

Exact operator self-energies from resummation of the Heisenberg equations of motion

C. F. Hart

*Institute for Modern Optics, Department of Physics and Astronomy,
University of New Mexico, Albuquerque, New Mexico 87131*

(Received 5 March 1984)

The Laplace-transformed Heisenberg equations of motion are resummed in such a way that the resulting iterative series expansion of any operator is given in terms of exact perturbed operator self-energies. We show how to incorporate this result into a recently introduced Liouvillian Green's-function and self-energy approach to nonequilibrium statistical mechanics. The spontaneous emission of a two-level atom is discussed as a simple example of this new resummation technique.

The behavior of nonequilibrium many-body systems is of considerable current interest. Quantum field-theoretic Green's functions and self-energies are important tools in calculating this behavior; however, standard temperature-time Green's-function perturbation techniques are, in general, inapplicable since they depend on specific properties of thermal equilibrium.¹ Recently, a new approach which combines Green's-function techniques with a systematic use of the Liouvillian and Liouville-space methods has been shown to be well suited to the development of nonequilibrium statistical mechanics.² This Liouvillian Green's-function and self-energy theory leads to a systematic procedure for the calculation of the dynamics of propagation, to arbitrary times $t > 0$, of correlations which are presumed known at $t = 0$.

In the Liouvillian Green's-function approach one uses Laplace-transform techniques to convert the Heisenberg equations of motion into coupled algebraic equations and then defines self-energies $\Sigma_\alpha(z)$ for the various excitations of the system.³ It is important to note that these self-energies $\Sigma_\alpha(z)$ are not the same as the usual self-energy superoperator which results from the decomposition of $(s + i\mathcal{L})^{-1}$, where \mathcal{L} is the Liouvillian, into a diagonal and nondiagonal part; rather, the $\Sigma_\alpha(z)$ also include environmental contributions arising from the nondiagonal part of $(s + i\mathcal{L})^{-1}$ (see Ref. 2 for further discussion of this point).

In Ref. 2 these generalized self-energy functions were calculated in a perturbation expansion in which each term depends on the unperturbed poles (eigenenergies) of the various operators. A problem can arise when attempting to solve certain problems using this technique. For example, if one calculates the resonance fluorescence (Mollow) spectrum⁴ of a two-level atom driven by a strong monochromatic field, using the method of Ref. 2, one finds that the linewidths of the three-peaked emission spectrum do not come out correctly. This can easily be shown to be directly attributable to the fact that the Liouvillian Green's-function approach of Ref. 2 is a perturbation expansion in terms of the *unperturbed* poles. In this paper we show that it is possible to improve the series expansion for $\Sigma_\alpha(z)$ by resumming the Heisenberg equations of motion in such a way that the new self-energy functions $\bar{\Sigma}_\alpha(z)$ are given by a perturbation expansion in which each term depends on the *exact* perturbed operator poles. This resummation procedure alleviates the aforementioned problem and the resulting, improved, Liouvillian Green's-function technique can then be

applied to other many-body problems.

This exact resummation of the Heisenberg equations of motion, though fairly simple, does not seem to have been done before in the way which is presented herein. It amounts to an exact (quasiperturbative) decomposition of the resolvent into diagonal and nondiagonal parts in the sense of van Hove.⁵ Such a decomposition is also achieved in the various projection operator methods,⁶ however, as discussed in Ref. 2 the present Liouvillian Green's-function approach has the advantage of explicitly including environmental effects in the self-energy functions. In other words, the present formalism fully incorporates the quantum statistical effects present in many-body systems. An explicit example of the usefulness of the inclusion of environmental effects in the self-energy is presented in the second paper of Ref. 2 where the line shift and width of a two-level atom in a finite-temperature radiation bath is derived.

Any operator \mathcal{O}_α satisfies the Heisenberg equations of motion

$$i\partial_t \mathcal{O}_\alpha(t) = [\mathcal{O}_\alpha(t), H] \equiv \mathcal{L} \mathcal{O}_\alpha(t) , \quad (1)$$

for H the total Hamiltonian (assumed time independent) and \mathcal{L} the associated Liouvillian (super) operator. We assume the existence of a linearly independent operator basis $B_m(t)$ such that the evolution of $\mathcal{O}_\alpha(t)$ may be expanded in terms of this basis:

$$\mathcal{L} \mathcal{O}_\alpha(t) = i\partial_t \mathcal{O}_\alpha(t) = \sum_m c(\alpha|m) B_m , \quad (2)$$

or, more generally,

$$i\partial_t B_n = \sum_m c(n|m) B_m . \quad (3)$$

The c -matrix elements $c(n|m)$ contain the dynamics of the system. We rewrite Eq. (3) as

$$i\partial_t B_n = \epsilon_n B_n + \sum'_m c(n|m) B_m , \quad (4)$$

where $\epsilon \equiv c(n|n)$ is usually chosen such that

$$\mathcal{L}_0 B_n = \epsilon_n B_n = [B_n, H_0]$$

for H_0 the unperturbed part of H and the prime on the summation excludes $m = n$. Taking the Laplace transform, where⁷

$$L(f(t); s) \equiv \tilde{f}(s) = \int_0^\infty dt f(t) e^{-st} ,$$

gives

$$(s + i\epsilon_n)\tilde{B}_n(s) = B_n(0) + (-i) \sum'_m c(n|m)\tilde{B}_m(s) . \quad (5)$$

The standard approach^{2,3} to using Eq. (5) is to iterate the expansion in a power series in the $c(n|m)$, in other words, substitute the expansion for $B_m(s)$ analogous to (5) into the right-hand side of (5), and so on. This gives a perturbation expansion for the $B_n(s)$ in terms of the unperturbed poles ϵ_m and initial values $B_m(0)$ and in the Liouvillian Green's-function approach also leads to the aforementioned expansion for the self-energies in terms of unperturbed poles.

Here, however, we shall proceed differently. Add to both

sides of Eq. (5) the term $\gamma_n(s)\tilde{B}_n(s)$ where $\gamma_n(s)$ is, as yet, undetermined:

$$[s + i\epsilon_n + \gamma_n(s)]\tilde{B}_n(s) = B_n(0) + (-i) \sum'_m c(n|m)\tilde{B}_m + \gamma_n(s)\tilde{B}_n(s) ,$$

or

$$\tilde{B}_n(s) = \frac{B_n(0)}{s + i\epsilon_n + \gamma_n(s)} + \frac{\gamma_n(s)\tilde{B}_n(s)}{s + i\epsilon_n + \gamma_n(s)} + \frac{(-i)}{s + i\epsilon_n + \gamma_n(s)} \sum'_m c(n|m)\tilde{B}_m(s) . \quad (6)$$

Next, iterate this expansion [defining $i\epsilon_n + \gamma_n(s) \equiv iE_n(s)$]

$$\begin{aligned} \tilde{B}_n(s) = & \frac{B_n(0)}{s + iE_n} + \frac{\gamma_n(s)\tilde{B}_n}{s + iE_n} + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)B_m(0)}{s + iE_m} + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)\gamma_m(s)\tilde{B}_m}{s + iE_m} \\ & + \frac{(-i)^2}{s + iE_n} \sum'_{m,l} \frac{c(n|m)c(m|l)\tilde{B}_l}{s + iE_m} \end{aligned}$$

and separate out of the last term the contribution for $l = n$ and $l \neq n$. Then

$$\begin{aligned} \tilde{B}_n = & \frac{B_n(0)}{s + iE_n} + \frac{\tilde{B}_n}{s + iE_n} \left[\gamma_n(s) + (-i)^2 \sum'_m \frac{c(n|m)c(m|n)}{s + iE_m} \right] + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)B_m(0)}{s + iE_m} + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)\gamma_m(s)\tilde{B}_m}{s + iE_m} \\ & + \frac{(-i)^2}{s + iE_n} \sum'_{m,l} \frac{c(n|m)c(m|l)\tilde{B}_l}{s + iE_m} , \end{aligned} \quad (7)$$

where the star on the summation implies that none of the summation indices are equal. This process can be continued indefinitely and we shall just write down the third-order term as an example:

$$\begin{aligned} \tilde{B}_n = & \frac{B_n(0)}{s + iE_n} + \frac{\tilde{B}_n}{s + iE_n} \left\{ \gamma_n(s) + (-i)^2 \sum'_m \frac{c(n|m)c(m|n)}{s + iE_m} + (-i)^3 \sum'_{m,l} \frac{c(n|m)c(m|l)c(l|n)}{(s + iE_m)(s + iE_l)} \right\} \\ & + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)B_m(0)}{s + iE_m} + \frac{(-i)}{s + iE_n} \sum'_m \frac{c(n|m)\tilde{B}_m}{s + iE_m} \left\{ \gamma_m(s) + (-i)^2 \sum'_l \frac{c(m|l)c(l|m)}{s + iE_l} \right\} \\ & + \frac{(-i)^2}{s + iE_n} \sum'_{m,l} \frac{c(n|m)c(m|l)B_l(0)}{(s + iE_m)(s + iE_l)} + \frac{(-i)^2}{s + iE_n} \sum'_{m,l} \frac{c(n|m)c(m|l)\gamma_l(s)\tilde{B}_l}{(s + iE_m)(s + iE_l)} \\ & + \frac{(-i)^3}{s + iE_n} \sum'_{m,l,k} \frac{c(n|m)c(m|l)c(l|k)\tilde{B}_k}{(s + iE_m)(s + iE_l)} . \end{aligned} \quad (8)$$

It is now clear that if we define

$$\gamma_n(s) \equiv - \sum_{l=2}^{\infty} (-i)^l \sum'_{m_1, \dots, m_l} \frac{c(n|m_1) \cdots c(m_{l-1}|n)}{(s + iE_{m_1}) \cdots (s + iE_{m_{l-1}})} , \quad (9)$$

all terms on the right-hand side which have any $\gamma_m(s)$ in the numerator are zero. We then have the exact result in terms of the true operator self-energies:

$$\tilde{B}_n = \frac{B_n(0)}{s + iE_n} + \frac{1}{s + iE_n} \sum_{l=1}^{\infty} (-i)^l \sum'_{m_1, \dots, m_l} \frac{c(n|m_1) \cdots c(m_{l-1}|m_l)\tilde{B}_{m_l}}{(s + iE_{m_1}) \cdots (s + iE_{m_l})} \equiv \frac{B_n(0)}{s + iE_n} + \bar{\Gamma} \frac{(-i)}{s + iE_n} \sum'_m c(n|m)\tilde{B}_m , \quad (10)$$

where the iterative $\bar{\Gamma}$ operation is defined by the explicit expression in terms of "starred" summations over distinct indices.

Several comments are in order. First, this procedure has effected an explicit separation of $(s + i\mathcal{L})^{-1}B_n(0)$ into a diagonal part, $[s + iE_n(s)]^{-1}B_n(0)$, and a nondiagonal part. Next, it should be noted from Eq. (9) that $\gamma_n(s)$ is given implicitly in terms of all other $\gamma_m(s)$ and, therefore, expression (9) is not just the usual perturbation series in

powers of the c -matrix elements. The $\gamma_m(s)$ can be computed iteratively by choosing some initial $\gamma_m^{[0]}(s)$ for the right-hand side of Eq. (9) to get $\gamma_n^{[1]}(s)$ and then iterating. If one is judicious enough in choosing the $\gamma_n^{[0]}(s)$ in any given problem, the higher-order $l=3, 4, \dots$ terms may be made small. This is analogous to Dyson's equations where one chooses a self-energy ansatz in some particular way (i.e., summing all ring or ladder diagrams) so that the resulting expansion contains the useful physics. Dyson-type

resummation methods are extensively used in many-body calculations (see, in particular, Ref. 1 and Breene, Ref. 6). The "starred" summation excludes all terms in which any two of the summation indices are the same—these are included in the definition of the $\gamma_n(s)$. It is important to realize, however, that in the iteration the same basis operator can be arrived at via different commutators. For example, a typical result might be $c(1|2)c(2|4)B_4(0)$ or $c(1|3)c(3|4)B_4(0)$ —this will be clear in the example given below. Finally, in order to incorporate these results into the Liouvillian Green's-function approach and to calculate environmental effects as described in Ref. 2, one needs only

$$\gamma_a^{[2]}(s) = \sum_{\lambda} \left[\frac{c(a|b_{\lambda})c(b_{\lambda}|a)}{s + iE_{b_{\lambda}}} + \frac{c(a|b_{\lambda}^{\dagger})c(b_{\lambda}^{\dagger}|a)}{s + iE_{b_{\lambda}^{\dagger}}} \right] + \frac{c(a|b_{\lambda}^{\dagger}n)c(b_{\lambda}^{\dagger}n|a)}{s + iE_{b_{\lambda}^{\dagger}n}}, \quad (12)$$

where $n \equiv a^{\dagger}a$ and

$$c(a|b_{\lambda})_{\lambda} = -c(b_{\lambda}|a) = c(a|b_{\lambda}^{\dagger}) = c(b_{\lambda}^{\dagger}|a) = -\frac{1}{2}c(a|b_{\lambda}^{\dagger}n) = \frac{1}{2}c(b_{\lambda}^{\dagger}n|a) = -iM_{\lambda},$$

$$\epsilon_{b_{\lambda}} = \lambda, \quad \epsilon_{b_{\lambda}^{\dagger}} = -\lambda, \quad E_{b_{\lambda}^{\dagger}} = -\lambda + \gamma_{b_{\lambda}^{\dagger}n}(s).$$

Note that for pure boson operators such as b_{λ}^{\dagger} or $b_{\lambda}^{\dagger}b_{\lambda}$ the corresponding $\gamma(s)$ is identically zero, whereas for mixed operators such as $b_{\lambda}^{\dagger}n$ this is not so. If we now choose as our initial iteration $E_{b_{\lambda}^{\dagger}n} \approx -\lambda$ and use the continuum limit $\sum_{\lambda} M_{\lambda}^2 \rightarrow \beta \int_0^{\Lambda} d\lambda \lambda$, where $\beta \equiv (2|\vec{d}|^2 \kappa^2 / 3\pi)$ for \vec{d} the dipole matrix element and Λ is a high-energy cutoff, Eq. (12) gives

$$\gamma_a^{[2]}(s) \approx \beta \int_0^{\Lambda} d\lambda \lambda \left[\frac{1}{s + i\lambda} + \frac{1}{s - i\lambda} \right]$$

$$= \beta s \ln \frac{s^2 + \Lambda^2}{s^2}. \quad (13)$$

If we look at the pole approximation to Eq. (13) where

$$s + i\epsilon_a + \gamma_a(s) \approx s + i\kappa + i\Delta + \Gamma,$$

we have $\Gamma = \beta\kappa\pi$ and $\Delta = -2\beta\kappa \ln(\Lambda/\kappa)$, the usual Weisskopf-Wigner decay and improved log-divergent nonrelativistic Lamb shift. The logarithmic branch cut behavior of $\gamma_a(s)$ in Eq. (13) is intimately connected with the

to replace the ϵ_n defined there by $E_n(s)$ and drop all terms in which the c -matrix elements have the same indices.

The spontaneous emission of a two-level atom illustrates our results nicely.^{2,3} The Hamiltonian is given by

$$H = \kappa a^{\dagger}a + \sum_{\lambda} \lambda b_{\lambda}^{\dagger}b_{\lambda} + i \sum_{\lambda} M_{\lambda} (b_{\lambda}^{\dagger} + b_{\lambda})(a - a^{\dagger}), \quad (11)$$

where a is a Fermi annihilation operator for the two-level atom, b_{λ} an annihilation operator for photons of wave vector \vec{k} (polarization index suppressed), and $\lambda = |\vec{k}|$ (see Ref. 3 for further detail). From Eq. (9) the order $l=2$ contribution to $\gamma_a(s)$, for example, is

Paley-Wiener theorem and affects both the very short and the very long time behavior.³ To illustrate our earlier point about arriving at the same operator basis element via different commutators, one may easily check that $a^{\dagger}(0)$ arises at second order from $c(a|b_{\gamma})c(b_{\gamma}|a^{\dagger})$, $c(a|b_{\gamma}^{\dagger})c(b_{\gamma}^{\dagger}|a)$, and $c(a|b_{\gamma}n)c(b_{\gamma}n|a^{\dagger})$.

For the spontaneous emission line-shape calculation just presented, it is clear that we did not need to use this new resummation procedure; however, for more complicated problems, especially for those where environmental effects are important, it is anticipated that the improved Liouvillian Green's-function approach will prove useful. As mentioned earlier, an important advantage of the derivation given herein is that it allows one to obtain approximations to the exact equations of motion in a manner similar to that used when approximating the self-energy via Dyson's equation. One can replace all $i\epsilon_n$ by the corresponding approximated $iE_n(s)$ calculated using Eq. (9) and truncate the equations of motion at some given order. This approach also seems well suited for computer calculations.

¹A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

²M. D. Girardeau, Phys. Rev. A **28**, 1056 (1983); M. D. Girardeau and C. F. Hart, *ibid.* **28**, 1072 (1983).

³C. F. Hart, Phys. Rev. A **28**, 186 (1983).

⁴B. R. Mollow, Phys. Rev. **188**, 1969 (1969).

⁵L. vanHove, Physica **21**, 901 (1955).

⁶A recent exposition of projection operator methods is H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Mechan-*

ics, Springer Tracts in Modern Physics, Vol. 95 (Springer-Verlag, New York, 1982). The Brussels School approach is given in R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley, New York, 1975). A good account of various different approaches with many references is R. G. Breene, Jr., *Theories of Spectral Line Shape* (Wiley, New York, 1981).

⁷We use a slightly different definition of the Laplace transform than that given in Ref. 2.