Exponential series expansion for correlation functions of many-body systems

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We demonstrate that in Hamiltonian many-body systems at equilibrium, any kind of time dependent correlation function $c(t)$ can always be expanded in a series of (complex) exponential functions of time when its Laplace transform $\tilde{C}(z)$ has single poles. The characteristic frequencies can be identified as the eigenfrequencies of the correlation. This is done without introducing the concepts of fluctuating forces and memory functions, due to Mori and Zwanzig and extensively used in the literature in the last decades. Our method is based on a different projection technique in the Hilbert space S of the system and shows that appropriate approximations of the exponential series are related to the contraction of S to a finite, usually small, number of dimensions. The time dependence of correlation functions is always described in detail by a multiple-exponential functionality also at long times. This result is therefore also valid for correlation functions of many-body Hamiltonian systems for which a power-law dependence, observed in restricted time ranges and predicted to be the asymptotic one, can be considered at most as a useful approximate modeling of long-time behavior.

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I. INTRODUCTION

Any kind of experimental spectroscopic study of the dynamical properties of a many-body system at thermal equilibrium is related to the time dependence of a correlation function of relevant variables. This is true for any possible probe acting within the linear response framework, such as, for example, either photons or particles interacting with nuclear, atomic, and molecular matter in the various aggregation states. In the theory, these correlation functions are given by means of the definition of a proper inner product (B,A) which characterizes the L^2 Hilbert space S of the variables of the system. We will consider the class of either classical or quantum-mechanical linear operators A and B corresponding to the variables of the many-body system under discussion. In this framework, the correlation function $c(t) = [B, A(t)]$, which represents either a cross correlation (for $A \neq B$) or an autocorrelation (for $A = B$), is studied starting from the Hamiltonian formalization of the dynamics given by the Liouville equation of motion $dA(t)/dt = iLA(t)$. The latter is a linear transformation determining the dynamics in S. The linear Hermitian operator L, in the classical dynamics of an N-particle system, is the Liouville operator $L = i\{H, \cdots\}$ where $\{\cdots, \cdots\}$ denotes the Poisson brackets, while in the quantum N-body case, $L = (1/\hbar)[H, \cdots]$ and $[\cdots, \cdots]$ denotes the commutator. The previous equation represents the Heisenberg equation, where H is the total Hamiltonian of the system.

For the complex spectrum of $c(t)$, given by $\tilde{C}(z) = \mathcal{L}[c(t)]$ where $\mathcal{L}$ denotes the Laplace transform, the most general approach up to now devised to the determination of a possible spectral form is the one by Mori and Zwanzig (MZ) [1–3]. This procedure starts from (i) the determination of a basis of vectors, also called "fluctuating forces," which is constructed by means of an *ad hoc* series of projection operators and (ii) the introduction of memory functions as autocorrelations of these basis vectors. Starting from these points, the theory shows that $c(t)$ satisfies a recurrence relation which is an integro-differential equation of the second-order Volterra type, usually indicated as the generalized Langevin equation (GLE). The GLE for $c(t)$ is linked by recurrence to a hierarchy of integro-differential equations for the memory functions. The solution to the problem is finally given by Laplace transforming the equation hierarchy to obtain a continued fraction representation of $\tilde{C}(z)$.

One limitation of the MZ theory is that the basis created in the projection procedure, i.e., the set of fluctuating forces, is not complete. In fact, the projection of the operators $A(t)$ or $B(t)$ onto the fluctuating-force basis contains a correlation integral which involves memory functions [4]. Therefore, this basis cannot be used as a general means of projection in S. Another difficulty in the MZ theory arises from the fact that each vector of the basis has a dynamics which is driven by a different linear transformation, even though within the Liouville equation scheme, so that dynamical behavior in the space S cannot be univocally characterized. Due to this last fact, the link between the various memory functions and the evolution of a generic property of the system under study becomes rather indirect and almost formal. The difficulty of understanding the physical meaning of the concepts of fluctuating forces and memory functions, and of the equation hierarchy in the MZ theory, induces a consequent difficulty in the interpretation of the continued fraction representation of the spectrum $\tilde{C}(z)$, which sometimes causes the application of improper approximations to the continued fraction itself.

Nevertheless, the construction of a suitable orthogonal set in S can be, in principle, realized following other routes, which can be chosen in order to avoid the difficulties presented by the MZ theory.

Here we will show that following the well-known Gram-Schmidt (GS) procedure as modified by Lee [5–7], an orthogonal and complete vector basis will be constructed in S, and we will give an explicit functional expression of correlation functions, showing that these can be written as a series of time dependent exponential functions. While Lee's approach was limited to the discussion of autocorrelations of Hermitian operators in order to deal with time-reversal symmetric $c(t)$, here we shall obtain a general result also for the case of cross correlations of possibly non-Hermitian operators.

This is a relevant generalization of what we have already shown for special cases, namely those of autocorrelations in classical [8] or quantum [9] systems. The result presented here has the role of a general theorem which can be applied to any one of the fields mentioned at the beginning. We will accomplish this result without introducing the fluctuating force and memory function concepts by using a hierarchy of differential equations and clarifying the connection between possible approximate forms of $c(t)$ and the contraction of the dimensionality of the Hilbert space under consideration. This theoretical derivation is contained in Sec. II, while the conclusions are summarized in Sec. III.

II. GENERAL THEORY

Let us start from the general time expansion representation of the operator $B(t)$ which can be immediately derived from the Liouville equation, i.e.,

$$B(t) = \exp(iLt)B = \sum_{\nu=0}^{\infty} \xi_\nu(t) B^{(\nu)}, \tag{1}$$

where $\xi_\nu(t) = t^\nu/\nu!$ are time dependent coefficients, and $B^{(\nu)} = (iL)^\nu B = [d^\nu B(t)/dt^\nu]_{t=0}$ are the time derivatives of $B(t)$ at $t = 0$ and $B^{(0)} \equiv B$. Here we assume, as it is usually done when Eq. (1) is used in theoretical physics, that all the $B^{(\nu)}$ exist and are univocally defined in terms of the variables of the system.

The time evolution of the N-body system, as mentioned before, can be studied in practice with reference to an appropriate correlation function between two observables defined in a Hilbert space S where Eq. (1) is a possible representation of the time behavior of the operators of the system. The detailed study clearly requires for two operators the assumption of a specific form for the inner product (B,A) and, consequently, the normalization and the metric of the space S. Here, for the moment, we do not need to specify the detailed form of the inner product (B,A).

We first observe that the solution of Eq. (1) gives $B(t)$ in terms of the complete set $\{B^{(\nu)}\}$ in S which, however, is not an orthogonal set.

Once a particular form of the inner product is defined in S, the GS process permits one to construct an orthogonal complete set $\{f_\nu\}$ out of $\{B^{(\nu)}\}$ and write $B(t)$ as an expansion in terms of $\{f_\nu\}$ with new time dependent coefficients in place of the $\{\xi_\nu(t)\}$. Since in the GS process one of the $\{f_\nu\}$ can be chosen arbitrarily, we start with the choice $f_0 = B$. The GS when applied to $\{B^{(\nu)}\}$ gives the first few f_ν as linear forms of the quantities $B^{(\nu)} = (iL)^\nu f_0$ and $f_0, \ldots, f_{\nu-1}$. In particular, we have $f_0 = B^{(0)} = B$; $f_1 = B^{(1)} - i\Omega_0 f_0 = iLf_0 - i\Omega_0 f_0$ where $i\Omega_0 = (B^{(1)}, B^{(0)})/(B^{(0)}, B^{(0)}) = (iLf_0, f_0)/(f_0, f_0)$; and $f_2 = iLf_1 - i\Omega_1 f_1 + \Delta_1 f_0$ with $\Delta_1 = -(iLf_1, f_0)/(f_0, f_0) = (f_1, f_1)/(f_0, f_0)$ and $i\Omega_1 = (iLf_1, f_1)/(f_1, f_1)$.

Instead of using the GS method applied to the $\{B^{(\nu)} = (iL)^\nu f_0\}$, the expressions of f_1 and f_2 suggest construction of the $\{f_\nu\}$ successively in terms of the $\{iLf_{\nu-1}\}$ which, in turn, results in combinations of the $B^{(\mu)}$ with $\mu \leqslant \nu$. Here we adopt this alternative procedure, showing that it permits one to arrive at a very useful recurrence relation.

Let us continue in the construction, first with f_3 and then in general. We start with the expression

$$f_3 = iLf_2 + X, \tag{2}$$

and search for the explicit expression of the vector X requiring orthogonality of f_3 with all the other previous vectors, i.e.,

$$(f_3, f_0) = (iLf_2, f_0) + (X, f_0) = 0, \tag{3a}$$

$$(f_3, f_1) = (iLf_2, f_1) + (X, f_1) = 0, \tag{3b}$$

$$(f_3, f_2) = (iLf_2, f_2) + (X, f_2) = 0. \tag{3c}$$

The first one, by using the property of L of being Hermitian and the expression of f_1, gives $(f_3, f_0) = -(f_2, f_1) - i\Omega_0(f_2, f_0) + (X, f_0) = 0$, where the first two terms vanish for the orthogonality of f_2 to both f_1 and f_0 so that X is orthogonal to f_0 as well. Then, Eqs. (3b) and (3c) allow one to write X as a linear combination of f_1 and f_2, leading to

$$f_3 = iLf_2 - i\Omega_2 f_2 + \Delta_2 f_1, \tag{4}$$

where $\Delta_2 = -(iLf_2, f_1)/(f_1, f_1) = (f_2, f_2)/(f_1, f_1)$ and $i\Omega_2 = (iLf_2, f_2)/(f_2, f_2)$.

In general, we can apply the same procedure to $f_{\nu+1}$ and have the recurrence relation

$$f_{\nu+1} = iLf_\nu - i\Omega_\nu f_\nu + \Delta_\nu f_{\nu-1}, \tag{5}$$

with $\Delta_\nu = (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$ and $i\Omega_\nu = (iLf_\nu, f_\nu)/(f_\nu, f_\nu)$. These formulas hold for $\nu \geqslant 1$ but can be extended to the case $\nu = 0$ if one defines $f_{-1} \equiv 0$, while Δ_0 is given a nonzero value explicitly defined later. The quantities Ω_ν and Δ_ν are real, with $\Delta_\nu > 0$.

Since the time evolution of all the vectors in S is governed by the same Liouville operator equation, the same time shift $\exp(iLt)$ applies to all of the members of the set $\{f_\nu\}$. Then, Eq. (5) can also be written as

$$f_{\nu+1}(t) = \frac{d}{dt} f_\nu(t) - i\Omega_\nu f_\nu(t) + \Delta_\nu f_{\nu-1}(t), \tag{6}$$

which is a differential recurrence relation connecting the time dependent orthogonal basis vectors created with our method.

Equation (5) can be used starting from f_0 to derive the explicit expressions of all the

$$f_\nu = f_\nu(B, B^{(1)}, \ldots, B^{(\nu)}; \Delta_1, \ldots, \Delta_{\nu-1}; \Omega_1, \ldots, \Omega_{\nu-1}). \tag{7}$$

If we now expand an operator $A(t)$ in terms of the set $\{f_\nu\}$ as

$$A(t) = \sum_{\nu=0}^{\infty} b_\nu^*(t) f_\nu, \tag{8}$$

the expansion coefficients are the normalized correlations $b_\nu^*(t) = (A(t), f_\nu)/(f_\nu, f_\nu)$ and for their complex conjugate we have $b_\nu(t) = (f_\nu, A(t))/(f_\nu, f_\nu)$. The first of these is just $b_0(t) = (B, A(t))/(f_0, f_0)$, which is the normalized version of the correlation function $c(t)$ that we are interested in. The respective zero-time values are $b_\nu(t = 0) = 0$ with $\nu > 0$ and $b_0(t = 0) = (B, A)/(f_0, f_0)$.

The substitution of Eq. (8) into the Liouville equation for $A(t)$ and the use of the recurrence relation in Eq. (5) permits

one to derive a differential recurrence relation also for the correlations $b_\nu(t)$, i.e.,

$$\frac{d}{dt}b_\nu(t) - i\Omega_\nu b_\nu(t) + \Delta_{\nu+1}b_{\nu+1}(t) - b_{\nu-1}(t) = 0, \quad (9)$$

for $\nu \geqslant 0$ and $b_{-1} = 0$.

The Laplace transformation of Eq. (9) gives

$$\tilde{b}_{\nu-1}(z) = (z - i\Omega_\nu)\tilde{b}_\nu(z) + \Delta_{\nu+1}\tilde{b}_{\nu+1}(z), \quad (10)$$

where $\nu \geqslant 0$ and we have defined $\tilde{b}_{-1}(z) = 1$. Equation (10) can also be written as

$$\tilde{b}_0(z) = \left[z - i\Omega_0 + \frac{\Delta_1\tilde{b}_1(z)}{\tilde{b}_0(z)}\right]^{-1}, \quad (11a)$$

$$\frac{\tilde{b}_\nu(z)}{\tilde{b}_{\nu-1}(z)} = \left[z - i\Omega_\nu + \frac{\Delta_{\nu+1}\tilde{b}_{\nu+1}(z)}{\tilde{b}_\nu(z)}\right]^{-1}, \quad (11b)$$

with $\nu \geqslant 1$. If we now define

$$\tilde{K}_0(z) = \tilde{b}_0(z), \quad (12a)$$

$$\tilde{K}_\nu(z) = \Delta_\nu\frac{\tilde{b}_\nu(z)}{\tilde{b}_{\nu-1}(z)}, \quad (12b)$$

from Eqs. (11) it follows that

$$\tilde{K}_0(z) = [z - i\Omega_0 + \tilde{K}_1(z)]^{-1}, \quad (13a)$$

$$\tilde{K}_\nu(z) = \Delta_\nu[z - i\Omega_\nu + \tilde{K}_{\nu+1}(z)]^{-1}. \quad (13b)$$

Recursive application of Eqs. (13) gives the continued fraction representation of any $\tilde{K}_\nu(z)$ with $\nu \geqslant 0$, which is also the form of the final result of the MZ theory, i.e.,

$$\tilde{K}_\nu(z) = \cfrac{\Delta_\nu}{z - i\Omega_\nu + \cfrac{\Delta_{\nu+1}}{z - i\Omega_{\nu+1} + \cfrac{\Delta_{\nu+2}}{z - i\Omega_{\nu+2} + \cdots}}}, \quad (14)$$

where, in the case $\nu = 0$, the definition $\Delta_0 = b_0(t = 0) = (B, A)/(f_0, f_0)$ is adopted.

It can be noted that in the time domain, Eqs. (13) correspond to

$$\dot{K}_\nu(t) - i\Omega_\nu K_\nu(t) + \int_0^t dt' K_{\nu+1}(t - t')K_\nu(t') = 0 \quad (15)$$

(with $\nu \geqslant 0$), i.e., to a set of recurrent differential equation of second-order Volterra type given in the MZ theory for the memory functions and usually named Langevin equations, which here appear to be just a direct consequence of the dynamical behavior expressed in Eq. (9) and shows that the solution of the many-body dynamics given by the complex spectral distribution (14) does not need the introduction of the concept of memory function, even though in some case it may be useful. From Eq. (15), we also see that $(f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1}) = \Delta_\nu = K_\nu(t = 0) > 0$ for $\nu > 0$.

It can be observed that $\tilde{K}_\nu(z)$ is defined with respect to the subspace $S_\nu \subset S = S_0$, which is also a Hilbert space, spanned, however, by $f_\nu, f_{\nu+1}, \ldots$. In the case of a Hermitian operator, the autocorrelation $(B, B(t))$ is easily shown to be an even function of time and all Ω_ν vanish identically, so that the expression given by Eq. (14) for $\tilde{K}_0(z)$ is identical to the one previously derived in special cases [5,8,9] for the relaxation function and to the one derived in the case of classical many-body systems [8]. It is worthwhile to notice here that in practical cases, the necessary approximations always reflect a termination of the continued fraction in Eq. (14) at an appropriate level, indicating, at the same time, a restriction of the dimensionality of the S_ν space considered.

The λth convergent of the continued fraction (14) can be expressed as ratios of polynomials in z [10]:

$$\tilde{K}_\nu^{(\lambda)}(z) = \Delta_\nu\frac{\det\mathbf{D}^{(\lambda,\nu+1)}(z)}{\det\mathbf{D}^{(\lambda,\nu)}(z)}, \quad (16)$$

where $\mathbf{D}^{(\lambda,\nu)}(z)$ is a $(\lambda - \nu)$-dimensional tridiagonal symmetric matrix whose elements are $D_{\alpha\alpha}^{(\lambda,\nu)} = z - i\Omega_{\alpha+\nu-1}$, $D_{\alpha\beta}^{(\lambda,\nu)} = i\Delta_{\alpha+\nu}^{1/2}\delta_{\alpha,\beta-1}$ where $1 \leqslant \alpha < \beta \leqslant \lambda - \nu$.

By taking the limit for $\lambda \to \infty$, Eq. (16) represents a meromorphic function with an infinite number of poles that can be written by applying the standard method of partial fraction decomposition as a uniformly convergent series [11], leading to

$$\tilde{K}_\nu(z) = \sum_{j=1}^{\infty}\frac{I_j^{(\nu)}}{z - z_j^{(\nu)}}, \quad (17)$$

where we have dropped the superscript λ, having taken the limit to infinity. Here, $\{z_j^{(\nu)}\} = \{z_1^{(\nu)}, z_2^{(\nu)}, \ldots\}$ is the set of poles [12], and the residues $I_j^{(\nu)}$ are

$$I_j^{(\nu)} = \lim_{z\to z_j^{(\nu)}}\left(z - z_j^{(\nu)}\right)\tilde{K}_\nu^{(}z). \quad (18)$$

Since the series in Eq. (17) is uniformly convergent, term-by-term Laplace antitransformation can be performed and we can write, for $t \geqslant 0$,

$$K_\nu(t) = \sum_{j=1}^{\infty} I_j^{(\nu)}\exp\left(z_j^{(\nu)}t\right). \quad (19)$$

Equations (17)–(19) refer, for simplicity, to the case in which all of the quantities $\{z_j^{(\nu)}\}$ are distinct poles of $\tilde{K}_\nu(z)$. It is well known, however, that the partial fraction decomposition method can handle the case of multiple poles as well. The expressions for $\tilde{K}_\nu(z)$ and $K_\nu(t)$, valid in the general case of multiple poles, are reported in the Appendix.

In Eq. (19), $I_j^{(\nu)}$ and $z_j^{(\nu)}$, with $\nu \geqslant 0$, appear as the amplitudes and the eigenfrequencies, respectively, of a normal mode representation of $K_\nu(t)$, and may be in general either real or complex, with $\mathrm{Re}(z_j^{(\nu)}) < 0$ in order to have, as usual, $K_\nu(t) \to 0$ for $t \to \infty$. (The case in which $\mathrm{Re}(z_j^{(\nu)}) = 0$ for a given j is also possible, as it corresponds to an oscillating time behavior where $K_\nu(t)$ remains, however, a bounded function.) In particular, for the correlation that we are interested in, we have

$$b_0(t) = (B, A(t))/(B, B) = \sum_{j=1}^{\infty} I_j^{(0)}\exp\left(z_j^{(0)}t\right). \quad (20)$$

Equation (20), which we shall denote as the exponential function (EF) solution of the dynamics of the many-body system, is the statement of the theorem.

Moreover, as it appears obvious from their respective definitions, all four sets $\{\Omega_\nu\}$, $\{\Delta_\nu\}$, $\{I_j^{(0)}\}$, and $\{z_j^{(0)}\}$ may be expressed in terms of the set of the normalized moments $M^{(k)} = (-i)^k (d^k b_0(t)/dt^k)_{t=0}$. In particular, from Eq. (20), it follows that $\{I_j^{(0)}\}$ and $\{z_j^{(0)}\}$ satisfy a set of relations of the form

$$\sum_{j=1}^{\infty} I_j^{(0)} \left(z_j^{(0)}\right)^k = i^k M^{(k)}, \tag{21}$$

for $k = 0,1,2,\ldots$. Equation (19) shows that an EF solution holds as well for any of the memory functions $K_\nu(t)$ related, in the MZ approach, to the correlation function $b_0(t)$, and the above considerations also apply to each of them.

The expansion (20) in an infinite sum of exponential functions is a fully general expression for the time behavior of the quantum-mechanical normalized correlation function $b_0(t)$, which is an alternative to the usual Maclaurin power expansion,

$$b_0(t) = \sum_{n=0}^{\infty} \frac{i^n M^{(n)}}{n!} t^n. \tag{22}$$

Both series (20) and (22) are exact and have the same convergence properties when all of the moments $M^{(k)}$ do exist and are finite, as it is usually assumed for any well-behaved physical correlation $b_0(t)$. Indeed, by Taylor expanding the exponentials in (20) and using (21), Eq. (22) is immediately obtained.

In some sense, however, the series (20) and (22) are complementary to each other when approximated by truncating summation after a few terms. The form (22) is useful in describing the behavior at short times, while Eq. (20) can be useful at longer times. In fact, approximations of Eq. (22) mean to retain few power terms, while to approximate Eq. (20) means to retain few exponentially decaying functions, which is the same as truncating the continued fraction given by Eq. (14) at a conveniently low level. Obviously, both approximations violate, at some level, the physical request that all frequency moments of $(B, A(t))$ must be determined and finite, limiting the number of relations (21) that can be used in practice in the analysis of either experimental or calculated correlations and spectra. This violation is also reflected in the fact that if the continued fraction expression of $\tilde{b}_0(z)$ is truncated by setting $\tilde{K}_\nu(z)$ to a constant value, then Eq. (12b) implies that $\tilde{b}_\nu(z)$ and $\tilde{b}_{\nu-1}(z)$ are linearly dependent, which is inconsistent and leads Lee to exclude a single-exponential behavior for $b_0(t)$ as shown in Refs. [6,13].

In a many-body system, the inner product used in the definition of a general two-variable correlation function is usually given by $(B, A(t)) = \mathrm{Tr}[BA^\dagger(t)\rho]$ where ρ is the statistical density operator given by $\rho = I$ in pure states, and by either $\rho = \exp(-\beta H)$ or $\rho = \exp[-\beta(H - \mu N)]$ at thermodynamic equilibrium in the canonical and grand-canonical ensemble, respectively. Here, $\beta = 1/(k_B T)$, where k_B is the Boltzmann constant, T is the temperature, μ is the chemical potential, I is the identity operator, and N is the particle number operator. When the results of linear response theory, such as either response or relaxation functions, are relevant for the discussion, the inner product can also be represented by the Kubo transform [14] $(B, A(t)) = \int_0^\beta d\lambda \mathrm{Tr}[B \exp(-\lambda\Gamma) A^\dagger(t) \exp(\lambda\Gamma)\rho]$ with $\Gamma = H$ and $\Gamma = H - \mu N$ in the canonical and grand-canonical ensemble, respectively.

III. CONCLUSIONS

The main result of this work can also be cast in the form of a theorem, as follows:

(1) Any correlation function $c(t) = (B, A(t))$ of a many-body system, either classical or quantum mechanical in first and in second quantization, at thermodynamic equilibrium, under the following hypotheses:

(i) the system is Hamiltonian;

(ii) an L^2 Hilbert space S of the system is defined;

(iii) the operators A and B are linear and correspond to dynamical variables of the system;

(iv) the Laplace transform $\tilde{C}(z)$ has single poles;

can be expanded in a series of time dependent exponential functions, with a characteristic set of complex frequencies which can be identified as the eigenfrequencies of the correlation and are functions of the moments of the related spectrum.

(2) At thermodynamic equilibrium, the eigenfrequencies depend on the state variables, for example density and temperature.

(3) The Laplace transform of the correlation turns out to be expressed by a corresponding series of complex functions of the form

$$\tilde{C}(z) = \sum_{j=1}^{\infty} \frac{I_j^{(0)}}{z - z_j^{(0)}}. \tag{23}$$

(4) Depending on the appropriate definition of the inner product in S, the correlation function can represent a property of either a classical or a quantum-mechanical system, in particular a correlation function, a response function, and a relaxation function in the linear response theory, or a Green function. The last one can be particularly useful in describing correlations and spectra of spins in magnetic systems and bosonic and fermionic systems in condensed matter. An example of an application to the relaxation function in a quantum system, namely, for the spectrum of velocity autocorrelation function in liquid hydrogen, was given in Ref. [9].

(5) The correlation functions can refer to statistical systems described either in pure quantum states or in the canonical or in the grand-canonical ensemble.

(6) The EF series expansion (20) of $b_0(t)$ provides a representation of its time behavior equivalent to, and as general as, the Maclaurin series (22). In the comparison with spectroscopic results, obtained either in time or frequency domain, the expansion is necessarily approximated with a finite number of terms and the cutoff directly reflects the restriction to a finite number of dimensions for the Hilbert space S in which we assume the dynamics can be actually represented. This approach can be particularly useful, in general, in long-time approximations of correlation functions as well as in low-frequency approximations of the related spectra.

(7) Our result shows that for describing the behavior of either the correlation function or its spectrum, there is no need to refer directly to the concepts of fluctuating forces and memory functions, or to the continued fraction approach that has been used so much in the past following Mori and Zwanzig. On the other hand, Eq. (19) shows that not only the correlation $b_0(t)$ but also a memory function of any order is expressed by an EF expansion. Then, proper approximations to the dynamic behavior can also be obtained by truncating the EF series representing a certain $K_\nu(t)$. It is important, however, to realize that such approximations correspond to projections of S onto finite-dimension subspaces that are, in general, different from those obtained by truncation of the series (20). In Ref. [9], we showed examples of both types, where the truncation of the exponential series is applied to either the correlation function itself or the second-order memory function. In properly approximated forms, the EF expansion has also been explicitly applied to the description of the dynamics of a variety of systems [15–22]. Moreover, an EF-based expression is assumed implicitly, though sometimes inadvertently, in all cases where an MZ continued fraction is truncated at some level in such a way as to give $\tilde{b}_0(z)$ the form of Eq. (16).

(8) As a consequence of the above theorem, the time dependence of a correlation function in Hamiltonian many-body systems is always rigorously given in the EF form also at long times. Power-law asymptotic behaviors are often used to describe long-time tails [23–26]. However, in some cases, the appearance of such time dependences is either not well assessed or limited to restricted time ranges and selected thermodynamic states [27,28]. In any case, from a general theoretical point of view, since the EF form is an exact representation, asymptotic power-law behaviors should be considered no more than effective approximate models for microscopic Hamiltonian dynamics correlations. It is, however, clear that asymptotic behavior can in practice be well represented by both EF and power laws, depending on the precision of the data under examination. On the other hand, there are non-Hamiltonian systems in which an EF behavior could not be adequate [29,30].

APPENDIX

When the jth pole $z_j^{(\nu)}$ is of order n_j, the partial fraction decomposition of Eq. (17) is written as

$$\tilde{K}_\nu(z) = \sum_{j=1}^{\infty} \sum_{\mu=1}^{n_j} \frac{I_{j\mu}^{(\nu)}}{\left(z - z_j^{(\nu)}\right)^\mu},$$

where the coefficients are given by

$$I_{j\mu}^{(\nu)} = \frac{1}{(n_j - \mu)!} \lim_{z \to z_j^{(\nu)}} \frac{d^{n_j-\mu}}{dz^{n_j-\mu}} \left[\left(z - z_j^{(\nu)}\right)^{n_j} \tilde{K}_\nu(z)\right].$$

In the time domain, Eq. (19) is replaced, in the general case, by

$$K_\nu(t) = \sum_{j=1}^{\infty} \sum_{\mu=1}^{n_j} I_{j\mu}^{(\nu)} \exp\left(z_j^{(\nu)} t\right) \frac{t^{\mu-1}}{(\mu-1)!}.$$

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