Formal Theory of Quantum Fluctuations from a Driven State*

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A formal apparatus is developed for dealing with quantum fluctuations in a driven (nonequilibrium) state. Phenomenological equations for the decay of the system from an arbitrary state to the driven state are presumed known. By assuming that at some initial time the system-reservoir density matrix can be factored, we establish that the spectrum of fluctuations is given by the Fourier transform of the solution of the phenomenological equations, i.e., the regression of fluctuations obey the "macroscopic" equations of motion even in the nonequilibrium case.

1. INTRODUCTION

WE have previously given an extensive classical discussion of the calculation of the spectrum of fluctuations from a steady nonequilibrium state.[1] In the present paper, we shall develop a natural extension of the previous method to quantum-mechanical systems. As before, our approach is "macroscopic" in the sense that we do not require a *complete* description, but shall assume that the future is determined by the presence of a suitably chosen set of variables (the Markoffian assumption). Microscopic approaches[2] have been used to provide rigorous proofs of *relationships* between noise and admittance, e.g., the Nyquist theorem, but an actual calculation of either quantity usually requires the development of a Markoffian approximation, e.g., a Boltzmann equation.

Our problem may be described abstractly as follows: We have a system interacting with a reservoir. The system-reservoir interaction causes the motion of the system to be damped, and introduces *fluctuations* into the system. The division into system plus reservoir is to be so chosen that all strong couplings are included within the system. Specifically, the system must be sufficiently large that the Dirac density matrix[3] of the system constitutes a set of Markoffian variables, i.e., the future of the density matrix elements must be predictable from their present values without specific knowledge of the reservoir density matrix. We assume, in short, that a set of "phenomenological" equations exist for the motion of the system. These could, for example, be derived by the methods of Bloch and Wangsness[4,5] in which system reservoir correlations are included in solving the dynamical equations that carry the system from time t to $t+\Delta t$ but are neglected at the initial time t.

For purposes of visualization, we may consider a localized electron in a crystal, in a paramagnetic resonance experiment. The spin states of the electron, and the electromagnetic field may be regarded as our system. Other spins and lattice vibrations provide the reservoir. It would be more precise for this problem (and absolutely necessary in a ferromagnetic resonance) to include all the spins as part of the system, leaving only the lattice vibrations as reservoir. As one makes the system more inclusive, the calculation becomes more rigorous but less tractable. In the limit, as the system becomes all inclusive, our methods become "microscopic" and our results rigorously correct, but only of formal value.

The first microscopic, quantum-mechanical treatment of driven systems has been given by Bernard and Callen.[6] Their treatment is limited to sufficiently weak driving fields that the system is only slightly off equilibrium, and perturbation methods are applicable. They obtain formal theorems relating the first- and second-order driven noise to third- and higher-order time-displaced correlation functions in the equilibrium state. There is as yet, however, no practical method of evaluating such higher moments.

By way of contrast, the discussion of noise in strongly driven quantum-mechanical systems, e.g., masers, is usually of a heuristic nature, or one which neglects off-diagonal elements of the density matrix.[7] We may, therefore, be forgiven if in this first systematic treatment we make the Bloch-Wangsness approximation of assuming that the density matrix of the system plus reservoir can be *factored* into system and reservoir matrices (at time t but not for the dynamics between t and $t+\Delta t$). The system can then be driven strongly. The motion of the reservoir is, in this approximation, uncorrelated with the system, although it is not necessarily at equilibrium, e.g., the effective temperature of the reservoir could be raised due to heating by the system. If the system is subject to alternating forces (as in a maser pump) the reservoir could have Fourier components at the pump frequency. [See Eq. (5.20).]

In a given physical situation, the factorization error can be made sufficiently small by making the system

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[1] M. Lax, Rev. Mod. Phys. 32, 25 (1960).

[2] H. B. Callen and T. A. Welton, Phys. Rev. 83, 34 (1951); R. Kubo, J. Phys. Soc. Japan 12, 570 (1957); M. Lax, Phys. Rev. 109, 1921 (1958), and other references given in reference 1.

[3] D. ter Haar, *Reports on Progress in Physics* (The Physical Society, London, 1961), Vol. 24, p. 304, and references therein.

[4] R. K. Wangsness and F. Bloch, Phys. Rev. 89, 728 (1953).

[5] F. Bloch, Phys. Rev. 102, 104 (1956); 105, 1206 (1957).

[6] W. Bernard and H. B. Callen, Rev. Mod. Phys. 31, 1017 (1959).

[7] For a review of maser noise work see J. Weber, Rev. Mod. Phys. 31, 681 (1959).

large enough to include all elements strongly affected by the driving force. A second approach would be to take account of the local perturbation of the reservoir by the system to first order. We postpone the latter procedure to a later discussion since it would also require a modification of the Bloch-Wangsness phenomenological equations.[4,5]

It may be of interest here to compare the assumptions made in this paper with our previous classical treatment of driven systems.[1]

1. We assume, as before, that the system is Markoffian.

2. This Markoffian character is assumed to arise because of a sufficiently weak coupling to a reservoir to permit factorization. The results, however, conceivably have a greater range of validity than required by this assumption. In the classical case, the reservoir is not explicitly mentioned, but in effect an equivalent assumption is tacitly made.

3. The assumption of stationarity made classically is now omitted since we wish to discuss systems driven by alternating driving forces. It would not be difficult to eliminate this assumption in the classical case by the methods developed here.

4. In the classical case, the assumption of quasilinearity was eliminated by introducing a discussion of distribution functions. In the quantum-mechanical case, our discussion is based on the density matrix and the equations are automatically linear.

Our principal result, Eq. (5.19), is that *even in the nonequilibrium case the regression of fluctuations obey the macroscopic equations of motion.* This result was first assumed by Onsager[8] in dealing with the equilibrium case. We have previously remarked[1] that this result should follow for any *Markoffian* system. The Nyquist theorem must, however, be modified since the fluctuations at *one* time are disturbed by the driving forces.[1]

It may be emphasized here that *only one approximation* is made in the entire paper—Eq. (5.18) or Eq. (5.20)—and it is this approximation that guarantees the desired Markoffian character of the system density matrix.

2. NOISE IN NONSTATIONARY SYSTEMS

If $\alpha(t)=I(t)-\langle I(t)\rangle$ represents a fluctuation in the variable I, the noise at frequency $f=(\omega/2\pi)$ for a stationary classical random variable is usually defined by[1]

$$G(f)=\lim_{T\to\infty}\frac{2}{T}\left|\int_0^T e^{-i\omega t}\alpha(t)dt\right|^2, \tag{2.1}$$

which, for sufficiently large T can be rewritten as

$$\begin{aligned}G(t)&=\frac{2}{T}\int_0^T dt\int_{-\infty}^{\infty}e^{-i\omega\tau}\langle\alpha(t+\tau)\alpha(t)\rangle d\tau\\&=2\int_{-\infty}^{\infty}e^{-i\omega\tau}\overline{\langle\alpha(t+\tau)\alpha(t)\rangle}d\tau,\end{aligned} \tag{2.2}$$

where $\langle\ \rangle$ represent an ensemble average, and the upper bar represents a time average.

For a nonstationary system the noise itself fluctuates in time and one would like to define a noise $G(f,t)$ at frequency f and time t. Even in classical systems, this is prevented by the Fourier relation between time and frequency dependence, which creates an analog of the Heisenberg uncertainty principle. One cannot measure frequency and time simultaneously with absolute precision, but only subject to errors obeying the uncertainty principle:

$$\Delta\omega\Delta t\gtrsim 1/2. \tag{2.3}$$

As a consequence, there is no unique function $G(f,t)$, but there is a variety of possible definitions which can differ from one another in detail, but presumably agree if one asks for the noise in a frequency$\times$time interval large compared to unity. One such definition suggested by Eq. (2.2) is

$$G(f,t)=2\int_{-\infty}^{\infty}\exp(-i\omega\tau)\langle\alpha(t+\tau)\alpha(t)\rangle d\tau, \tag{2.4}$$

which has the desirable characteristics

$$G(f)=\overline{G(f,t)}, \tag{2.5}$$

$$\begin{aligned}\langle[\alpha(t)]^2\rangle&=\frac{1}{2}\int_{-\infty}^{\infty}G(f,t)df\\&=\int_0^{\infty}\tfrac{1}{2}[G(f,t)+G(-f,t)]df;\end{aligned} \tag{2.6}$$

i.e., the fluctuations at a given frequency (time) can be obtained by integrating $G(f,t)$ over time (frequency).

A similar nonuniqueness difficulty occurs in defining a phase-space function $G(p,q)$ in quantum mechanics, since position q and momentum p obey a Heisenberg uncertainty principle. This problem is discussed by Wigner and Moyal.[9] They make a choice for the phase-space problem which for our frequency time space is equivalent to the "symmetrical" choice:

$$G(f,t)=2\int_{-\infty}^{\infty}\exp(-i\omega\tau)\langle\alpha(t+\tfrac{1}{2}\tau)\alpha(t-\tfrac{1}{2}\tau)\rangle d\tau. \tag{2.7}$$

For the stationary case there is no distinction between Eqs. (2.6) and (2.7), and furthermore, both then yield

[8] L. Onsager, Phys. Rev. **37**, 405 (1931); **38**, 2265 (1931). For a recent critical discussion of the Onsager regression hypothesis see A. Shimony, thesis, Princeton University, 1962 (unpublished).

[9] E. Wigner, Phys. Rev. **40**, 749 (1932); J. E. Moyal, Proc. Cambridge Phil. Soc. **45**, 99 (1949).

results independent of time and equivalent to the usual definition, Eq. (2.2).

All of the above-mentioned alternatives, including the results of any physical measurement through a filter system, can be expressed as a suitable integral of the form

$$G=\int\int K(t,t')\langle\alpha(t)\alpha(t')\rangle dtdt', \tag{2.8}$$

although for Eq. (2.2) one might need to take the limit as $T\to\infty$ after using a $K(t,t',T)$. A definition of noise suitable for quantum mechanics[10] replaces $\alpha(t)\alpha(t')$ by the Hermitian operator

$$\alpha(t)\alpha(t')\to\tfrac{1}{2}[\alpha(t)\alpha(t')+\alpha(t')\alpha(t)], \tag{2.9}$$

i.e., the anticommutator; whereas, the linear response of the system to an external driving force involves commutators.[2] All of the desired results can, therefore, be obtained from a computation of $\langle\alpha(t)\alpha(t')\rangle$ or, more generally, of $\langle\alpha^\mu(t)\alpha^\nu(t')\rangle$. The succeeding sections are devoted, therefore, to a study of such correlation functions.

3. AN INTUITIVE TREATMENT OF DENSITY MATRIX FLUCTUATIONS

In this section, we present an elementary but unconventional treatment of fluctuations in quantum-mechanical systems. The treatment is unconventional because we regard the fluctuations as taking place not in the variables, but in the density matrix. The latter, as customarily defined, is already an ensemble average, and does not fluctuate. Let us use $\sigma_{ij}(t)$ to denote the conventional density matrix of the system for states i and j, and $\boldsymbol{\sigma}_{ij}(t)$ the corresponding operator random variable, whose quantum expectation takes a different value for each member of the ensemble of systems. The mean value of any observable I with the matrix elements I_{ij} in some representation of the system, can be written at time t as

$$\langle I(t)\rangle=\mathrm{Tr}[I\sigma(t)]=\sum I_{ij}\sigma_{ji}(t) \tag{3.1}$$

and a fluctuation from this mean value can be written as

$$\alpha(t)=I(t)-\langle I(t)\rangle=\sum I_{ij}\Delta\boldsymbol{\sigma}_{ji}(t), \tag{3.2}$$

where

$$\Delta\boldsymbol{\sigma}_{ji}(t)=\boldsymbol{\sigma}_{ji}(t)-\sigma_{ji}(t) \tag{3.3}$$

represents a fluctuation of the density matrix operator from its mean value. The noise can then be expressed via Eqs. (2.4)–(2.8) in terms of

$$\langle\alpha(t)\alpha(t')\rangle=\sum I_{ij}I_{kl}\langle\Delta\boldsymbol{\sigma}_{ji}(t)\Delta\boldsymbol{\sigma}_{lk}(t')\rangle. \tag{3.4}$$

As in Eqs. (2.12)–(2.14) of our classical treatment[1] the mean in Eq. (3.4) may be taken in two steps. First, one takes the mean of the $\Delta\boldsymbol{\sigma}$ at the later time subject to the condition that the $\Delta\boldsymbol{\sigma}$'s at the earlier time are known. Thus, for $t>t'$, we can write

$$\langle\Delta\boldsymbol{\sigma}_{ji}(t)\rangle_{\sigma(t')}=\sum O_{qp}{}^{ji}(t,t')\Delta\boldsymbol{\sigma}_{qp}(t') \tag{3.5}$$

where $O_{qp}{}^{ji}(t,t')$ can be obtained by solving the phenomenological equations for $\Delta\boldsymbol{\sigma}$ (which will be identical to those for $\boldsymbol{\sigma}$ in a linear problem). We shall not enter here upon a discussion of the derivation of the phenomenological equations. We only remark that the work of Bloch and Wangsness leads one to expect that the phenomenological equations take the form

$$d\sigma_{ji}/dt+i\sum_k(E_{jk}\sigma_{ki}-\sigma_{jk}E_{ki})=-\Gamma_{ji;nm}\sigma_{nm}, \tag{3.6}$$

where the E_{jk} represents the matrix elements of the system energy (possibly modified by second-order "Lamb" shifts produced by the reservoir) and the Γ's are damping terms produced by the reservoir. In the stationary case, the E's and Γ's are independent of time and the solution of the initial value problem has the property of invariance under a time displacement:

$$O_{qp}{}^{ji}(t,t')=O_{qp}{}^{ji}(t-t'), \tag{3.7}$$

but when periodic or more generally time-dependent forces are present, this invariance is lost.

Actually, for our purposes, we do not even need to require that the equation for the O's takes the linear form, Eq. (3.6). All that is necessary for the validity of Eq. (3.5) is that the phenomenological equation for the O's be linearizable about the driven state, so that the fluctuations $\Delta\boldsymbol{\sigma}$ from the driven state obey linear equations.

Equations (3.4) and (3.5) yield

$$\langle\alpha(t)\alpha(t')\rangle=\sum I_{ij}I_{kl}O_{qp}{}^{ji}(t,t')\langle\Delta\boldsymbol{\sigma}_{qp}(t')\Delta\boldsymbol{\sigma}_{lk}(t')\rangle \tag{3.8}$$

for $t>t'$. For $t<t'$, we interchange the dummy indices (ji) with (lk) and make use of Eq. (3.5) with t and t' interchanged:

$$\langle\alpha(t)\alpha(t')\rangle=\sum I_{ij}I_{kl}O_{qp}{}^{ji}(t',t)\langle\Delta\boldsymbol{\sigma}_{lk}(t)\Delta\boldsymbol{\sigma}_{qp}(t)\rangle. \tag{3.9}$$

From our previous classical discussion of fluctuations in occupation numbers [Eq. (12.36) of reference 1], we expect that

$$\langle\Delta\boldsymbol{\sigma}_{qq}\Delta\boldsymbol{\sigma}_{kk}\rangle=\delta_{qk}\sigma_{kk}-\sigma_{qq}\sigma_{kk}, \tag{3.10}$$

where all σ's are evaluated at the same time. The quadratic term on the right-hand side arises from the constant

$$\mathrm{Tr}\sigma=\textstyle\sum_k\sigma_{kk}=1. \tag{3.11}$$

If contact were made with a particle reservoir (in addition to a heat reservoir), these quadratic terms could be omitted.

The only general relation invariant under an arbitrary change of basis, which agrees with Eq. (3.10) for the diagonal fluctuation is

$$\langle\Delta\boldsymbol{\sigma}_{qp}\Delta\boldsymbol{\sigma}_{lk}\rangle=a\delta_{qk}\sigma_{lp}+(1-a)\delta_{lp}\sigma_{qk}-\sigma_{qp}\sigma_{lk}, \tag{3.12}$$

with a arbitrary. The requirement that this result be unchanged in the order of $\Delta\boldsymbol{\sigma}_{qp}$ and $\Delta\boldsymbol{\sigma}_{lk}$ is inter-

[10] H. Ekstein and N. Rostoker, Phys. Rev. **100**, 1023 (1955).

changed leads to $a=\frac{1}{2}$. We find in the next section, however, that the $\boldsymbol{\sigma}_{qp}$ are to be interpreted properly as operators, and $\langle\ \rangle$ as a weighted trace, so that order is important, and the correct result is found to be $a=1$, i.e.,

$$\langle\Delta\boldsymbol{\sigma}_{qp}(t')\Delta\boldsymbol{\sigma}_{lk}(t')\rangle=\delta_{qk}\sigma_{lp}(t')-\sigma_{qp}(t')\sigma_{lk}(t'). \quad (3.13)$$

If Eq. (3.13) is inserted into Eq. (3.8) and use is made of the relationship

$$\sum O_{qp}{}^{ji}(t,t')\sigma_{qp}(t')=\sigma_{ji}(t), \quad (3.14)$$

then Eq. (3.8) reduces to

$$\langle\alpha(t)\alpha(t')\rangle=\sum I_{ij}I_{kl}[O_{kp}{}^{ji}(t,t')\sigma_{lp}(t')-\sigma_{ji}(t)\sigma_{lk}(t')], \quad (3.15)$$

or

$$\langle\alpha(t)\alpha(t')\rangle=\langle I(t)I(t')\rangle-\langle I(t)\rangle\langle I(t')\rangle, \quad (3.16)$$

and the terms in Eqs. (3.15) and (3.16) correspond to one another in view of Eq. (3.1).

We note that Eq. (3.14) is consistent with Eq. (3.5) only if the equation for σ is linear, but Eqs. (3.9) and (3.13) can be combined *without assuming linearity*.

The correctness of our analysis up to this point may be verified by applying it to a closed system describable by a Hamiltonian $H(t)$ for which all operations can, at least formally, be carried out. In this case, the density matrix obeys the exact equation

$$i\partial\sigma/\partial t=[H(t),\sigma], \quad (3.17)$$

with the conventional choice $\hbar=1$. If the time evolution operator $U=U(t,t')$ is defined by the Schrödinger equation and the initial condition:

$$idU/dt=H(t)U, \quad (3.18)$$

$$U(t',t')=1, \quad (3.19)$$

then it is readily verified that the time evolution of the density matrix obeys

$$\sigma(t)=U(t,t')\sigma(t')U^{-1}(t,t'), \quad (3.20)$$

or

$$\sigma_{ji}(t)=\sum U_{jk}\sigma_{kp}(t')(U^{-1})_{pi}. \quad (3.21)$$

Comparison with Eq. (3.5) or (3.14) reveals that for this case

$$O_{kp}{}^{ji}(t,t')=U_{jk}(t,t')U^{-1}(t,t')_{pi}. \quad (3.22)$$

Let us now verify Eq. (3.15) by inserting Eq. (3.22) into its first term to obtain

$$\langle I(t)I(t')\rangle=U^{-1}(t,t')_{pi}I_{ij}U(t,t')_{jk}I_{kl}\sigma_{lp}(t') =\mathrm{Tr}[I(t,t')I\sigma(t')], \quad (3.23)$$

where

$$I(t,t')=U^{-1}(t,t')IU(t,t'). \quad (3.24)$$

The answer we wish to obtain, however, has the conventional form

$$\langle I(t)I(t')\rangle=\mathrm{Tr}[I(t)I(t')\sigma(-\infty)], \quad (3.25)$$

where

$$I(t)=U^{-1}(t,-\infty)IU(t,-\infty), \quad (3.26)$$

and we regard the time-dependent part of the Hamiltonian as having been turned on gradually in the distant part.

We shall now transform Eq. (3.23) into a more general form which includes Eq. (3.25) as a special case:

$$\langle I(t)I(t')\rangle=\mathrm{Tr}[U^{-1}(t,t')IU(t,t') \times IU(t',t_0)\sigma(t_0)U^{-1}(t',t_0)]. \quad (3.27)$$

By permuting the last factor to the left and utilizing the group property

$$U(t,t_0)=U(t,t')U(t',t_0), \quad (3.28)$$

Eq. (3.27) can be written in general form:

$$\langle I(t)I(t')\rangle=\mathrm{Tr}[I(t,t_0)I(t',t_0)\sigma(t_0)] \quad (3.29)$$

for *any* choice of t_0, with $I(t,t_0)$ defined by Eq. (3.24). The choice $t_0=-\infty$ leads to Eq. (3.25) and verifies the correctness of our procedure. The choice $t_0=t'$ returns one to Eq. (3.23). For use in a Markoffian approximation, one would always choose t_0 equal to the earlier of the two times, t and t'.

We may remark that if in Eq. (3.12) we had chosen $a=0$ instead of $a=1$, we would have obtained instead the incorrect result

$$\langle I(t)I(t')\rangle=\mathrm{Tr}[I(t',t_0)I(t,t_0)\sigma(t_0)]. \quad (3.30)$$

Thus, the choice $a=1$ is ordained and the lack of symmetry in Eq. (3.12) with $a\neq\frac{1}{2}$ definitely suggests that we regard $\boldsymbol{\sigma}_{qp}$ not as random variables but as random operators. This possibility will be developed in the next section by the introduction of a second quantized notation. In Sec. 5, we shall see that the present approach is an approximation in a more general framework, involving the system in interaction with a reservoir.

4. A SECOND QUANTIZED TREATMENT OF DENSITY MATRIX FLUCTUATIONS AT ONE TIME

Because of the expectation that the $\boldsymbol{\sigma}_{ji}$ can be represented by operators, we shall introduce a second quantized treatment of the system. Although it is not necessary to do so at the same time, we shall also introduce a reservoir and assume that the system and reservoir interact. If φ_i and φ_j are system states and the system operator I has the matrix element

$$I_{ij}=(\varphi_i,I\varphi_j) \quad (4.1)$$

coupling them, then the second quantized operator corresponding to I, written boldface, is

$$\mathbf{I}=\sum I_{ij}a_i{}^{\dagger}a_j, \quad (4.2)$$

where $a^{\dagger}$ and a are the usual creation and destruction operators which obey

$$[a_r,a_s{}^{\dagger}]_{\pm}=\delta_{rs}, \quad (4.3)$$

where commutation or anticommutation rules in Eq. (4.3) lead to the same results since we are dealing with only one system

$$N\equiv\sum a_i^\dagger a_i=1. \tag{4.4}$$

If we restrict ourselves to the reduced Hilbert space $N=1$ for all initial and final states, then all operators (see Appendix A) can be reduced to the bilinear form shown in Eq. (4.2).

If ϱ denotes the density matrix of system plus reservoir, second quantized with respect to the system, then

$$\langle I\rangle=\mathrm{Tr}(\mathbf{I}\varrho), \tag{4.5}$$

or

$$I=\sum I_{ij}\sigma_{ji}=\mathrm{Tr}_S(I\sigma), \tag{4.6}$$

with

$$\sigma_{ji}=\mathrm{Tr}(a_i^\dagger a_j\varrho) \tag{4.7}$$

as the appropriate definition of the (reduced) density matrix of the system and the subscript S refers to a trace over the system.

Because of the bilinear nature of all operators, we can write

$$\varrho=\sum a_i^\dagger a_j\nu_{ij}(R), \tag{4.8}$$

where the R in parenthesis is to remind us that $\nu_{ij}(R)$ is an operator in the reservoir variables. We can append a factor $\delta_{N,1}$ or simply remember that in all subsequent calculations, we are restricted to $N=1$ states.

If we combine Eqs. (4.7) and (4.8), trace separately over system and reservoir, and make use of the lemma

$$\mathrm{Tr}_S(a_s^\dagger a_r a_i^\dagger a_j)=\delta_{ri}\delta_{js}, \tag{4.9}$$

Equation (A6), we obtain the more conventional definition

$$\sigma_{rs}=\mathrm{Tr}_R\nu_{rs}(R) \tag{4.10}$$

of a system density matrix as a trace of the complete density matrix over the reservoir variables. Similarly, the second quantized system density matrix can be defined and expressed as

$$\mathbf{S}=\mathrm{Tr}_R\varrho=\sum a_i^\dagger a_j\sigma_{ij} \tag{4.11}$$

in view of Eqs. (4.8) and (4.10).

Equation (4.7) indicates that the operator $a_i^\dagger a_j$ whose mean value is σ_{ji} corresponds to the random variable $\boldsymbol{\sigma}_{ji}$ of the preceding section. Thus, with

$$\boldsymbol{\sigma}_{ji}=a_i^\dagger a_j,$$

we have

$$\langle\Delta\boldsymbol{\sigma}_{qp}\Delta\boldsymbol{\sigma}_{lk}\rangle=\mathrm{Tr}[(a_p^\dagger a_q-\sigma_{qp})(a_k^\dagger a_l-\sigma_{lk})\varrho]. \tag{4.12}$$

Trace first over the reservoir which reduces ϱ to the system matrix $\mathbf{S}$ of Eq. (4.11) and insert the latter:

$$\begin{aligned}\langle\Delta\boldsymbol{\sigma}_{qp}\Delta\boldsymbol{\sigma}_{lk}\rangle=\sum_{ij}[&\mathrm{Tr}(a_p^\dagger a_q a_k^\dagger a_l a_i^\dagger a_j)\\&-\sigma_{qp}\,\mathrm{Tr}(a_k^\dagger a_l a_i^\dagger a_j)-\mathrm{Tr}(a_p^\dagger a_q a_i^\dagger a_j)\sigma_{lk}\\&+\mathrm{Tr}(a_i^\dagger a_j)\sigma_{qp}\sigma_{lk}]\sigma_{ij}\end{aligned} \tag{4.13}$$

$$\begin{aligned}=\sum_{ij}[&\delta_{qk}\delta_{li}\delta_{jp}-\sigma_{qp}\delta_{li}\delta_{jk}-\delta_{qi}\delta_{jp}\sigma_{lk}\\&+\delta_{ij}\sigma_{qp}\sigma_{lk}]\sigma_{ij}.\end{aligned} \tag{4.14}$$

In Eq. (4.13) the trace "Tr" is over the system only and Eq. (4.14) is obtained by using the lemma proven in Appendix A that traces yield a contribution only if the first and last indices are identical, and the intermediate indices are equal in successive pairs. Equation (4.14) reduces directly to the result previously conjectured in Eq. (3.13) [whose consistency was verified in Eqs. (3.23)–(3.29)].

5. SECOND QUANTIZED TREATMENT OF TIME EVOLUTION AND AUTOCORRELATION

The mean of a time-dependent observable $I(t)$ can be written

$$\langle\mathbf{I}(t)\rangle=\mathrm{Tr}[\mathbf{I}(t,t')\varrho(t')], \tag{5.1}$$

where

$$\mathbf{I}(t,t')=\mathbf{U}^{-1}(t,t')\mathbf{I}\mathbf{U}(t,t') \tag{5.2}$$

and

$$\varrho(t')=\mathbf{U}(t',-\infty)\varrho\mathbf{U}(t',-\infty). \tag{5.3}$$

Here, $\mathbf{U}(t,t')$ is the time evolution operator of *system plus reservoir*. The definition, Eq. (3.18) is still applicable with $H(t)$ now representing the Hamiltonian of system plus reservoir plus interaction in second quantized notation. Equation (5.1), with arbitrary t' can be obtained from the conventional definition [namely, Eq. (5.1) with $t'=-\infty$] by the same arguments used to derive Eq. (3.29). Equation (5.1) is equivalent to the conventional statement

$$\langle\mathbf{I}(t)\rangle=\sum I_{ij}\sigma_{ji}(t), \tag{5.4}$$

providing the time-dependent density matrix of the system is defined by

$$\sigma_{ji}(t)=\mathrm{Tr}[\mathbf{U}^{-1}(t,t')a_i^\dagger a_j\mathbf{U}(t,t')\varrho(t')]. \tag{5.5}$$

The choices $t'=-\infty$ and $t'=t$ lead to the conventional and convenient definitions:

$$\sigma_{ji}(t)=\mathrm{Tr}[a_i(t)a_j(t)\varrho(-\infty)], \tag{5.6}$$

$$\sigma_{ji}(t)=\mathrm{Tr}[a_i^\dagger a_j\varrho(t)], \tag{5.7}$$

respectively. If we regard the driving forces as having been turned on gradually in the past, then $\varrho(-\infty)$ can be defined to be the equilibrium density matrix of the system-reservoir complex in the absence of driving forces, but the presence of interactions. [One can also turn on the system-reservoir interactions gradually and take $\varrho(-\infty)$ to be the equilibrium density matrix of the system, times that of the reservoir.] This procedure throws the burden of labor on $a_i^\dagger(t)a_j(t)$ which must succeed in demonstrating how a system plus reservoir in equlibrium (possibly without interaction) is transformed into a driven, interacting system. Equation (5.7) is a more convenient definition since no explicit reference is made to an equilibrium state, but the time evolution in the driven state can be considered.

If we define

$$\varrho(t)=\sum a_r^\dagger a_s\nu_{rs}(R,t), \tag{5.8}$$

then

$$\sigma_{rs}(t)=\mathrm{Tr}_R\nu_{rs}(R,t) \tag{5.9}$$

is an immediate consequence of Eq. (5.7). We shall find it convenient therefore, to define

$$f_{rs}(R,t)=\nu_{rs}(R,t)/\sigma_{rs}, \tag{5.10}$$

with

$$\mathrm{Tr}_R f_{rs}(R,t)=1. \tag{5.11}$$

Let us now investigate the time evolution formally by applying Eq. (5.5) together with

$$\mathbf{U}^{-1}(t,t')a_i^\dagger a_j\mathbf{U}(t,t')=\sum A_{pq}{}^{ij}(R,t,t')a_p^\dagger a_q, \tag{5.12}$$

which is a consequence of the bilinearity of all operators in our subspace. The result is

$$\sigma_{ji}(t)=\sum O_{qp}{}^{ji}(t,t')\sigma_{qp}(t'), \tag{5.13}$$

where

$$O_{qp}{}^{ji}(t,t')=\mathrm{Tr}_R[A_{pq}{}^{ij}(R,t,t')f_{qp}(R,t')]. \tag{5.14}$$

We are now in a position to investigate autocorrelation and determine to what extent it is expressible in terms of the O functions. If we parallel the notation of Eq. (3.23), we can write

$$\langle I(t)I(t')\rangle=\mathrm{Tr}[\mathbf{I}(t,t')\mathbf{I}\varrho(t')], \tag{5.15}$$

$$\langle I(t)I(t')\rangle=\sum I_{ij}I_{kl}\,\mathrm{Tr}\times[\mathbf{U}^{-1}(t,t')a_i^\dagger a_j\mathbf{U}(t,t')a_k^\dagger a_l\varrho(t')]. \tag{5.16}$$

If we insert Eqs. (5.12) and (5.8), we obtain the rigorous result,

$$\langle I(t)I(t')\rangle=\sum I_{ij}I_{kl}\mathrm{Tr}_R[A_{pk}{}^{ij}(R,t,t')f_{lp}(R,t')]\sigma_{lp}(t'), \tag{5.17}$$

appropriate for $t>t'$.

If we now make the *only* approximation of the present paper,

$$f_{lp}(R,t')\approx f(R,t'), \tag{5.18}$$

then with the help of Eq. (5.14) we can write

$$\langle I(t)I(t')\rangle=\sum I_{ij}I_{kl}O_{kp}{}^{ji}(t,t')\sigma_{lp}(t'), \tag{5.19}$$

in agreement with the result of our previous heuristic approach—see the first term in Eq. (3.15). The second term of Eq. (3.15), namely, $\langle I(t)\rangle\langle I(t')\rangle$ follows, of course, from Eq. (5.4) without requiring any approximations.

The approximation, Eq. (5.18) is equivalent in Eq. (5.8) to the factorization:

$$\varrho(t)\approx\mathbf{S}(t)f(R,t), \tag{5.20}$$

where

$$\mathbf{S}(t)=\sum a_r^\dagger a_s\sigma_{rs}(t) \tag{5.21}$$

is the second quantized density matrix of the system. It is clear that both $\mathbf{S}(t)$ and $f(R,t)$ could have periodic parts, correlated in time, because of a periodic driving force. What is neglected in Eq. (5.18) is the ability of the reservoir density matrix to vary in a way which correlates with the system states.

6. GENERALIZATIONS AND SPECIALIZATIONS

Our results of the previous section can be immediately generalized to the case of a set of operators $I^\mu(t)$ by defining

$$I^\mu(t)=\sum I_{ij}{}^\mu\sigma_{ji}(t). \tag{6.1}$$

Equation (5.19) takes the form

$$\langle I^\mu(t)I^\nu(t')\rangle=\sum I_{ij}{}^\mu I_{kl}{}^\nu O_{kp}{}^{ji}(t,t')\sigma_{lp}(t') \tag{6.2}$$

and Eq. (5.13) leads to:

$$\langle I^\mu(t)\rangle=\sum I_{ij}{}^\mu O_{qp}{}^{ji}(t,t')\sigma_{qp}(t'). \tag{6.3}$$

If, now, we *assume* that the set of variables $I^\mu(t)$ constitute a linear Markoffian set in the sense that

$$\langle I^\mu(t)\rangle=\sum_\nu G^{\mu\nu}(t,t')\langle I^\nu(t')\rangle, \tag{6.4}$$

then the insertion of

$$\langle I^\nu(t')\rangle=\sum I_{pq}{}^\nu\sigma_{qp}(t') \tag{6.5}$$

together with (6.3) into Eq. (6.4) leads to the requirement

$$\sum_{ij}I_{ij}{}^\mu O_{qp}{}^{ji}(t,t')=\sum_\nu G^{\mu\nu}(t,t')I_{pq}{}^\nu. \tag{6.6}$$

The use of Eq. (6.6) in (6.2) with $\nu=\lambda$ leads immediately to

$$\langle I^\mu(t)I^\nu(t')\rangle=\sum_\lambda G^{\mu\lambda}(t,t')\langle I^\lambda(t')I^\nu(t')\rangle. \tag{6.7}$$

The comparison of Eqs. (6.4) and (6.7) is equivalent to the statement that for a set of Markoffian variables $I^\mu(t)$, the regression of fluctuations is identical to the decay of a macroscopic signal.[8] [Equation (5.19) is this same statement for the complete set of operators $a_i^\dagger a_j$.]

It may seem that the results just derived are limited to first and second moments—i.e., the mean motion and fluctuations therefrom. However, our procedure, in fact, yields the complete distribution function or all moments (at two times). For example, all moments of a quantity $Q(t)$ can be obtained by setting I equal to the characteristic function

$$I(t)=\exp[fQ(t)]. \tag{6.8}$$

The coefficient of f^n in $\langle I(t)\rangle$ yields $\langle[Q(t)]^n\rangle$. Similarly, one could evaluate

$$\langle\exp[fQ(t)]\exp[gP(t')]\rangle \tag{6.9}$$

to get all moments at two times involving Q and P. Such seemingly more complicated cases can be dealt with readily by making use of the essential bilinearity of all operators via Eq. (A14). It is this bilinearity that guarantees that the equations of motion for the set of operators $a_i^\dagger a_j$ are *linear*. This linearity is achieved by using a very *large* set of operators. We can illustrate the nature of our operators by noting that a harmonic oscillator, with creation and destruction operators $A^\dagger$ and A obeying

$$[A,A^\dagger]=1 \tag{6.10}$$

and possessing the usual eigenstates

$$A^\dagger A|n\rangle = n|n\rangle \tag{6.11}$$

with

$$A^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle; \quad A|n\rangle = n^{1/2}|n-1\rangle, \tag{6.12}$$

can be expressed in our notation by setting

$$A^\dagger = \sum_{n=0}^{\infty} (n+1)^{1/2} a_{n+1}^\dagger a_n, \tag{6.13}$$

$$A = \sum_{n=1}^{\infty} n^{1/2} a_{n-1}^\dagger a n, \tag{6.14}$$

so that Eq. (A3) leads to

$$A^\dagger A = \sum_{n=1}^{\infty} n a_n^\dagger a_n \tag{6.15}$$

and

$$\langle A^\dagger A\rangle = \sum n\sigma_{nn}, \tag{6.16}$$

where σ_{nn} is the probability that the harmonic oscillator is in its nth excited state.

The use of Eq. (A14) or (A15) permits us to exploit linearity in the form

$$\exp(\mu A^\dagger A) = \sum_n a_n^\dagger a_n \exp(\mu n), \tag{6.17}$$

$$\langle \exp(\mu A^\dagger A)\rangle = \sum \sigma_{nn} \exp(\mu n). \tag{6.18}$$

Thus, the complete distribution function for $A^\dagger A$ at time t is specified by $\sigma_{nn}(t)$.

Note added in proof. Subject to the one approximation of factorization (5.20) our conclusion (5.19) relating the regression of fluctuations to the solution (5.13) of the "macroscopic" equations of motion remains valid even for *non-Markoffian systems*. Equation (5.13) relating $\sigma(t)$ to its earlier value $\sigma(t')$ appears to imply that the system is Markoffian. However, the Green's function $0(t,t')$ depends on the history of the system implicitly through $f_{qp}(R,t')$ since the "present" status of the reservoir may depend on the history of the system. The author is indebted to J. R. Klauder for this last remark.

APPENDIX A. ALGEBRA OF SECOND QUANTIZATION FOR ONE SYSTEM

Operator $a_j^\dagger$ creates a system in state j; operator a_i destroys a system in state i (or causes a vanishing result if state i is initially empty). Operators which contain as many creation as destruction operators leave $N \equiv \sum a_s^\dagger a_s =$ the number of systems unchanged and are the only ones allowed in our algebra. We may use the commutation rules to rearrange any polynomial so that creation and destruction operators alternate, with a destruction operator acting first.

Since any of the state vectors with $N=1$ has only one state occupied, it can be destroyed by the successive action of two destruction operators:

$$a_j a_k|N=1\rangle = 0, \tag{A1}$$

or, more generally,

$$(\text{any operator}) a_j (\text{any operator not involving } a_j^\dagger) \times a_k|N=1\rangle = 0. \tag{A2}$$

We therefore obtain the following lemma:

Lemma 1. If a polynomial operator is arranged to have a destruction operator in the right hand or first position followed by a creation operator, then a destruction operator, etc., then each destruction operator, except for the first, must be immediately preceded by the same creation operator or the result vanishes. For example:

$$a_i^\dagger a_j a_k^\dagger a_l = \delta_{jk} a_i^\dagger a_l, \tag{A3}$$

$$a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n = \delta_{jk}\delta_{lm} a_i^\dagger a_n. \tag{A4}$$

Since $a_i^\dagger a_j$ has no diagonal elements unless $i=j$, we have

$$\mathrm{Tr} a_i^\dagger a_j = \delta_{ij}, \tag{A5}$$

$$\mathrm{Tr} a_i^\dagger a_j a_k^\dagger a_l = \delta_{jk}\delta_{li}, \tag{A6}$$

$$\mathrm{Tr} a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n = \delta_{jk}\delta_{lm}\delta_{ni}, \tag{A7}$$

and we arrive at:

Lemma 2. The trace of a polynomial operator is unity if the intermediate indices are equal in pairs as described in Lemma 1 and if the first and last indices are equal.

Theorem 1. All allowed operators are bilinear. (This is an immediate consequence of Lemma 1.)

If

$$\mathbf{A} = \sum A_{ij} a_i^\dagger a_j, \tag{A8}$$

$$\mathbf{B} = \sum B_{kl} a_k^\dagger a_i, \tag{A9}$$

it follows from Eq. (A3) that we can write

$$\mathbf{AB} = \sum A_{ij} B_{jl} a_i^\dagger a_l = \sum (AB)_{il} a_i^\dagger a_l, \tag{A10}$$

or more briefly

$$\mathbf{AB} \to AB; \tag{A11}$$

and obviously

$$\mathbf{A}+\mathbf{B} \to A+B, \tag{A12}$$

so that generally

$$f(\mathbf{A},\mathbf{B}) \to f(A,B), \tag{A13}$$

i.e.,

$$f(\mathbf{A},\mathbf{B}) = \sum f(A,B)_{ij} a_i^\dagger a_j. \tag{A14}$$

As an especially useful example,

$$\exp(it\mathbf{H}) = \sum [\exp(itH)]_{ij} a_i^\dagger a_j \tag{A15}$$

or

$$\exp(it\mathbf{H}) = \sum \{\delta_{ij} + [\exp(itH) - 1]_{ij}\} a_i^\dagger a_j. \tag{A16}$$

Combining Eqs. (A5) and (A10), we also obtain

$$\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr} AB,$$

indicating the close correspondence between the quantized and unquantized notations.