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Calculation of Correlation Functions in the Weak Coupling Approximation

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We have previously pointed out (1996, *Phys. Rev. Lett.* **77**, 798) that in the calculation of a correlation function $C(t)$ by means of the fluctuation–dissipation theorem, much insight could be gained by writing the Fourier transform of $C(t)$ as of the Fourier transform of the relaxation function multiplying the *universal* power spectrum of quantum noise at temperature T. Here, we show how this factorization leads to an immediate simplifying approach in the weak coupling limit near resonance. In particular, the time decay dependencies which appear are those associated with the Onsager *classical* regression theorem. Also, we throw further light on our previous assertion that there is *never* a quantum regression theorem. © 1999 Academic Press

Correlation functions are an integral component of the literature of statistical physics [1, 2] and they have applications in many different branches of physics. In particular, they arise in the work of Callen and Welton on the fluctuation–dissipation theorem [3, 4] and the work of Kubo *et al.* [1] on linear response theory. The relationship between correlation functions and relaxation (after-effect) functions has also proved to be very useful [1, 5].

Another pillar of nonequilibrium statistical physics is the famous Onsager regression hypothesis [6], which he used to obtain his equally famous reciprocity law of kinetic coefficients. This hypothesis states that "the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process" [6] and it should be emphasized that it is a statement of classical statistical physics. In fact, in the classical limit and for macroscopic variables corresponding to a dynamical variable of the system, the fluctuation–dissipation theorem is a proof of the Onsager regression hypothesis [5].

Correlation functions are pervasive in Quantum Optics and one often needs to study the correlation of many operators at different times. In particular, they arise

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in the study of driven systems and, in a pioneering study, Lax [7, 8] showed that, using only what he referred to as the Markovian approximation, many simplifications arise so that, for example, a two-time correlation function could be calculated from a single-time correlation function. However, the latter feature of the Lax formulation led subsequent authors to refer to this as the quantum regression theorem [9] and this is referred to extensively as such in all the modern textbooks [10–14]. However, we have recently pointed out that there is in fact no quantum regression theorem but, nevertheless, we hasten to add that the results of Lax [5] are correct and extremely useful, particularly in the realm of quantum optics. But they are useful, not because they constitute a quantum regression theorem, but because they exploit the basic fact that quantum optics deals with weak coupling systems. In fact, it is this emphasis on weak coupling which motivates our present study. This arises from the observation which we made in Ref. [5] that the quantum generalization of the classical Onsager regression theorem [6] is the fluctuation–dissipation theorem, as a consequence of which use of the latter theorem is the preferred way to calculate quantum correlation functions $C(t)$. Here, we wish to expand on these remarks and, in particular, demonstrate the great simplicity which immediately arises in the case of weak coupling. In addition, we throw further light on why there is no quantum regression theorem by carrying out an explicit calculation. With the notation of Ref. [1] the result is best stated in the form

$$\tilde{C}(\omega)=u(\omega)\,\tilde{A}(\omega), \tag{1}$$

where $\tilde{A}(\omega)$ and $\tilde{C}(\omega)$ are the Fourier transforms of the relaxation function and the correlation function, respectively, and $u(\omega)$ is the *universal* power spectrum of quantum noise at temperature T. Explicitly

$$u(\omega)=\frac{\hbar\omega}{2}\coth\frac{\hbar\omega}{2kT}=\hbar\omega\left(N(\omega)+\frac{1}{2}\right) \tag{2}$$

is the Planck energy plus zero-point energy and $N(\omega)$ is the mean number of photons with frequency ω. Also,

$$C(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\,\tilde{C}(\omega)\,e^{-i\omega t}, \tag{3}$$

with a similar expression for $\tilde{A}(\omega)$ in terms of $A(t)$. In the classical limit $u(\omega)\to kT$ and is thus independent of frequency with the result that the inverse Fourier transform of (1) leads to the result $C(t)\to kT\,A(t)$ and hence $C(t)$ has the same time dependence as $A(t)$, which is the classical Onsager result. More generally, $C(t)$ will not be proportional to $A(t)$, which is to say that there is no quantum regression theorem.

It should be emphasized that the result given in (1), which expresses the Callen–Welton theorem in the form involving the relaxation function, is a very general result. Here, for the purpose of illustration, we consider an oscillator of frequency ω_0 in an arbitrary dissipative environment. In the case of weak coupling ($\gamma \ll \omega_0$, where γ is a typical decay rate and ω_0 is the oscillator frequency), it is still useful to write the correlation function in the form given in (1). This is because, for the weakly damped oscillator, $\tilde{A}(\omega)$ is sharply peaked about $\omega_0 = \sqrt{K/m}$, the natural frequency of the undamped oscillator (see, for example, Eq. (27) of Ref. [5] and (6) below and also [16] and [17]).

If this peak is sufficiently narrow (weak coupling), then in the neighborhood of the peak one can evaluate $u(\omega)$ at the peak and write

$$\tilde{C}(\omega) \cong u(\omega_0)\, \tilde{A}(\omega). \tag{4}$$

Thus, in the weak coupling approximation, $\tilde{C}(\omega)$ is also sharply peaked and, in the neighborhood of the peak, is proportional to $\tilde{A}(\omega)$. What one sees is the spectrum of quantum noise, $u(\omega)$, through a filter, $\tilde{A}(\omega)$. *This spectrum of quantum noise is universal.* Only the relaxation function depends upon the parameters of the particular system being considered. If we use this approximation in the expression (3) for C(t), we find

$$\begin{aligned} C(t) &\approx u(\omega_0) \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, \tilde{A}(\omega)\, e^{-i\omega t} \\ &= u(\omega_0)\, A(t) \\ &= \frac{u(\omega_0)}{kT}\, C_{cl}(t), \end{aligned} \tag{5}$$

where $C_{cl}(t) = kT\, A(t)$ is the classical (in the sense that it obeys the classical Onsager regression hypothesis) result. Thus, in this approximation, $C(t)$ has the same time dependence as $A(t)$. In fact, $C(t)$ is actually the classical result multiplied by a constant $(\hbar\omega_0/2kT)\coth(\hbar\omega_0/2kT)$; i.e., it obeys the *classical* regression theorem despite the fact that there are $\hbar$ terms in the constant factor. As we shall demonstrate below, the quantum factor that appears is not associated with the presence of dissipation. The important point is that $C(t)$ has the same time dependence as $A(t)$. In addition (and this is the real power of the fluctuation–dissipation theorem), the relaxation function is generally a quantity which is much easier to calculate than the correlation function [5].

Up to now, we have been discussing correlation functions and their associated relaxation functions from a very general point of view. Next, we consider a specific example which in fact is very relevant in numerous investigations, viz., the *position* autocorrelation function for the case of a quantum oscillator in an Ohmic dissipative environment for which the expression for the relaxation function is given by [5]

$$\tilde{A}(\omega) = \frac{2\gamma}{m\{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2\}}, \tag{6}$$

where $\omega_0 = \sqrt{K/m}$ is the natural frequency of the undamped oscillator and γ is the frequency-independent damping parameter. It is clear that, in the weak coupling limit ($\gamma \ll \omega_0$), $\tilde{A}(\omega)$ is sharply peaked about ω_0, justifying our expression (4). Consider now the position autocorrelation function

$$C(t-t') = \tfrac{1}{2}\langle x(t)\, x(t') + x(t')\, x(t)\rangle. \tag{7}$$

Thus, using (5) and (6), we obtain the weak coupling result for Ohmic dissipation:

$$C(t) \cong \frac{\gamma}{\pi m}\, u(\omega_0) \int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega t}}{(\omega_0^2-\omega^2)^2+\gamma^2\omega^2}. \tag{8}$$

Henceforth, we will take $t>0$. However, we see from (7) that $C(-t) = C(t)$ and thus our final results for $C(t)$ may be generalized to all t values by simply replacing t by $|t|$. The integral in (8) is readily evaluated using contour integration (and recalling that $\omega \to \omega + i0^+$) with the result

$$C(t) \cong \frac{\hbar}{2m\omega_0} \coth(\hbar\omega_0/2kT)\, e^{-(\gamma/2)\,t} \left(\cos\omega_1 t + \frac{\gamma}{2\omega_1}\sin\omega_1 t\right), \tag{9}$$

where

$$\omega_1 = \{\omega_0^2 - (\gamma/2)^2\}^{1/2}. \tag{9a}$$

Thus, we have obtained $C(t)$ essentially by calculating $A(t)$, which, in the present context, is simply proportional [5] to $\langle x(t)\rangle_f$, where $\langle x(t)\rangle_f$ describes how the expectation value of x evolves when a constant force f (which was applied in the distant past so that the system came to equilibrium at temperature T) is removed at $t=0$. In other words, the calculation of a correlation function, which involves the expectation value of two operators, has been reduced, in the weak coupling approximation, to the calculation of the expectation value of a single operator. However, such a result does *not* constitute a quantum regression theorem.

It is of interest to *check* this weak coupling result with an *exact* calculation. Using the exact expression (1), we have

$$\begin{aligned} C(t) &= \frac{\hbar\gamma}{2\pi m} \int_{-\infty}^{\infty} d\omega\, \frac{\omega\coth(\hbar\omega/2kT)}{(\omega^2+i\gamma\omega-\omega_0^2)(\omega^2-i\gamma\omega-\omega_0^2)}\, e^{-i\omega t} \\ &\equiv C^{(1)}(t) + C^{(2)}(t), \end{aligned} \tag{10}$$

where $C^{(1)}$ is the contribution of the poles of $\tilde{A}(\omega)$, while $C^{(2)}$ is the contribution of the poles of the hyperbolic cotangent;

$$C^{(1)}(t) = \frac{\hbar}{2m\omega_1}\, e^{-(\gamma/2)\,t}\, \frac{\sinh(\hbar\omega_1/kT)\cos\omega_1 t + \sin(\hbar\gamma/2kT)\sin\omega_1 t}{\cosh(\hbar\omega_1/kT) - \cos(\hbar\gamma/2\mathrm{kT})} \tag{11}$$

and

$$C^{(2)}(t) = -\frac{4\gamma\omega_1}{2\pi} \sum_{n=1}^{\infty} \frac{n\Omega^2 e^{-n\Omega t}}{(\omega_0^2 + n^2\Omega^2)^2 - n^2\Omega^2\gamma^2}, \tag{12}$$

where

$$\Omega = \frac{2\pi kT}{\hbar} = \left(\frac{T}{1.1 \times 10^{-12}\mathrm{K}}\right) \mathrm{s}^{-1}. \tag{13}$$

Noting that typical values of γ in quantum optics range from $\approx 3 \times 10^{10}\,\mathrm{s}^{-1}$ for collisional broadening to $\approx 10^5\,\mathrm{s}^{-1}$ and less for lasers [18], whereas a typical ω_0 value is $10^{16}\,\mathrm{s}^{-1}$, we see that the weak coupling approximation is extremely good. Also, in the present context, we see that only for $T \to 0$ does $C^{(2)}(t)$ make a non-negligible contribution. In fact, it is clear that, since $\gamma \ll \Omega$ even at 1 K, $C^{(2)}(t) \ll C^{(1)}(t)$ and, in the weak coupling limit ($\gamma \ll \omega_0$), $C^{(1)}(t)$ reduces to the right-hand side of (9). This verifies both the correctness and the simplicity of the approach outlined above.

It is of interest to note that, in general, $C^{(1)}(t)$ obeys the Onsager regression hypothesis [6] which states that "the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible processes." However, $C^{(2)}(t)$ does not obey this hypothesis and in fact it is precisely this term which gives rise to the right-hand side of Eq. (12) of Ref. [5], thereby manifesting its non-compliance with the Onsager hypothesis. Nevertheless, since this term does not contribute if one assumes weak coupling and moderate temperatures (room temperature, for example), it is immediately clear why the result given for $C(t)$ in (8) obeys the Onsager hypothesis.

On the other hand, for $\mathrm{T} = 0$ and in the long-time limit, the dominant contribution comes from $C^{(2)}(t)$ and, using a procedure similar to that used in the derivation of Eq. (15) of Ref. [5], we obtain $C(t) \sim t^{-2}$; i.e., it exhibits a long-time tail. This is in contrast to the exponential decay exhibited by the temperature-independent quantity $A(t)$. Thus, we have a striking example of how quantum effects destroy the linear classical relation between $C(t)$ and $A(t)$.

The above calculation concentrated on the case of Ohmic dissipation. However, as we have recently shown [19], it is of interest to note that it is also relevant to the case of a charged oscillator in a *radiation field* where now γ has the specific value $\omega_0^2\tau_e$ (where M is the renormalized mass) and $\tau_e = (2e^2/3Mc^3) \approx 6 \times 10^{-24}$ s. Also, the radiation field is a good example of the fact that off-peak effects can also make important contributions. In particular, we have shown that there is an important contribution from high-frequency ($\omega \gg \omega_0$) components, which give rise, among other effects, to a thermal shift in the energy levels [20]. In addition, at $\mathrm{T} = 0$, the dominant contribution comes from $\mathrm{C}^{(2)}(\mathrm{t})$ and we find in fact that $\mathrm{C}(0)$ is dominated by quantum effects and is actually logarithmically divergent.

Finally, we emphasize the generality of our approach. Whereas, in the example above, we calculated correlation functions for the displacement operator, it is clear that the analysis is actually very general [4, 5, 15]. In particular, results similar to those found for the coordinates may be found for momentum operators and for creation and annihilation operators. Thus, consider

$$\begin{aligned} C_{a^+a}(t-t') &\equiv \tfrac{1}{2}\langle a^+(t)\, a(t') + a^+(t')\, a(t)\rangle \\ &= \mathrm{Re}\langle a^+(t)\, a(t')\rangle, \end{aligned} \tag{14}$$

where, as usual,

$$a = \frac{m\omega_0 x + ip}{(2m\hbar\omega_0)^{1/2}}, \qquad a^+ = \frac{m\omega_0 x - ip}{(2m\hbar\omega_0)^{1/2}}. \tag{15}$$

Hence, from the fact [15] that $p = m(dx(t)/dt)$ it readily follows that

$$C_{a^+a} = \frac{1}{x_0^2}\, C_{xx} + \frac{1}{p_0^2}\, C_{pp} + R(t-t'), \tag{16}$$

where $p_0 = (2m\hbar\omega_0)^{1/2} = m\omega_0 x_0$ and $R(t-t')$ involves the commutator of $x(t)$ and $p(t')$, explicit results for which are given in Ref. 21.

If one takes Fourier transforms and uses the fact that $\tilde{p}(\omega) = i\omega m\tilde{x}(\omega)$, it follows that

$$\begin{aligned} \tilde{C}_{a^+a}(\omega) &= \left\{\frac{1}{x_0^2} + \frac{m^2}{p_0^2}\,\omega^2\right\} \tilde{C}_{xx}(\omega) + \tilde{R}(\omega) \\ &= \frac{1}{x_0^2}\left\{1 + \frac{\omega^2}{\omega_0^2}\right\} \tilde{C}_{xx}(\omega) + \tilde{R}(\omega) \\ &= \frac{m}{2\hbar\omega_0}\,(\omega_0^2 + \omega^2)\, \tilde{C}_{xx}(\omega) + \tilde{R}(\omega). \end{aligned} \tag{17}$$

Thus, we obtain, in the weak coupling limit,

$$C_{a^+a}(t) = \frac{m}{2\hbar\omega_0}\left\{\omega_0^2 - \frac{d^2}{dt^2}\right\} C_{xx}(t) - \frac{1}{2}\cos(\omega_0 t)\, e^{-(\gamma/2)\,t}, \tag{18}$$

where $C_{xx}(t)$ is given by (7) [the subscripts "xx" having been added for further clarity]. Hence, for the particular case of the Ohmic model in the weak coupling limit, it is immediately clear, from (19) and (9), that

$$\begin{aligned} C_{a^+a}(t) &= N(\omega_0)\, e^{-(\gamma/2)\,t} \cos\omega_0 t \\ &= N(\omega_0)\cos\omega_0 t. \end{aligned} \tag{19}$$

Thus $C_{a^+a}(t)$ exhibits the characteristic time decay $\exp\{-(\gamma/2)\,t\}$ associated with $C_{xx}(t)$ and $A(t)$.

Finally, we turn to the origin of the quantum factors appearing in the various correlation functions. For this purpose, we take $t = t'$ and then (9) and (20) reduce to

$$\langle x^2(t)\rangle = \frac{\hbar}{2m\omega_0}\coth(\hbar\omega_0/2kT) = \frac{\hbar}{m\omega_0}\left(N(\omega_0) + \frac{1}{2}\right) \tag{20}$$

and

$$\langle a^+(t)\, a(t)\rangle = N(\omega_0), \tag{21}$$

which will be recognized as nothing but the familiar results for a *free* oscillator. Thus, in the calculation of correlation functions for the oscillator in the weak coupling limit, the *quantum* effects that appear are those associated with the free oscillator whereas the important *classical* time-dependent terms result from the determination of the relaxation function; in other words, the formalism and apparatus of quantum dissipation play an essential role only in the determination of the time decay terms.

In conclusion, we stress the fact that either in (a) the high temperature limit or (b) the weak coupling limit near resonance, $u(\omega)$ becomes independent of ω, in which case $C(t)$ obeys the Onsager relation. In case (b), quantum features remain but nevertheless, there is no quantum regression theorem and in fact, all the correlation and response functions exhibit the same Onsager classical time behavior. Furthermore, we note that if we are dealing with a system with more than one resonance, such as the Mollow spectrum [9], then we simply get additive contributions from each of the resonances, with the appropriate resonant frequencies and decay constants. If exact results need to be derived, then (1) must be used; i.e., "the correct generalization of the Onsager relation is the fluctuations–dissipation theorem" [5].

It should be emphasized that there is *never* a quantum regression theorem. Thus, it is not true to say that weak coupling implies that we have an approximate quantum regression theorem; the correct statement is that weak coupling implies classical regression. We feel that part of the confusion in the literature stems from the fact that the various relationships derived between one-time and two-time correlations have been incorrectly characterized; they should be identified as resulting simply from a weak coupling approximation. By contrast, the relationship between the two-operator quantity C(t) and the one-operator quantity A(t) is a very special kind. In the classical limit, it says that "the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process" [6]. In other words, it says that, if a system is close to equilibrium, there is no way of knowing if it was taken out of equilibrium by an external force (in which situation the relaxation function A(t) comes into play) or by a spontaneous fluctuation (in which case C(t) comes into play). In the example given above, the time scale for both processes is given, in the classical case only, by $(\gamma/2)^{-1}$; in the quantum case, there are additional time scales, as is manifest in (12).

Finally, we emphasize that our remarks have been confined to equilibrium or near-equilibrium systems. Strongly driven systems will be discussed elsewhere [21].

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