throughout this paper all coupling constants are assumed to have been made real by the appropriate choice of the arbitrary phases for the vector-mode functions in the expansion of the field.) The creation, annihilation operator pairs a^{\dagger} , a and b^{\dagger} , bobey boson commutation relations, and the interaction hamiltonian is given in the rotating-wave approximation. (In a future publication we will relax this condition.)

The above type of coupling is found in the parametric frequency converter (Louisell *et al* 1961) and also in polaritons (Loudon 1969) which exhibit strong photon-phonon coupling.

Following the discussion of the previous section, we should now be able to obtain the required master equation by the direct application of equation (2.2) using the hamiltonian defined above. Having converted this equation into the Schrödinger picture, this leads us to a master equation for the reduced density operator ρ of the form

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H_{\rm S}, \rho] + \left(\frac{\partial \rho}{\partial t}\right)^{\rm a}_{\rm irrev} + \left(\frac{\partial \rho}{\partial t}\right)^{\rm b}_{\rm irrev}$$
(3.2)

where

$$\left(\frac{\partial \rho}{\partial t} \right)_{irrev}^{a,b} = \exp\left(-\frac{iH_s}{\hbar} t \right) \left(\frac{\partial \tilde{\rho}}{\partial t} \right)^{a,b} \exp\left(\frac{iH_s}{\hbar} t \right)$$

$$\left(\frac{\partial \tilde{\rho}}{\partial t} \right)^{a,b} = -\frac{1}{\hbar^2} \int_0^t \operatorname{Tr}_{\mathbf{R}_{a,b}}([V_{a,b}(t), [V_{a,b}(t'), \tilde{\rho}f_0(\mathbf{R}_{a,b})]]) dt'$$

$$(3.3)$$

with

$$V_{\mathbf{a},\mathbf{b}}(t) = \exp\left(\frac{\mathbf{i}(H_{\mathbf{S}} + H_{\mathbf{R}})}{\hbar}t\right) H_{\mathbf{a},\mathbf{b}\mathbf{R}_{\mathbf{a},\mathbf{b}}} \exp\left(-\frac{\mathbf{i}(H_{\mathbf{S}} + H_{\mathbf{R}})}{\hbar}t\right).$$
(3.4)

After making the standard assumptions regarding the properties of the reservoirs and the form of the reservoir interactions $H_{a_{R_a}}$ and $H_{b_{R_b}}$ (Weidlich and Haake 1965a, b, Haake 1969), substitution of the hamiltonians into equations (3.2)–(3.4) followed by a certain amount of tedious but straightforward algebra leads to the master equation[†]

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{1}{\mathrm{i}\hbar} \left[\hbar \omega_0 a^{\dagger} a + \hbar \omega_0 b^{\dagger} b + \hbar \kappa (a^{\dagger} b + a b^{\dagger}), \rho \right] + \frac{1}{4} (\gamma_A^a + \gamma_B^a) ([a, \rho a^{\dagger}] + [a\rho, a^{\dagger}]) \\ &+ \frac{1}{4} (\gamma_A^a - \gamma_B^a) ([a, \rho b^{\dagger}] + [b\rho, a^{\dagger}]) + \frac{1}{2} (\gamma_A^a \bar{n}_A^a + \gamma_B^a \bar{n}_B^a) ([a\rho, a^{\dagger}] + [a^{\dagger}, \rho a]) \\ &+ \frac{1}{4} (\gamma_A^a \bar{n}_A^a - \gamma_B^a \bar{n}_B^a) ([a^{\dagger}, \rho b] + [a\rho, b^{\dagger}] + [b^{\dagger}, \rho a] + [b\rho, a^{\dagger}]) \\ &+ \frac{1}{4} (\gamma_A^b + \gamma_B^b) ([b, \rho b^{\dagger}] + [b\rho, b^{\dagger}] + \frac{1}{4} (\gamma_A^b - \gamma_B^b) ([b, \rho a^{\dagger}] + [a\rho, b^{\dagger}]) \\ &+ \frac{1}{2} (\gamma_A^b \bar{n}_A^b + \gamma_B^b \bar{n}_B^b) ([b\rho, b^{\dagger}] + [b^{\dagger}, \rho b]) \\ &+ \frac{1}{4} (\gamma_A^b \bar{n}_A^b - \gamma_B^b \bar{n}_B^b) ([b^{\dagger}, \rho a] + [b\rho, a^{\dagger}] + [a^{\dagger}, \rho b] + [a\rho, b^{\dagger}]). \end{aligned}$$
(3.5)

The terms with coefficients involving $\gamma_{A,B}^{a,b}$ are damping terms, the damping constants being defined by

$$\gamma_{\mathbf{A},\mathbf{B}}^{\mathbf{a},\mathbf{b}} = 2\pi g_{\mathbf{a},\mathbf{b}}(\omega_{j}^{\mathbf{a},\mathbf{b}})|\kappa^{\mathbf{a},\mathbf{b}}(\omega_{j}^{\mathbf{a},\mathbf{b}})|^{2}\Big|_{\omega_{j}^{\mathbf{a},\mathbf{b}}=\omega_{\mathbf{A},\mathbf{B}}}$$
(3.6)

where

$$\omega_{\mathbf{A},\mathbf{B}} = \omega_0 \pm \kappa. \tag{3.7}$$

Here $g_a(\omega_j^a)$ is the frequency spectrum for the reservoir R_a and $\kappa^a(\omega_j^a)$ is the coupling constant between mode a and the component of R_a corresponding to the eigenvalue ω_j^a . $g_b(\omega_j^b)$ and $\kappa^b(\omega_j^b)$ are similarly defined. We note that since the reservoirs are assumed to have a reasonably flat frequency spectrum, $\gamma_A^{a,b}$ and $\gamma_B^{a,b}$ will differ little unless the coupling is strong and hence $\kappa/\omega_0 \sim 1$. The greatest effect of the coupling in the irreversible part of the master equation will appear in the terms with coefficients involving $\bar{n}_{A,B}^{a,b}$, which for reservoirs in thermal equilibrium at a temperature T are given by

$$\bar{n}_{\mathbf{A},\mathbf{B}}^{\mathbf{a},\mathbf{b}} = \bar{n}^{\mathbf{a},\mathbf{b}}(\omega_{j}^{\mathbf{a},\mathbf{b}})\Big|_{\omega_{j}^{\mathbf{a},\mathbf{b}}=\omega_{\mathbf{A},\mathbf{B}}} = \left\{\exp(\hbar\omega_{j}^{\mathbf{a},\mathbf{b}}/kT) - 1\right\}^{-1}\Big|_{\omega_{j}^{\mathbf{a},\mathbf{b}}=\omega_{\mathbf{A},\mathbf{B}}}$$
(3.8)

and therefore become highly frequency sensitive as $\hbar\omega_{A,B}$ approaches the thermal energy kT. The effect on fluctuation terms is also relatively small if $\hbar\omega_{A,B} \gg kT$.

† During the preparation of this paper it was drawn to our attention that Agarwal (1973) has derived using identical methods such a master equation for coupled boson systems.

1556

Using standard techniques, the master equation (3.5) may be used to solve for timedependent expectation values of system observables. For the system considered above, these may also be obtained from the explicit solutions for the operator equations which are available via the method illustrated in the appendix.

4. The Fokker-Planck equation

Extensive use of the Fokker-Planck equation technique has been made in quantummechanical damping studies. This equation has distinct advantages over the master equation in operator form for the investigation of quantum statistics, since it is a cnumber equation and hence may be solved in closed form. In order to convert our master equation (3.5) into a Fokker-Planck equation, we must assume that the reduced density operator $\rho(t)$ possesses a time-dependent P representation (Glauber 1963a, b) defined by

$$\rho(t) = \int \frac{|\alpha, \beta\rangle \langle \alpha, \beta|}{\pi^2} P(\alpha, \beta, t) d^2 \alpha d^2 \beta$$
(4.1)

where the coherent states $|\alpha, \beta\rangle$ are simultaneous eigenstates of the operators *a* and *b*. Then utilizing standard techniques (see Haken 1969, Louisell 1969), $P(\alpha, \beta, t)$ can be shown to satisfy the Fokker-Planck equation

$$\begin{aligned} \frac{\partial P(\alpha, \beta, t)}{\partial t} &= \left\{ \left(\frac{\gamma_{A}^{a} + \gamma_{B}^{a}}{4} + i\omega_{0} \right) \frac{\partial}{\partial \alpha} \alpha + \left(\frac{\gamma_{A}^{a} + \gamma_{B}^{a}}{4} - i\omega_{0} \right) \frac{\partial}{\partial \alpha^{*}} \alpha^{*} \right. \\ &+ \left(\frac{\gamma_{A}^{b} + \gamma_{B}^{b}}{4} + i\omega_{0} \right) \frac{\partial}{\partial \beta} \beta + \left(\frac{\gamma_{A}^{b} + \gamma_{B}^{b}}{4} - i\omega_{0} \right) \frac{\partial}{\partial \beta^{*}} \beta^{*} \\ &+ \left(\frac{\gamma_{A}^{a} - \gamma_{B}^{a}}{4} + i\kappa \right) \frac{\partial}{\partial \alpha} \beta + \left(\frac{\gamma_{A}^{a} - \gamma_{B}^{a}}{4} - i\kappa \right) \frac{\partial}{\partial \alpha^{*}} \beta^{*} \\ &+ \left(\frac{\gamma_{A}^{b} - \gamma_{B}^{b}}{4} + i\kappa \right) \frac{\partial}{\partial \beta} \alpha + \left(\frac{\gamma_{A}^{b} - \gamma_{B}^{b}}{4} - i\kappa \right) \frac{\partial}{\partial \beta^{*}} \alpha^{*} \\ &+ \left(\frac{\gamma_{A}^{a} \bar{n}_{A}^{a} + \gamma_{B}^{a} \bar{n}_{B}^{a}}{2} \right) \frac{\partial^{2}}{\partial \alpha \partial \alpha^{*}} + \left(\frac{\gamma_{A}^{b} \bar{n}_{A}^{b} + \gamma_{B}^{b} \bar{n}_{B}^{b}}{2} \right) \frac{\partial^{2}}{\partial \beta \partial \beta^{*}} \\ &+ \left(\frac{\gamma_{A}^{a} \bar{n}_{A}^{a} - \gamma_{B}^{a} \bar{n}_{B}^{a}}{4} + \frac{\gamma_{A}^{b} \bar{n}_{A}^{b} - \gamma_{B}^{b} \bar{n}_{B}^{b}}{4} \right) \left(\frac{\partial^{2}}{\partial \alpha \partial \beta^{*}} + \frac{\partial^{2}}{\partial \beta \partial \alpha^{*}} \right) \right\} P(\alpha, \beta, t). \end{aligned}$$
(4.2)

For a Fokker-Planck equation of the form

$$\frac{\partial P(\lbrace x_i \rbrace, t)}{\partial t} = -\sum_i \frac{\partial}{\partial x_i} \{ A_i(\lbrace x_i \rbrace) P(\lbrace x_i \rbrace, t) \} + \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \{ D_{ij}(\lbrace x_i \rbrace) P(\lbrace x_i \rbrace, t) \}$$
(4.3)

the detailed balance conditions are (Graham and Haken 1971, Agarwal 1972, Risken 1972)

$$\frac{\partial}{\partial x_j} \sum_k (D^{-1})_{ik} \left(A_k^{(i)} - \sum_l \frac{\partial D_{kl}}{\partial x_l} \right) = \frac{\partial}{\partial x_i} \sum_k (D^{-1})_{jk} \left(A_k^{(i)} - \sum_l \frac{\partial D_{kl}}{\partial x_l} \right)$$

$$\sum_i \left\{ \frac{\partial A_i^{(r)}}{\partial x_i} + A_i^{(r)} \sum_j (D^{-1})_{ij} \left(A_j^{(i)} - \sum_k \frac{\partial D_{jk}}{\partial x_k} \right) \right\} = 0$$
(4.4)

where

$$A_i^{(r)} = \frac{1}{2} \{ A_i(\{x_i\}) \mp A_i(\{\tilde{x}_i\}) \} \qquad A_i^{(i)} = \frac{1}{2} \{ A_i(\{x_i\}) \pm A_i(\{\tilde{x}_i\}) \}.$$
(4.5)

Here $\{\tilde{x}_i\}$ are the variables obtained from $\{x_i\}$ under time reversal and the upper or lower sign is taken according to whether x_i is even or odd under time reversal.

It may readily be shown that for the case of thermal equilibrium, the detailed balance conditions are satisfied by the Fokker-Planck equation (4.2). Master equations for coupled systems derived from equation (1.2) do not in general satisfy detailed balance except in the particular case where the interaction hamiltonian H_{AB} commutes with the free hamiltonian $H_A + H_B$ (Carmichael and Walls to be published).

The Green function solution to our Fokker-Planck equation (4.2) arises under the condition that both field modes are initially in coherent states. A method for constructing this Green function solution for Fokker-Planck equations of the type above is given by Wang and Uhlenbeck (1945). For identical reservoirs it assumes the form

$$P(\alpha, \beta, t; \alpha_{0}, \beta_{0}, 0) = \exp\left(-\frac{\frac{1}{2}|(\alpha + \beta) - (\alpha_{0} + \beta_{0})\exp\{-(\frac{1}{2}\gamma_{A} + i\omega_{A})t\}|^{2}}{\bar{n}_{A}\{1 - \exp(-\gamma_{A}t)\}}\right) [\bar{n}_{A}\{1 - \exp(-\gamma_{A}t)\}]^{-1} \times \exp\left(-\frac{\frac{1}{2}|(\alpha - \beta) - (\alpha_{0} - \beta_{0})\exp\{-(\frac{1}{2}\gamma_{B} + i\omega_{B})t\}|^{2}}{\bar{n}_{B}\{1 - \exp(-\gamma_{B}t)\}}\right) [\bar{n}_{B}\{1 - \exp(-\gamma_{B}t)\}]^{-1}$$

$$(4.6)$$

where we have put $\gamma_{A,B}^a = \gamma_{A,B}^b = \gamma_{A,B}$ and $\bar{n}_{A,B}^a = \bar{n}_{A,B}^b = \bar{n}_{A,B}$, from which it may be readily shown that the stationary solution for the density operator is of the form

$$\rho = \exp\left(-\frac{H_{a} + H_{b} + H_{ab}}{kT}\right). \tag{4.7}$$

That is, the system relaxes to the correct steady state corresponding to the full hamiltonian $H_a + H_b + H_{ab}$.

5. A two-level atom coupled to a single electromagnetic field mode

In this section we consider a single two-level atom coupled at resonance to a single mode of the electromagnetic field. The field mode is damped by coupling to a thermal reservoir. This is a nonlinear problem for which the Heisenberg equations of motion (2.11) cannot be solved, hence we shall derive the master equation for the matrix elements of the reduced density operator.

Using the notation of equation (2.1), the system hamiltonian is given by

$$H_{\rm S} = H_{\rm F} + H_{\rm A} + H_{\rm FA} = \hbar\omega_0 a^{\dagger} a + \frac{1}{2}\hbar\omega_0 \sigma_z + \hbar\kappa(a\sigma_+ + a^{\dagger}\sigma_-)$$
(5.1)

where the interaction term H_{FA} is given in the rotating wave approximation. The creation and annihilation operators a^{\dagger} , a for the field mode obey boson commutation relations and the pseudospin operators for the atom obey the anticommutation relations

$$[\sigma_{\pm}, \sigma_{-}]_{\pm} = 1$$

$$[\sigma_{\pm}, \sigma_{z}]_{\pm} = 0.$$
(5.2)

The field mode is damped through coupling to a thermal reservoir

$$H_{\rm FR} = a\Gamma_{\rm R}^{\dagger} + a^{\dagger}\Gamma_{\rm R} \tag{5.3}$$

where the Γ_{R} , Γ_{R}^{\dagger} represent the reservoir operators.

As for the preceding problem the master equation may be obtained directly from equation (2.2), and is given in the Schrödinger picture by

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H_{\rm S}, \rho] + \left(\frac{\partial \rho}{\partial t}\right)_{\rm irrev}$$
(5.4)

where

$$\left(\frac{\partial\rho}{\partial t}\right)_{irrev} = \exp\left(-\frac{iH_s}{\hbar}t\right)\frac{\partial\tilde{\rho}}{\partial t}\exp\left(\frac{iH_s}{\hbar}t\right)$$

$$\frac{\partial\tilde{\rho}}{\partial t} = -\frac{1}{\hbar^2}\int_0^t \operatorname{Tr}_{\mathbf{R}}([V(t), [V(t'), \tilde{\rho}f_0(\mathbf{R})]]) dt'$$

$$(5.5)$$

with

$$V(t) = \exp\left(\frac{i(H_{\rm S} + H_{\rm R})}{\hbar}t\right) H_{\rm FR} \exp\left(-\frac{i(H_{\rm S} + H_{\rm R})}{\hbar}t\right).$$
(5.6)

We cannot obtain the explicit operator form of this equation since the nonlinear Heisenberg equations of motion are not solvable. However, if we adopt the representation defined by the basic kets $|m, \xi\rangle$, where $m = 0, 1, \ldots$ represents the occupation number of the field mode and $\xi = \pm 1$ represents the upper and lower levels of the atom, we are able to derive equations for the matrix elements $\rho_{m,\xi,n,\eta}$ of the reduced density operator via the equation

$$\frac{\partial \rho_{m,\xi,n,\eta}}{\partial t} = \left\langle m, \xi \middle| \left\{ \frac{1}{\mathrm{i}\hbar} [H_{\mathrm{S}}, \rho] + \left(\frac{\partial \rho}{\partial t} \right)_{\mathrm{irrev}} \right\} \middle| n, \eta \right\rangle.$$
(5.7)

For simplicity we only consider the diagonal elements $\rho_{n,+,n,+}$, $\rho_{n+1,-,n+1,-}$ here. Treating the reservoir in standard fashion, all system operators are expanded in terms of their representatives and the orthonormality of the basic vectors used to write the integrand of the irreversible term (5.5) in terms of the factors

$$\left\langle r, \xi \left| \exp \left(\pm \frac{iH_{s}}{\hbar}(t-t') \right) \right| s, \eta \right\rangle$$

If we then make use of the 'transition probabilities' (Jaynes and Cummings 1963)

$$\left\langle r, + \left| \exp\left(\pm \frac{\mathrm{i}H_{\mathrm{s}}}{\hbar}t\right) \right| s, + \right\rangle = \delta_{r,s} \exp\{\pm \mathrm{i}\omega_{0}(r+\frac{1}{2})t\} \cos\kappa(r+1)^{1/2}t$$

$$\left\langle r, - \left| \exp\left(\pm \frac{\mathrm{i}H_{\mathrm{s}}}{\hbar}t\right) \right| s, - \right\rangle = \delta_{r,s} \exp\{\pm \mathrm{i}\omega_{0}(r-\frac{1}{2})t\} \cos\kappa r^{1/2}t$$

$$\left\langle r, + \left| \exp\left(\pm \frac{\mathrm{i}H_{\mathrm{s}}}{\hbar}t\right) \right| s, - \right\rangle = \pm \mathrm{i}\delta_{r,s-1} \exp\{\pm \mathrm{i}\omega_{0}(r+\frac{1}{2})t\} \sin\kappa(r+1)^{1/2}t$$

$$\left\langle r, - \left| \exp\left(\pm \frac{\mathrm{i}H_{\mathrm{s}}}{\hbar}t\right) \right| s, + \right\rangle = \pm \mathrm{i}\delta_{r,s+1} \exp\{\pm \mathrm{i}\omega_{0}(r-\frac{1}{2})t\} \sin\kappa r^{1/2}t$$

we arrive after long and tedious algebraic manipulation at the two equations

$$\frac{\partial \rho_{n,+,n,+}}{\partial t} = -i\kappa(n+1)^{1/2}(\rho_{n+1,-,n,+}+\rho_{n,+,n+1,-}) - \rho_{n,+,n,+}(\gamma_{A}^{(+)}+\delta_{A}^{(+)}+\delta_{B}^{(+)}) -\frac{1}{2}(\rho_{n+1,-,n,+}+\rho_{n,+,n+1,-})(\gamma_{A}^{(-)}+\delta_{A}^{(-)}+\delta_{B}) + \rho_{n+1,+,n+1,+}(\gamma_{B}^{(+)}+\delta_{B}^{(+)}) +\frac{1}{2}(\rho_{n+2,-,n+1,+}+\rho_{n+1,+,n+2,-})(\gamma_{B}^{(-)}+\delta_{B}^{(-)}) + \rho_{n-1,+,n-1,+}\delta_{A}^{(+)} +\frac{1}{2}(\rho_{n,-,n-1,+}+\rho_{n-1,+,n,-})\delta_{A}$$
(5.9)

where

$$\begin{split} \gamma_{A}^{(\pm)} &= \frac{1}{4} (\gamma_{3} \pm \gamma_{4}) \left\{ n^{1/2} (n+1)^{1/2} + n \right\} - \frac{1}{4} (\gamma_{1} \pm \gamma_{2}) \left\{ n^{1/2} (n+1)^{1/2} - n \right\} \\ \gamma_{B}^{(\pm)} &= \frac{1}{4} (\gamma_{7} \pm \gamma_{8}) \left\{ (n+1)^{1/2} (n+2)^{1/2} + (n+1) \right\} - \frac{1}{4} (\gamma_{5} \pm \gamma_{6}) \left\{ (n+1)^{1/2} (n+2)^{1/2} - (n+1) \right\} \\ \delta_{A}^{(\pm)} &= \frac{1}{4} (\gamma_{3} \bar{n}_{3} \pm \gamma_{4} \bar{n}_{4}) \left\{ n^{1/2} (n+1)^{1/2} + n \right\} - \frac{1}{4} (\gamma_{1} \bar{n}_{1} \pm \gamma_{2} \bar{n}_{2}) \left\{ n^{1/2} (n+1)^{1/2} - n \right\} \\ \delta_{B}^{(\pm)} &= \frac{1}{4} (\gamma_{7} \bar{n}_{7} \pm \gamma_{8} \bar{n}_{8}) \left\{ (n+1)^{1/2} (n+2)^{1/2} + (n+1) \right\} \\ &- \frac{1}{4} (\gamma_{5} \bar{n}_{5} \pm \gamma_{6} \bar{n}_{6}) \left\{ (n+1)^{1/2} (n+2)^{1/2} - (n+1) \right\} \\ \delta_{A} &= \frac{1}{4} (\gamma_{3} \bar{n}_{3} - \gamma_{4} \bar{n}_{4}) \left\{ n^{1/2} (n+1)^{1/2} + n \right\} + \frac{1}{4} (\gamma_{1} \bar{n}_{1} - \gamma_{2} \bar{n}_{2}) \left\{ n^{1/2} (n+1)^{1/2} - n \right\} \\ \delta_{B} &= \frac{1}{4} (\gamma_{7} \bar{n}_{7} - \gamma_{8} \bar{n}_{8}) \left\{ (n+1)^{1/2} (n+2)^{1/2} + (n+1) \right\} \\ &+ \frac{1}{4} (\gamma_{5} \bar{n}_{5} - \gamma_{6} \bar{n}_{6}) \left\{ (n+1)^{1/2} (n+2)^{1/2} - (n+1) \right\} \end{split}$$

with

$$\gamma_{i} = 2\pi g(\omega_{j}) |\kappa(\omega_{j})|^{2} \Big|_{\omega_{j} = \omega_{i}} \qquad i = 1, \dots, 8$$

$$\bar{n}_{i} = \bar{n}(\omega_{j}) \Big|_{\omega_{j} = \omega_{i}} \qquad (5.11)$$

and

$$\omega_{1,2} = \omega_0 \pm \kappa ((n+1)^{1/2} + n^{1/2})$$

$$\omega_{3,4} = \omega_0 \pm \kappa ((n+1)^{1/2} - n^{1/2})$$

$$\omega_{5,6} = \omega_0 \pm \kappa ((n+2)^{1/2} + (n+1)^{1/2})$$

$$\omega_{7,8} = \omega_0 \pm \kappa ((n+2)^{1/2} - (n+1)^{1/2}),$$
(5.12)

and

$$\frac{\partial \rho_{n+1,-,n+1,-}}{\partial t} = -i\kappa(n+1)^{1/2}(\rho_{n,+,n+1,-}-\rho_{n+1,-,n,+}) - \rho_{n+1,-,n+1,-}(\Gamma_{A}^{(+)} + \Delta_{A}^{(+)} + \Delta_{B}^{(+)})
- \frac{1}{2}(\rho_{n,+,n+1,-} + \rho_{n+1,-,n,+})(\Gamma_{A}^{(-)} + \Delta_{A}^{(-)} + \Delta_{B}) + \rho_{n+2,-,n+2,-}(\Gamma_{B}^{(+)} + \Delta_{B}^{(+)})
+ \frac{1}{2}(\rho_{n+1,+,n+2,-} + \rho_{n+2,-,n+1,+})(\Gamma_{B}^{(-)} + \Delta_{B}^{(-)}) + \rho_{n,\cdots,n,-}\Delta_{A}^{(+)}
+ \frac{1}{2}(\rho_{n-1,+,n,-} + \rho_{n,-,n-1,+})\Delta_{A}$$
(5.13)

where

$$\begin{split} \Gamma_{A}^{(\pm)} &= \frac{1}{4} (\gamma_{3} \pm \gamma_{4}) \{ (n+1) + n^{1/2} (n+1)^{1/2} \} + \frac{1}{4} (\gamma_{1} \pm \gamma_{2}) \{ (n+1) - n^{1/2} (n+1)^{1/2} \} \\ \Gamma_{B}^{(\pm)} &= \frac{1}{4} (\gamma_{7} \pm \gamma_{8}) \{ (n+2) + (n+1)^{1/2} (n+2)^{1/2} \} + \frac{1}{4} (\gamma_{5} \pm \gamma_{6}) \{ (n+2) - (n+1)^{1/2} (n+2)^{1/2} \} \\ \Delta_{A}^{(\pm)} &= \frac{1}{4} (\gamma_{3} \bar{n}_{3} \pm \gamma_{4} \bar{n}_{4}) \{ (n+1) + n^{1/2} (n+1)^{1/2} \} + \frac{1}{4} (\gamma_{1} \bar{n}_{1} \pm \gamma_{2} \bar{n}_{2}) \{ (n+1) - n^{1/2} (n+1)^{1/2} \} \\ \Delta_{B}^{(\pm)} &= \frac{1}{4} (\gamma_{7} \bar{n}_{7} \pm \gamma_{8} \bar{n}_{8}) \{ (n+2) + (n+1)^{1/2} (n+2)^{1/2} \} \\ + \frac{1}{4} (\gamma_{5} \bar{n}_{5} \pm \gamma_{6} \bar{n}_{6}) \{ (n+2) - (n+1)^{1/2} (n+2)^{1/2} \} \\ \Delta_{A} &= \frac{1}{4} (\gamma_{3} \bar{n}_{3} - \gamma_{4} \bar{n}_{4}) \{ (n+1) + n^{1/2} (n+1)^{1/2} \} - \frac{1}{4} (\gamma_{1} \bar{n}_{1} - \gamma_{2} \bar{n}_{2}) \{ (n+1) - n^{1/2} (n+1)^{1/2} \} \\ \Delta_{B} &= \frac{1}{4} (\gamma_{7} \bar{n}_{7} - \gamma_{8} \bar{n}_{8}) \{ (n+2) + (n+1)^{1/2} (n+2)^{1/2} \} \\ - \frac{1}{4} (\gamma_{5} \bar{n}_{5} - \gamma_{6} \bar{n}_{6}) \{ (n+2) - (n+1)^{1/2} (n+2)^{1/2} \} . \end{split}$$

The first term on the right-hand side of each of these equations describes the reversible motion of the system, the remaining terms the irreversible motion.

It is easily seen that in the weak-coupling limit $\kappa \to 0$, both the above equations reduce to

$$\frac{\partial \rho_{n,n}}{\partial t} = -\gamma \{ n\rho_{n,n} - (n+1)\rho_{n+1,n+1} \} - \gamma \bar{n} \{ (2n+1)\rho_{n,n} - (n+1)\rho_{n+1,n+1} - n\rho_{n-1,n-1} \}$$
(5.15)

where

$$\gamma = 2\pi g(\omega_j) |\kappa(\omega_j)|^2 \Big|_{\omega_j = \omega_0}$$

$$\bar{n} = \bar{n}(\omega_j) \Big|_{\omega_j = \omega_0}$$
(5.16)

which is the equation for an uncoupled damped field mode and the expression obtained for the irreversible term if the factorization ansatz is used. Apart from the modifications to the drift coefficients $\gamma_{A,B}^{(+)}$, $\Gamma_{A,B}^{(+)}$ and the diffusion coefficients $\delta_{A,B}^{(+)}$, $\Delta_{A,B}^{(+)}$ appearing in equations (5.8) and (5.12), the difference between the irreversible terms of our new equations and equation (5.15) lies in the prediction of a dependence of the diagonal elements on the nondiagonal elements. These nondiagonal elements are related to the atomic transition probabilities, and this dependence arises out of the atomic transitions involved in the crosscoupling of the atom to the reservoir. This destroys the property of the usual Pauli-type master equation where diagonal matrix elements are coupled only to diagonal matrix elements. The nondiagonal terms are only important for the matrix elements corresponding to low-field mode population, for example, spontaneous emission, since for large n

$$\gamma_{A,B}^{(-)} = \delta_{A,B}^{(-)} = \delta_{A,B} = 0$$
 and $\Gamma_{A,B}^{(-)} = \Delta_{A,B}^{(-)} = \Delta_{A,B} = 0$

and the irreversible part of both equations reduces to that obtained using the factorization ansatz.

As with the previous example, under the assumption of a nearly flat frequency spectrum all the γ_i (5.10) differ little except for large κ , and hence

$$\gamma_{\mathbf{A},\mathbf{B}}^{(-)} = \Gamma_{\mathbf{A},\mathbf{B}}^{(-)} \simeq 0$$
 (5.17)

and

$$\gamma_{\mathbf{A}}^{(+)} \simeq \gamma_{n}$$

$$\gamma_{\mathbf{B}}^{(+)} \simeq \gamma(n+1) \simeq \Gamma_{\mathbf{A}}^{(+)}$$
(5.18)
$$\Gamma_{\mathbf{B}}^{(+)} \simeq \gamma(n+2).$$

The main effect arises in the diffusion terms when the resonant energy $\hbar\omega_0$ is of the order of the thermal energy kT of the reservoir.

6. Conclusions

We have derived a master equation for dissipating coupled systems which includes the coupling to all orders in the irreversible part of the master equation. This is shown to remove certain deficiencies contained in the usual derivation of the master equation for coupled systems. In particular our master equation satisfies detailed balance and yields the correct canonical form for the steady-state density operator. Future applications of this technique include a derivation of the laser master equation without employing the usual factorization ansatz between atoms and field in deriving the irreversible part of the master equation.

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Appendix

We consider two coupled harmonic oscillators a and b and for simplicity consider only one of these oscillators to be coupled to a heat bath consisting of an infinite number of harmonic oscillators $\{r_i\}$. The total hamiltonian is then

$$H = \hbar \omega a^{\dagger} a + \hbar \omega b^{\dagger} b + \hbar \kappa (a^{\dagger} b + a b^{\dagger}) + \hbar \sum_{j} \omega_{j} r_{j}^{\dagger} r_{j} + \hbar \sum_{j} g_{j} b r_{j}^{\dagger} + \hbar \sum_{j} g_{j}^{*} b^{\dagger} r_{j}$$
(A.1)

where κ and g_j are coupling constants and the operators a, b and $\{r_j\}$ all obey boson commutation relations.

The Heisenberg equations of motion derived from the above hamiltonian are

$$\frac{da}{dt} = -i\omega a - i\kappa b$$

$$\frac{db}{dt} = -i\omega b - i\kappa a - i\sum_{j} g_{j}r_{j}$$

$$\frac{dr_{j}}{dt} = -i\omega_{j}r_{j} - ig_{j}^{*}b.$$
(A.2)

Taking the Laplace transforms of the above equations we obtain

$$(s + i\omega)\overline{a}(s) = a - i\kappa\overline{b}(s)$$

$$(s + i\omega)\overline{b}(s) = b - i\kappa\overline{a}(s) - i\sum_{j} g_{j}\overline{r}_{j}(s)$$

$$(s + i\omega_{j})\overline{r}_{j}(s) = r_{j} - ig_{j}^{*}\overline{b}(s)$$
(A.3)

where

$$\bar{o}(s) = \int_0^\infty e^{-st} o(t) \, \mathrm{d}t$$

and o is the operator in the Schrödinger picture at t = 0. The solution to these equations for $\bar{a}(s)$ and $\bar{b}(s)$ may be derived in approximate form using a Wigner-Weiskopff type method (see Louisell 1964)

$$\bar{a}(s) = \left(s + i\omega + \frac{|\kappa|^2}{s + i\omega + (\Sigma_j |g_j|^2)/(s + i\omega_j)}\right)^{-1} \times \left(a - \frac{i\kappa b}{s + i\omega + (\Sigma_j |g_j|^2)/(s + i\omega_j)} - \frac{\kappa \sum_j g_j r_j}{(s + i\omega_j)(s + i\omega + (\Sigma_j |g_j|^2)/(s + i\omega_j)}\right)$$
(A.4)
$$\bar{b}(s) = \left(s + i\omega + \sum_j \frac{|g_j|^2}{s + i\omega_j} + \frac{|\kappa|^2}{s + i\omega}\right)^{-1} \left(b - \frac{i\kappa a}{s + i\omega} - i\sum_j \frac{g_j r_j}{s + i\omega_j}\right).$$
(A.5)

The inverse transform of these equations may readily be shown to be

$$a(t) e^{i\omega t} = \frac{\exp(-\frac{1}{4}\gamma t)}{\lambda} \{ (\lambda \cos \lambda t - \frac{1}{4}\gamma \sin \lambda t)a - i\kappa \sin \lambda tb \} \\ \times \frac{-\kappa \sum_{j} g_{j}r_{j}}{(\frac{1}{4}\gamma - i\Delta_{j})^{2} + \lambda^{2}} \left\{ \exp(-i\Delta_{j}t) + \exp(-\frac{1}{4}\gamma t) \left(\cos \lambda t - (\frac{1}{4}\gamma - i\Delta_{j})\frac{\sin \lambda t}{\lambda} \right) \right\} (A.6) \\ b(t) e^{i\omega t} = \frac{\exp(-\frac{1}{4}\gamma t)}{\lambda} \{ (\lambda \cos \lambda t - \frac{1}{4}\gamma \sin \lambda t)b - i\kappa \sin \lambda ta \} \\ -i\sum_{j} g_{j}r_{j} \left[-\frac{i\Delta_{j}}{(\frac{1}{4}\gamma - i\Delta_{j})^{2} + \lambda^{2}} \exp(-i\Delta_{j}t) + \exp(-\frac{1}{4}\gamma t) \left\{ \frac{i\Delta_{j}}{(\frac{1}{4}\gamma - i\Delta_{j})^{2} + \lambda^{2}} \cos \lambda t + \frac{1}{\lambda} \left(1 + \frac{i\Delta_{j}(\frac{1}{4}\gamma - i\Delta_{j})}{(\frac{1}{4}\gamma - i\Delta_{j})^{2} + \lambda^{2}} \right) \sin \lambda t \right\} \right] (A.7)$$

where

$$\lambda = \{\kappa^2 - (\frac{1}{4}\gamma)^2\}^{1/2}, \qquad \Delta_j = \omega_j - \omega$$

and

$$\gamma = 2\pi |g_k|^2 \rho(\omega_k) \bigg|_{\omega_k = \omega}$$

where $\rho(\omega_k)$ is the mode density of the bath oscillators, and we have neglected the small frequency shift terms

$$\Delta \omega = -\mathscr{P}\left(\int_{-\infty}^{\infty} \frac{|g_k|^2 \rho(\omega_k)}{\omega_k - \omega} d\omega_k\right).$$

T

In both these solutions the part involving the operators a and b corresponds exactly to the classical solution for one damped oscillator coupled to an undamped oscillator. However, both solutions a(t) and b(t) contain a dependence on the bath operators r_j . This is necessary in a quantum-mechanical calculation to preserve the canonical commutation relations. The oscillator b which is coupled directly to the bath has a coupling constant with the bath operators proportional to g_j . The oscillator a which is not coupled directly to the heat bath contains a second order dependence on the heat bath operators proportional to κg_i .

As $t \to \infty$ both oscillators decay exponentially into the heat bath, the exponential decay being modulated by the factors $e^{\pm i\lambda t}$. For $\frac{1}{4}\gamma > \kappa$ this damped oscillation becomes pure damping, that is, the system is overdamped. The interdependence of all the interacting components readily apparent in the operator solutions clearly illustrates the weakness of the factorization ansatz in the derivation of the master equation.

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