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## Master equation derivation of quantum regression theorem

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**Abstract.** The master equation approach is used to relate the calculation of correlation functions to the calculation of single-time expectation values. The quantum regression theorem is shown to result on neglecting a certain term. The properties of this neglected term are briefly discussed.

In the calculation of averages of products of operators at two different times (correlation functions) in non-equilibrium situations, the quantum regression theorem plays an important role (Lax 1963, 1968, Haken and Wiedlich 1967, and the references quoted therein). It was much used in the development of the theory of resonance fluorescence (Mollow 1969) and recently it was assumed in the master equation treatment of the interaction of quantum systems with stochastic perturbations (Agarwal 1979). Particular derivations for resonance fluorescence have been given by Mollow (1975a, b). In this paper we adopt a more general master equation approach and derive not only the quantum regression theorem but the corrections to it. These are briefly discussed. The basic idea of the quantum regression theorem is as follows. The correlation function  $\langle A(t')B(t) \rangle$ , where  $A$  and  $B$  are quantum mechanical operators and  $\langle \dots \rangle$  denotes the expectation value, may be written

$$\langle A(t')B(t) \rangle \equiv \text{Tr}[\rho(0)A(t')B(t)] = \text{Tr}[\Omega(t, t')B] \quad (1)$$

where

$$\Omega(t, t') \equiv U(t, t')[\rho(t')A]U^{-1}(t, t'), \quad (2)$$

$$A(t) = U^{-1}(t, 0)AU(t, 0), \quad (3)$$

$$\rho(t) = U(t, 0)\rho(0)U^{-1}(t, 0), \quad (4)$$

$\rho(t)$  being the density matrix at time  $t$  and  $U(t, t')$  being the time development operator

$$U(t, t') = \exp[-iH(t-t')]. \quad (5)$$

$H$  is the full Hamiltonian of the system, assumed to be time independent. Expression (1) is analogous to the expression for single-time expectation values,

$$\langle B(t) \rangle = \text{Tr}[\rho(t)B] \quad (6)$$

with  $\rho(t)$  replaced by  $\Omega(t, t')$ . Furthermore, it is obvious from (2) and (4) that  $\rho(t)$  and  $\Omega(t, t')$ , regarded as functions of  $t$ , satisfy the same differential equation:

$$dx/dt = [H, x], \quad x = \rho, \Omega. \quad (7)$$

Thus if the equations of motion for the density matrix can be solved, then  $\Omega(t, t')$  can also be found, and two-time averages may be obtained from single-time averages. (For an example of the application of the theorem, see Mollow (1969).)

Actually, the situation in practice is more complicated than this, because it is usually possible to split the whole system into a sub-system of interest (called henceforth simply the 'system', S) and a sub-system of secondary interest (the 'reservoir', R) with a corresponding decomposition of the Hamiltonian

$$H = (H_S + H_R) + H_{SR} \equiv H_0 + H_1, \tag{8}$$

$H_1 \equiv H_{SR}$  being the interaction between the system and the reservoir. It is then more convenient to work with the reduced density matrix for the system alone,  $\rho_S$ :

$$\rho_S \equiv \text{Tr}_R(\rho), \quad \rho_R \equiv \text{Tr}_S(\rho), \tag{9}$$

where  $\text{Tr}_R$  denotes a trace over the variables of the reservoir and  $\text{Tr}_S$  a trace over the system variables. One cannot use the arguments of the second paragraph because  $\rho_S$  does not satisfy an equation of the form (7).

To find the equations satisfied by  $\rho_S(t)$  we briefly summarise the arguments of Zwanzig (1964). We introduce the projection operator,

$$\mathcal{P} \equiv \rho_R(0) \text{Tr}_R \tag{10}$$

and the quantities  $\rho_1$  and  $\rho_2$  obtained from  $\rho$  as follows:

$$\rho_1 \equiv \mathcal{P}\rho, \quad \rho_2 \equiv (1 - \mathcal{P})\rho. \tag{11}$$

$\rho_S(t)$  may be obtained from  $\rho_1(t)$  simply by tracing it over R:  $\rho_S(t) = \text{Tr}_R \rho_1(t)$ . The Laplace transform,  $\rho(z)$ , of  $\rho(t)$ , defined by

$$\rho(z) = \int_0^\infty e^{-zt} \rho(t) dz, \tag{12}$$

satisfies the Laplace transform of equation (7):

$$z\rho(z) - \rho(0) = -i\mathcal{L}\rho \tag{13}$$

where  $\mathcal{L}\rho \equiv H\rho - \rho H$  defines the Liouvillean operator  $\mathcal{L}$ . By acting on equation (13) with  $\mathcal{P}$  and  $1 - \mathcal{P}$  one obtains the equations

$$z\rho_1(z) - \rho_1(0) = -i\mathcal{P}\mathcal{L}\rho_1(z) - i\mathcal{P}\mathcal{L}\rho_2(z), \tag{14}$$

$$z\rho_2(z) - \rho_2(0) = -i(1 - \mathcal{P})\mathcal{L}\rho_1(z) - i(1 - \mathcal{P})\mathcal{L}\rho_2(z), \tag{15}$$

which have the formal solution

$$\left( z + i\mathcal{P}\mathcal{L} + \mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} (1 - \mathcal{P})\mathcal{L} \right) \rho_1(z) = \rho_1(0) - i\mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} \rho_2(0). \tag{16}$$

On tracing this equation over R one obtains the equation satisfied by  $\rho_S$ .

It is natural and customary to assume that if the interaction is 'switched on' at  $t = 0$  the initial density matrix  $\rho(0)$  factorises:

$$\rho(0) = \rho_S(0) \times \rho_R(0); \tag{17}$$

it then follows that  $\rho_2(0) = 0$ , since

$$\rho_2(0) = (1 - \mathcal{P})\rho(0) = \rho(0) - \rho_R(0)\rho_S(0) = 0. \tag{18}$$

Thus the final term in equation (16) vanishes, and we obtain

$$\left( z + i\mathcal{P}\mathcal{L} + \mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} (1 - \mathcal{P})\mathcal{L} \right) \rho_1(z) = \rho_1(0). \tag{19}$$

This is the desired equation for  $\rho_1(z)$ . For examples of its use see e.g. Swain (1980).

Assuming that  $A$  and  $B$  are system operators only (this is natural as we have assumed  $S$  is the sub-system of principal interest) and noting that  $\text{Tr} \equiv \text{Tr}_R \text{Tr}_S$ , one may write (6) and (1) as

$$\langle B(t) \rangle = \text{Tr}_S[(\text{Tr}_R \rho_1(t))B], \tag{20}$$

$$\langle A(t')B(t) \rangle = \text{Tr}_S[(\text{Tr}_R \Omega_1(t, t'))B], \tag{21}$$

where  $\Omega_1(t, t')$  is defined analogously to  $\rho_1(t)$ :  $\Omega_1 \equiv \mathcal{P}\Omega$ .

To be definite, we assume that we are interested in evaluating the correlation function  $\langle A(t')B(t) \rangle$  for the case  $t \geq t'$ . Then we assume

$$\Omega(t, t') = 0 \quad \text{for } t < t'. \tag{22}$$

One may then define the Laplace transform  $\Omega(z, t)$  analogously to equation (12), and repeat the steps leading to equation (16), when we obtain

$$\left( z + i\mathcal{P}\mathcal{L} + \mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} (1 - \mathcal{P})\mathcal{L} \right) \Omega_1(z, t) = \Omega_1(t', t') + \Phi(z, t) \tag{23}$$

where

$$\begin{aligned} \Phi(z, t) &= -i\mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} \Omega_2(t', t') \\ &= -i\mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} [\rho(t') - \rho_R(0)\rho_S(t')]A. \end{aligned} \tag{24}$$

Thus  $\Omega(z, t)$  satisfies equation (23), which is formally identical to equation (19), *apart from the final term*,  $\Phi(z, t)$ . This term represents a driving force due to the perturbation of the reservoir by the system. When it can be neglected, the quantum regression theorem holds.

We make the following comments.

(1) Equation (23) is an exact relation: it is not necessary to invoke either the Born or Markov approximations or to make any assumptions about the form of the Hamiltonian (apart from time independence).

(2)  $\Phi(z, t)$  represents the difference of the expectation value of an operator taken with the exact density matrix  $\rho(t')$  and the 'approximate' density matrix  $\rho_R(0)\rho_S(t')$ . One therefore expects it to be small. In fact, Mollow (1969) in his original treatment of resonance fluorescence obtained the quantum regression theorem by assuming that the composite density matrix factorises for all time and that, when calculating system averages, the effect of the system on the reservoir density matrix is negligible. (Later papers (Mollow 1975a, b) gave a justification of this procedure for resonance fluorescence.) These assumptions are equivalent to taking

$$\rho(t') = \rho_R(0)\rho_S(t'), \quad \text{all } t', \tag{25}$$

and it is evident from equation (24) that this is sufficient to cause the vanishing of  $\Phi(z, t)$ .

(3) One can use equation (15) to set

$$\rho_2(z) = -i[z + i(1 - \mathcal{P})\mathcal{L}]^{-1} \mathcal{P}\mathcal{L}\rho_1(z). \quad (26)$$

Inverting this, one obtains

$$\rho_2(t') = -i \int_0^{t'} d\tau e^{-i(1-\mathcal{P})\mathcal{L}\tau} \mathcal{P}\mathcal{L}\rho_1(t-\tau) \quad (27)$$

and thus one can express  $\Phi(z, t')$  in terms of  $\rho_S(t)$ , the system density matrix:

$$\Phi(t', z) = -\mathcal{P}\mathcal{L} \frac{1}{z + i(1 - \mathcal{P})\mathcal{L}} \int_0^{t'} d\tau e^{-i(1-\mathcal{P})\mathcal{L}\tau} \mathcal{P}\mathcal{L}\rho_R(0)\rho_S(t' - \tau), \quad (28)$$

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