Subdynamics, Fokker-Planck equation, and exponential decay of relaxation processes

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The problem of relaxation is studied via the microscopic Hamiltonian model of an impurity (or particle of interest) embedded in a linear chain of harmonic oscillators. When the mass of the particle of interest is sufficiently larger than that of the "bath" particle and the system is classical, the velocity autocorrelation function of the particle of interest is known to consist of the sum of an exponentially decaying term and a nonexponential contribution with a slow tail of oscillatory nature. The damping of the exponential decay is determined by using a renormalization procedure within the context of the generalized Langevin equation. By expressing the "bath" coordinates in terms of normal modes and using a scalar product of the Kubo type, it is shown that the classical Liouvillian becomes formally equivalent to the quantum-mechanical Hamiltonian introduced by Friedrichs to study unstable quantum-mechanical states. In the case of a finite number N of particles (or $2N$ normal modes) the excited state of the Friedrichs model largely overlaps an "eigenstate" $|S\rangle$, the "eigenvalue" of which is straightforwardly expressed in terms of the model parameters. It is shown that in the continuum limit ($N=\infty$) this "eigenvalue" becomes complex and its imaginary part coincides with the renormalized damping above. It is also shown that the projection approach to the Fokker-Planck equation leads precisely to the same renormalized damping coefficient. The major conclusion is that the Fokker-Planck description refers to the stochastic dynamics of a sort of dressed variable rather than that of the merely bare velocity. Furthermore, we conclude that whereas the decay of the autocorrelation function of the bare velocity cannot be exponential in accordance with the general remarks by Lee [Phys. Rev. Lett. **51**, 1227 (1983)], the decay of the dressed variable is an exact exponential. It is argued that to establish a contact with real experiments, the Kubo approach to the linear response to an external excitation should be reformulated and that this might naturally lead to the basic tenets of the subdynamics of Prigogine and coworkers. The relations between the present and a former approach to the Fokker-Planck equation to be associated to non-Markovian processes are studied.

I. INTRODUCTION

The problem of assessing whether or not the time decay of a relaxation process is rigorously exponential has been the subject of recent investigations. For a more detailed discussion of the basic literature on this important issue we refer the reader to the recent work of Lee,[1] who showed that the decay of relaxation process with a rigorous Hamiltonian origin cannot be rigorously exponential, since this would conflict with the fulfillment of a rigorous sum rule, established on the basis of recurrence relations stemming from the genuine Hamiltonian nature of the microscopic interaction among the component of the physical system under study.

On the other hand, recent research work carried out by Der on the establishment of a time local Langevin equation[2-4] shows that under precise circumstances this can be done by relying on a sort of slowest eigenvalue,[2] which implies again the introduction of a rigorous exponential behavior. This seems to contrast not only with the point of view of Lee, but also with very simple Hamiltonian models such as that of a particle linearly coupled to a chain of harmonic oscillators. In this case well-known analytical expressions for autocorrelation functions are available, which, in accordance with the general remarks of Lee, reveal indeed a nonexponential nature.[5-7] Let us focus on the case of an impurity embedded in a linear chain of particles. This is the model under investigation in this paper. It is well known that even in the case where the impurity is characterized by a mass very large compared with that of the bath particles, the time decay of the autocorrelation function of the velocity of the impurity exhibits a significant deviation from the exponential behavior in the long-time region, in addition to a deviation from the exponential behavior in the short-time region. In this long-time region the decay process is characterized indeed by a sort of damped oscillatory regime. This would lead to the conclusion that the exponential decay is the result of an approximation and the Fokker-Planck equation, which leads to an exponential behavior, is itself an approximated equation of motion.

The major aim of this paper is to show that the Fokker-Planck equation actually corresponds to studying the motion of a sort of dressed variable, or, adopting a quantum-mechanical language, of a "dressed state" and the conflict with the rigorous nonexponential character of a correlation function is only apparent. The correlation function corresponds to the decay of a bare state, whereas the Fokker-Planck equation describes the relaxation process of a dressed state. If the time-scale separation between system and bath is rendered infinitely large, the two descriptions tend to coincide. When the time-scale separation between system and bath is not infinitely large, or, equivalently, the time scale of the bath does not vanish, the two descriptions lead to different predictions. This involves the subtle problem of how to actually carry out a true experiment. According to Prigogine and co-workers,[8(a)] this is an aspect of great relevance which also applies to the problem of measurement in quantum mechanics. This dressed state we are talking about coincides indeed with the concept of subdynamics introduced by Prigogine and co-workers.[8(a)] Concerning this aspect, the element of originality of our treatment relies on the use of the Schrödinger picture, which has the capability of rendering the derivation of the dressed state very transparent.

The tendency of a system to precipitate in a dressed state characterized by a rigorously exponential decay has already been noticed some years ago in a different context[9,10] and has been the subject of intense discussions by Prigogine and co-workers.[8(a)] If this were proved to be a general property of the interaction between a microscopic system and a macroscopic measurement apparatus, the Fokker-Planck equation, as resulting from the renormalized procedure of Ref. 11 and exhaustively illustrated for the first time in the present paper, would become a theoretical tool of greater interest.

The paper is organized as follows. Section II is devoted to deriving the renormalized drift coefficient within the generalized Langevin picture. In Sec. III we show that the classical Liouvillian of a linear chain with an impurity mass, expressed in the Hilbert space generated by the Kubo scalar product, is equivalent to the quantum-mechanical Hamiltonian of the Friedrichs model.[8(b)] Furthermore, using this equivalence, we determine the "dressed" state $|S\rangle$ resulting in a rigorously exponential decay. Section IV is devoted to showing that the Fokker-Planck equation provides a description of the statistical properties of the "dressed" variable S rather than the "bare" variable velocity v. Connections with a former approach to the Fokker-Planck equation are discussed in the Appendix. Concluding remarks are found in Sec. V.

II. SHORT REVIEW OF THE STANDARD RESULTS ON THE DYNAMICS OF AN IMPURITY EMBEDDED IN A LINEAR CHAIN OF HARMONIC OSCILLATORS

In this paper we study a physical system described by the following Hamiltonian:

$$\mathcal{H}=\sum_{i=-N}^{N}\frac{p_i^2}{2m_i}+\frac{k}{2}\sum_{i=-N}^{N-1}(q_{i+1}-q_i)^2 , \qquad (2.1)$$

where $m_i=m$ if $i\neq 0$ and $m_i=M$ if $i=0$. By using the continued-fraction procedure of Ref. 12 we can easily evaluate the correlation function of the moment p_0, defined as follows:

$$\Phi_0(t)\equiv\frac{\langle p_0p_0(t)\rangle}{\langle p_0^2\rangle}=\frac{1}{\langle p_0^2\rangle}\int d\Gamma\, p_0p_0(t)\rho_{\rm eq}(\Gamma) , \qquad (2.2)$$

where the time evolution of the moment p_0 is driven by

$$\frac{\partial}{\partial t}p_0(t)=-\mathcal{L}p_0(t) , \qquad (2.3)$$

$\mathcal{L}$ being the classical Poisson bracket associated with the Hamiltonian of Eq. (2.1), and the equilibrium distribution, on which the average of Eq. (2.2) is carried out, is given the canonical form

$$\rho_{\rm eq}\propto\exp(-\mathcal{H}/k_BT) . \qquad (2.4)$$

We adopted the synthetic notation $d\Gamma=dp_0dp_1\cdots dq_0dq_1\cdots$. By adopting the quantumlike formalism of Ref. 12 the correlation function of Eq. (2.2) can be rewritten as follows:

$$\Phi_0(t)=\langle f_0|f_0(t)\rangle/\langle f_0|f_0\rangle , \qquad (2.5)$$

where the "quantum-mechanical" state $|f_0\rangle$ must be identified with the variable p_0. The scalar product follows the following general definition:

$$\langle A|B\rangle\equiv\int d\Gamma\, A^*(\Gamma)B(\Gamma)\rho_{\rm eq}(\Gamma) , \qquad (2.6)$$

where A and B denote two generic functions of the phase space Γ.

From the theory of Ref. 12 we also derive that $\Phi_0(t)$ obeys the following equation of motion:[13]

$$\dot\Phi_0(t)=-\Delta_1^2\int_0^t d\tau\,\Phi_1(\tau)\Phi_0(t-\tau) , \qquad (2.7)$$

where

$$\Delta_1^2=-\langle\tilde f_1|f_1\rangle/\langle\tilde f_0|f_0\rangle=2k/M \qquad (2.8)$$

and

$$\Phi_1(t)=\langle\tilde f_1|f_1(t)\rangle/\langle\tilde f_1|f_1\rangle=2\frac{J_1(\omega_0t)}{\omega_0t} . \qquad (2.9)$$

$|f_1\rangle$ and $\langle\tilde f_1|$ denote the right and left states of the generalized Mori chain built up according to the rules of Ref. 12. Note that the memory kernel of Eq. (2.7) is nothing but the correlation function of the state $|f_1\rangle$ regarded as being driven only by the interaction with the remaining states of the infinite Mori chain.

By iteration of this procedure,[12,14,15(a)] it is possible to show that

$$\Phi_0(t)=\frac{1}{2\pi i}\int_C\frac{e^{zt}}{(1-\mu)z+\mu(z^2+\omega_0^2)^{1/2}} , \qquad (2.10)$$

where

$$\mu=m/M \qquad (2.11)$$

and

$$\omega_0^2=4k/m . \qquad (2.12)$$

C denotes the integration path along a straight line parallel to the imaginary axis on the right side of the singularities of the integrand.

In a very recent paper Lee *et al.*[15(b)] shows that a zero-temperature two-dimensional interacting electron gas at long wavelengths is characterized by the same correlation function, the mass difference $m-M$ acting as the electron-electron interaction. For $\mu<1$ the explicit expression of Φ_0 reads[16(a)]

$$\Phi_0(t)=\frac{\mu}{\pi}\int_{-1}^{+1}\frac{(1-x^2)^{1/2}\cos(x\omega_0 t)}{(1-2\mu)x^2+\mu^2}dx \ . \tag{2.13}$$

In the long-time region this exact expression has been rewritten by Ullersma[5] and Phillipson[6] as the sum of an exponentially decaying function and a correction to it. More in general, throughout the whole time interval $\Phi_0(t)$ can be rewritten as follows:[16(b),17]

$$\Phi_0(t)=\frac{1-\mu}{1-2\mu}\exp\left[-\frac{\mu\omega_0 t}{\sqrt{1-2\mu}}\right]+\frac{2\mu}{\pi}\int_1^{\infty}\frac{\sin(x\omega_0 t)(x^2-1)^{1/2}}{(1-2\mu)x^2+\mu^2}dx \ . \tag{2.14}$$

Equation (2.14) has been derived as follows. First of all we made on the integral of Eq. (2.13) the following change of integration variable $x\rightarrow x\omega_0 t$. The new integral is evaluated by integrating from $-\infty$ to $+\infty$ minus the integral from $-\infty$ to $-\omega_0 t$ and that from $\omega_0 t$ to $+\infty$. The former contribution is precisely the exponential function appearing in Eq. (2.14).

Equation (2.14) shows that the rigorous nonexponential decay of Eq. (2.13), agreeing with the general remarks of Lee,[1] can be seen as the sum of an exponential decay plus a correction term. The aim of this paper is to show that this way of splitting the exact expression of Eq. (2.13) is not arbitrary. On the one hand, we can show that it is completely equivalent to the result of a fully renormalized Fokker-Planck equation. On the other hand, both the exponential decay provided by the first term of Eq. (2.14) and the Fokker-Planck equation derived with the approach illustrated in Sec. IV correspond to the dynamics of a dressed state $|S\rangle$. This dressed state $|S\rangle$ will be introduced in Sec. III.

From Laplace transforming Eq. (2.7) we find that the function $\Phi_0(t)$ is characterized by a pole λ in the second Riemann sheet, fulfilling the following relation:

$$\lambda=\Delta_1^2\hat{\Phi}_1(-\lambda) \ , \tag{2.15}$$

where $\hat{\Phi}_1(-\lambda)$ denotes the Laplace transform of $\Phi_1(t)$ evaluated at $-\lambda$. The next step to get the explicit expression of this pole, consists of using Eq. (2.9) and carrying out the analytical continuation of $\hat{\Phi}_1(z)$ on the left half-plane. This leads to the following result:

$$\lambda=\frac{\mu\omega_0}{\sqrt{1-2\mu}} \ . \tag{2.16}$$

It is remarkable that we found this exponential contribution to the decay of $\Phi_0(t)$ without any assumption on the time-scale separation between the system and its "bath." Later we shall show that λ can be regarded as the "eigenvalue" of an "eigenstate" $|S\rangle$ with the following remarkable feature. When the system is initially prepared in the state $|S\rangle$ the time evolution of its projection on the state $|f_0\rangle$ is exactly given by an exponentially decaying function with the damping λ of Eq. (2.16). It is worth stressing that the Mori theory leading to Eq. (2.7) aims at determining the bare correlation function of Eq. (2.5). Within this context, therefore, the damped exponential is certainly an approximation. After introducing a suitably dressed correlation function—see Sec. III—it will become clear that its exponential decay with that damping is actually an exact result.

III. EQUIVALENCE BETWEEN THE CLASSICAL CHAIN OF HARMONIC OSCILLATORS AND THE QUANTUM-MECHANICAL FRIEDRICHS MODEL

First of all, on the Hamiltonian of Eq. (2.1) the boundary condition $q_{-N}=q_{N+1}$ is imposed. Then with the change of indices $i\rightarrow i+N$, it is replaced by the following Hamiltonian:

$$\mathcal{H}=\frac{p_0^2}{2M}+\sum_{i=1}^{2N}\frac{p_i^2}{2m}+\frac{k}{2}\sum_{i=1}^{2N-1}(q_i-q_{i+1})^2+\frac{k}{2}(q_1^2+q_{2N}^2)+kx^2-kx(q_1+q_{2N}) \ . \tag{3.1}$$

The system consists of $2N$ particles with mass m and one particle of interest (the impurity) with mass M. After carrying out the change of indices above the coordinate of the particle of interest is

$$q_0=x=q_{2N+1} \ . \tag{3.2}$$

Let us split the Hamiltonian $\mathcal{H}$ into a part of interest $\mathcal{H}_a$, an interaction $\mathcal{H}_I$, and an "irrelevant" part $\mathcal{H}_b$, as follows:

$$\mathcal{H}=\mathcal{H}_a+\mathcal{H}_I+\mathcal{H}_b \ , \tag{3.3}$$

where

$$\mathcal{H}_a=\frac{p_0^2}{2M}+\frac{M}{2}\Omega^2x^2 \ , \tag{3.4}$$

$$\mathcal{H}_I=-kx(q_1+q_{2N}) \ , \tag{3.5}$$

and

$$\mathcal{H}_b=\sum_{i=1}^{2N}\frac{p_i^2}{2m}+\frac{k}{2}\sum_{i=1}^{2N-1}(q_i-q_{i+1})^2+\frac{k}{2}(q_1^2+q_{2N}^2) \ . \tag{3.6}$$

Note that the frequency defined by

$$\Omega^2\equiv 2k/M=\mu\omega_0^2/2 \tag{3.7}$$

fixes the macroscopic time scale $T\equiv 1/\Omega$.

Let us diagonalize $\mathcal{H}_b$ with the following transformation of coordinates and momenta, borrowed from the paper of Cukier *et al.*:[17]

$$q_i=\sum_{i=1}^{2N}T_{il}q_l' \ , \qquad p_i=\sum_{i=1}^{2N}T_{il}p_l' \ , \tag{3.8}$$

where the coefficients T_{il} of this transformation are defined by

$$T_{il}=\left[\frac{2}{2N+1}\right]^{1/2}\sin\left[\frac{il\pi}{2N+1}\right] . \tag{3.9}$$

It is shown that the transformation matrix $\underline{T}$ fulfills the property

$$\underline{T}^{-1}=\underline{T} . \tag{3.10}$$

When written in terms of these normal modes the Hamiltonian $\mathcal{H}$ reads

$$\mathcal{H}=\mathcal{H}_a+\sum_{i=1}^{2N}\frac{p_i'^2}{2m}+\frac{m}{2}\omega_i^2 q_i'^2+\sum_{i=1}^{2N}\epsilon_i q_i' x , \tag{3.11}$$

where the coupling strengths ϵ_i are defined by

$$\epsilon_i=\begin{cases}-2k\left[\frac{2}{2N+1}\right]^{1/2}\sin\left[\frac{i\pi}{2N+1}\right] & \text{(for odd } i)\\ 0 \quad \text{(for even } i) .\end{cases} \tag{3.12}$$

The frequencies ω_i are given by

$$\omega_i=\omega_0\sin\left[\frac{\pi i}{2(2N+1)}\right], \quad i=1,\dots,2N . \tag{3.13}$$

In terms of the new coordinates we obtain the following equations of motion:

$$\begin{aligned}\dot{x}&=\frac{p_0}{M}=v ,\\ \dot{p}_0&=-M\Omega^2 X-\sum_{i=1}^{2N}\epsilon_i q_i' ,\\ \dot{q}_i'&=\frac{p_i'}{m} ,\\ \dot{p}_i'&=-m\omega_i^2 q_i'-\epsilon_i x .\end{aligned} \tag{3.14}$$

Let us now adopt a mixed representation where the coordinates q_i' are replaced by the new coordinates

$$y_i=q_i'+x\frac{\epsilon_i}{m\omega_i^2} , \tag{3.15}$$

while still referring ourselves to the old velocities defined by

$$v_i'=\frac{p_i'}{m} . \tag{3.16}$$

We thus obtain the new equations of motion

$$\begin{aligned}\dot{x}&=v ,\\ \dot{v}&=-\left[\Omega^2-\sum_{i=1}^{2N}\frac{\epsilon_i^2}{mM\omega_i^2}\right]x-\sum_{i=1}^{2N}\frac{\epsilon_i y_i}{M} ,\\ \dot{y}_i&=v_i'+v\frac{\epsilon_i}{m\omega_i^2} ,\\ \dot{v}_i'&=-\omega_i^2 y_i .\end{aligned} \tag{31.7}$$

Due to the translational invariance of the original Hamiltonian, the variables x and v turn out to be decoupled from one another, i.e., we have

$$\Omega_{\text{eff}}^2\equiv\Omega^2-\sum_{i=1}^{2N}\frac{\epsilon_i^2}{mM\omega_i{}^2}=0 . \tag{3.18}$$

Note that the Hamiltonian, written in terms of these mixed coordinates, reads

$$\mathcal{H}=\frac{M}{2}v^2+\sum_{i=1}^{2N}\frac{p_i'^2}{2m}+\frac{m}{2}\omega_i^2 y_i^2 . \tag{3.19}$$

Let us now carry out a further change of variables. This is as follows:

$$\begin{aligned}\xi_i^+&\equiv v_i'+i\omega_i y_i ,\\ \xi_i^-&\equiv v_i'-i\omega_i y_i .\end{aligned} \tag{3.20}$$

In terms of these new variables the set of Eq. (3.17) becomes

$$\begin{aligned}\dot{x}&=v ,\\ \dot{v}&=-\sum_{i=1}^{2N}\frac{\epsilon_i}{2iM\omega_i}(\xi_i^+-\xi_i^-) ,\\ \dot{\xi}_i^+&=i\omega_i\xi_i^++i\frac{\epsilon_i}{m\omega_i}v ,\\ \dot{\xi}_i^-&=-i\omega_i\xi_i^--i\frac{\epsilon_i}{m\omega_i}v .\end{aligned} \tag{3.21}$$

First of all let us stress that the basis set $|v\rangle|\xi_i\rangle$ is characterized by the orthogonality properties

$$\langle\xi_i^+|\xi_i^-\rangle=0 \quad \text{for any } i , \tag{3.22}$$

$$\langle\xi_i^\mu|\xi_j^{\mu'}\rangle=0, \quad \mu=+,-;\ \mu'=+,- \quad \text{for } i\neq j , \tag{3.23}$$

$$\langle v|\xi_i^\mu\rangle=0, \quad \text{for any pair of } \mu \text{ and } i . \tag{3.24}$$

Equation (3.22) expresses the result of energy equipartition. Equation (3.23) results from the fact that the normal modes are independent from each other; see Eq. (3.19). The third equation, Eq. (3.24), depends on the fact that the new variables ξ_i^μ, also depending on x [see Eq. (3.15)], are, however, certainly independent of v. Equations (3.22)–(3.24) show that this is a suitable orthogonal basis set to expand the operator $\mathcal{L}$. After proper normalization, the matrix $\underline{A}$ with components

$$A_{r,k}=-i\langle e_r|\mathcal{L}|e_k\rangle , \tag{3.25}$$

where we follow the ordering

$$\begin{aligned}&|e_0\rangle=|v\rangle,\ |e_1\rangle=|\xi_1^+\rangle,\ |e_2\rangle=|\xi_1^-\rangle ,\\ &|e_3\rangle=|\xi_2^+\rangle,\ |e_4\rangle=|\xi_2^-\rangle,\dots ,\end{aligned}$$

appears to read as follows:

$$\underline{A}=\begin{vmatrix} 0 & -\frac{\epsilon_1}{\omega_1}\frac{1}{\sqrt{2mM}} & +\frac{\epsilon_1}{\omega_1}\frac{1}{\sqrt{2mM}} & -\frac{\epsilon_2}{\omega_2}\frac{1}{\sqrt{2mM}} & +\frac{\epsilon_2}{\omega_2}\frac{1}{\sqrt{2mM}} & \cdots \\ -\frac{\epsilon_1}{\omega_1}\frac{1}{\sqrt{2mM}} & -\omega_1 & 0 & 0 & 0 & \cdots \\ +\frac{\epsilon_1}{\omega_1}\frac{1}{\sqrt{2mM}} & 0 & \omega_1 & 0 & 0 & \cdots \\ -\frac{\epsilon_2}{\omega_2}\frac{1}{\sqrt{2mM}} & 0 & 0 & -\omega_2 & 0 & \cdots \\ +\frac{\epsilon_2}{\omega_2}\frac{1}{\sqrt{2mM}} & 0 & 0 & 0 & \omega_2 & \cdots \\ \cdots & & & & & \end{vmatrix} . \tag{3.26}$$

In this basis set the variable x is not included, since we are here interested in determining the dynamical properties of v and, due to Eq. (3.18), these do not depend on the dynamics of x.

We are in a position to identify $|v\rangle$ with the unstable quantum-mechanical state $|e\rangle$, and the states $|\xi_n^{\pm}\rangle$ with the quantum-mechanical states $|\pm n\rangle$ of the Friedrichs model.[8(b)] Then, the classical Liouville operator $-i\mathcal{L}$ turns out to be equivalent to the quantum-mechanical Hamiltonian operator $\mathcal{H}$ defined by

$$\mathcal{H}=w_e|e\rangle\langle e|+\sum_{\substack{m=-2N\\ m\neq 0}}^{2N} w_m|m\rangle\langle m|+\sum_{\substack{m=-2N\\ m\neq 0}}^{2N} V_{em}|e\rangle\langle m| + \sum_{\substack{m=-2N\\ m\neq 0}}^{2N} V_{em}^{*}|m\rangle\langle e| , \tag{3.27}$$

where

$$\begin{aligned} &w_e=0 ,\\ &w_m=-\omega_m, \quad m>0\\ &w_m=\omega_m, \quad m<0\\ &V_{em}=-\frac{\epsilon_i}{\omega_i\sqrt{2mM}}, \quad m>0\\ &V_{em}=\frac{\epsilon_i}{\omega_i\sqrt{2mM}}, \quad m<0 . \end{aligned} \tag{3.28}$$

Let us now discuss how to use the Hamiltonian $\mathcal{H}$ of Eq. (3.27) to determine the state $|S\rangle$ with an "imaginary energy" $-i\lambda$ with λ coinciding with the renormalized damping coefficient of Eq. (2.16). The Hamiltonian $\mathcal{H}$ of Eq. (3.27) refers to a case of a finite number of Friedrichs states $|m\rangle$, as a result of considering in our original classical model a finite number of particles.

The leading idea of our approach is as follows. First of all, let us note that the frequencies of our normal modes are maintained within the finite range $(0,\omega_0)$. Correspondingly, the unperturbed energies of the Friedrichs states are limited by the lower bound $w_{\min}=-\omega_0$ and the upper bound $w_{\max}=\omega_0$. As a consequence of this, upon increase of N the energy spectrum tends to a continuum. We are in a position to determine an "eigenstate" of $\mathcal{H}$, the "eigenenergy" of which in the continuous limit is precisely $-i\lambda$.

Let us consider the state $|S\rangle$ defined by

$$|S\rangle=|e\rangle+\sum_{\substack{m=-2N\\ m\neq 0}}^{2N}\frac{V_{em}^{*}|m\rangle}{z-w_m} , \tag{3.29}$$

It is straightforward to show that $|S\rangle$ is an eigenstate of $\mathcal{H}$ with eigenenergy z. This eigenvalue, in turn, is provided by the implicit equation[8(c)]

$$z=\sum_{\substack{m=-2N\\ m\neq 0}}^{2N}\frac{|V_{em}|^2}{z-w_m} . \tag{3.30}$$

It is immediately seen that if the memory kernel Φ_1 of the generalized Langevin equation of the preceding section is explicitly written in this representation, it reads

$$\Phi_1(t)=\sum_m |V_{em}|^2 e^{-iw_m t} . \tag{3.31}$$

If we apply now the renormalized expression of Eq. (2.16) and take the relation $\lambda=iz$ into account, we see that this important expression leads to precisely Eq. (3.30).

Note that the results we are commenting on are of very general nature and are not confined to the case of a "bath" chain with equal masses and couplings. This conditions basically served the purpose of resulting in analytical expressions for the transformation coordinates above. After carrying out the normal-mode transformation above, in terms of generic transformation matrices, the memory kernal $\Phi_1(t)$ always turns out to be written under the form of Eq. (3.31). We obtain thus the following general and important result. The renormalized transport coefficient λ, as derived from the generalized Langevin equations, is not easily recognized as the eigenvalue of a certain eigenstate. *After carrying out the transformation to the Friedrichs representation, this transport coefficient is immediately recognized as being the eigenvalue associated with an eigenstate, and the general expression for this eigenstate is immediately derived and it is indeed Eq. (3.29).*

It must also be stressed that before reaching the continuum limit, the solution to Eq. (3.30) is always given by $2N+1$ real values of z, as it is obvious, because of the Hermitian nature of the matrix $\underline{A}$. Thus, so to speak, the related parameter $\lambda = iz$ is not a genuine transport coefficient. This is made to become a real transport coefficient in the continuum limit, via a suitable use of the technique of analytic continuation. Let us, therefore, explore this important physical condition.

Let us make this calculation in the special case of our linear chain of particles. In this case, due to Eq. (3.12), the contributions of even m vanish and the continuum limit is attained via the following expression:

$$\sum_{\substack{m=-2N \\ m\neq 0}}^{2N} |V_{em}|^2 f(w_m) = \int_{-\omega_0}^{\omega_0} dw |V(w)|^2 f(w) \frac{dm}{dw} . \tag{3.32}$$

From Eqs. (3.28), (3.12), and (3.13) we obtain

$$|V(w)|^2 = \frac{\mu}{2N+1}(\omega_0^2 - w^2) . \tag{3.33}$$

dm/dw is evaluated by inversion of Eq. (3.13). This leads us to

$$\frac{dm}{dw} = \frac{2N+1}{\pi} \frac{1}{(\omega_0^2 - w^2)^{1/2}} . \tag{3.34}$$

Let us substitute Eqs. (3.33) and (3.34) into Eq. (3.32); we are led to the following prescription:

$$\sum_{\substack{m=-2N \\ m\neq 0}}^{2N} |V_{em}|^2 f(w_m) = \int_{-\omega_0}^{\omega_0} dw \frac{\mu}{\pi}(\omega_0^2 - w^2)^{1/2} f(w) . \tag{3.35}$$

By using this prescription to evaluate the eigenvalue z in the continuum limit, from Eq. (3.30) we obtain

$$z = \int_{-\omega_0}^{\omega_0} dw \frac{\mu}{\pi} \frac{(\omega_0^2 - w^2)^{1/2}}{z - w} . \tag{3.36}$$

The integral on the right-hand side (rhs) of Eq. (3.36) must be evaluated by analytical continuation. From the cut on the real axis we obtain

$$z = \mu z - i\mu(\omega_0^2 - z^2)^{1/2} , \tag{3.37}$$

which means

$$z = -i \frac{\mu\omega_0}{\sqrt{1-2\mu}} . \tag{3.38}$$

Equation (3.38) provides for $\lambda = iz$, precisely the same as expression as Eq. (2.16). The "eigenstates" $|S\rangle$ and $\langle S|$ corresponding to the "eigenvalues" of Eq. (3.38) are derived by expressing in the continuum limit the state of Eq. (3.29) and the left state associated to it.

Note that the projector over the space spanned by the state $|S\rangle$,

$$\Pi = |S\rangle \frac{1}{\langle S|S\rangle} \langle S| , \tag{3.39}$$

being Hermitian, seems to be a special case of that of the Prigogine and co-workers.[8(a),18] If the "wave function" of our system, $|\varphi(t)\rangle$, at the initial time $t=0$, satisfies the property

$$\Pi |\varphi(0)\rangle = |\varphi(0)\rangle , \tag{3.40}$$

the subsequent decay is rigorously exponential. This is so because Eq. (3.40) means that the "wave function" lies completely on the subspace characterized by an exponential decay. We have thus shown that an initial condition exists, resulting in a time behavior which exactly coincides with the exponential contribution to the correlation function $\Phi_0(t) = \langle f_0 | f_0(t) \rangle / \langle f_0 | f_0 \rangle$ of Eq. (2.5), i.e., the first term on the rhs of Eq. (2.14).

IV. THE FOKKER-PLANCK EQUATION

Let us apply the projection technique of Refs. 19–21 to derive the Fokker-Planck equation describing the equation of motion of the probability distribution of the velocity $v = p_0/M$ of the Brownian particle of the Hamiltonian system of Eq. (2.1). Let us use the relative coordinates R_i defined by

$$R_i = q_i - q_{i-1} . \tag{4.1}$$

Then the Liouvillian $\mathcal{L}$ associated with the Hamiltonian of Eq. (2.1) can be written as

$$\mathcal{L} = -\sum_{i=-\infty}^{\infty} (v_i - v_{i-1}) \frac{\partial}{\partial R_i} + \frac{k}{m_i}(R_{i+1} - R_i) \frac{\partial}{\partial v_i} , \tag{4.2}$$

with $m_i = m$ for $i \neq 0$ and $m_i = M$ for $i=0$. Since the variable of interest is $v = v_0$, we are immediately led to the following repartition of $\mathcal{L}$:

$$\mathcal{L} = \mathcal{L}_a + \mathcal{L}_b + \mathcal{L}_1 , \tag{4.3}$$

where

$$\mathcal{L}_a = 0 , \tag{4.4}$$

$$\mathcal{L}_1 = -v \left[\frac{\partial}{\partial R_0} - \frac{\partial}{\partial R_1} \right] - \frac{k}{M}(R_1 - R_0) \frac{\partial}{\partial v} , \tag{4.5}$$

the latter being also written in the fully equivalent way

$$\mathcal{L}_1 = v \left[\left[\frac{\partial}{\partial R_1} + \frac{kR_1}{k_B T} \right] - \left[\frac{\partial}{\partial R_0} + \frac{kR_0}{k_B T} \right] \right] - \frac{k}{M}(R_1 - R_0) \left[\frac{\partial}{\partial v} + \frac{Mv}{k_B T} \right] . \tag{4.6}$$

By using the usual projection projector P, defined by

$$P\rho(v,b;t) = \rho_{\text{eq}}(b) \int db\, \rho(v,b;t) , \tag{4.7}$$

where $\rho(v,b;t)$ denotes the probability distribution of the variables v and b, b expressing the set of the remainder variables of our Hamiltonian system, and $\rho_{\text{eq}}(b)$ the equilibrium distribution of these "irrelevant variables." Let us also use the properties

$$P\mathcal{L}_b = \mathcal{L}_b P = P\mathcal{L}_1 P = 0 \tag{4.8}$$

[the last equality depends on the nature of the Hamiltonian $\mathcal{H}$, studied in this paper, the other two are a general property of the operator of Eq. (4.7)] and let us follow the prescription described in details in Ref. 21. Then we get for the probability distribution of v, $\sigma(v;t) = \int db\, \rho(v,b;t)$, the following equation of motion:

$$\frac{\partial \sigma(v,t)}{\partial t} = \int_0^t d\tau\, \mathcal{K}(t-\tau)\sigma(v,\tau) , \tag{4.9}$$

where the memory kernel $\mathcal{K}$ is defined by

$$\mathcal{K}(t-\tau) = \frac{1}{\rho_{\text{eq}}(b)} P\mathcal{L}_1(t) T \times \exp\left[Q \int_\tau^t \mathcal{L}_1(t')dt' \right] Q\mathcal{L}_1(\tau)P \tag{4.10}$$

with

$$Q \equiv 1 - P , \quad \mathcal{L}_1(t) \equiv e^{-\mathcal{L}_b t}\mathcal{L}_1 e^{\mathcal{L}_b t} , \tag{4.10'}$$

and T denotes a time-ordered exponential.[21] Note that this equation is rigorously exact only if the initial condition

$$\rho(b,v;0) = \rho_{\text{eq}}(b)\sigma(v;0) \tag{4.11}$$

is assumed to be true.

Let us now make the basic assumption that the time scale of the bath is fast enough as to allow Eq. (4.9) to approach for $t \to \infty$ the Markovian structure

$$\frac{\partial \sigma(v;t)}{\partial t} = \mathcal{D}\sigma(v;t) , \tag{4.12}$$

where $\mathcal{D}$ is an operator, the exact expression of which is still to be determined. From Eq. (4.12), we have

$$\sigma(t-\tau) = e^{-\mathcal{D}\tau}\sigma(t) , \tag{4.13}$$

which, replaced in the second term on the rhs of Eq. (4.9), results in

$$\frac{\partial}{\partial t}\sigma(v;t) = \left[\int_0^t \mathcal{K}(\tau) e^{-\mathcal{D}\tau} d\tau \right] \sigma(v;t) . \tag{4.14}$$

By replacing the upper limit of time integration with ∞ and comparing Eq. (4.14) with the term on the rhs of Eq. (4.12), we obtain the following implicit equation for the operator $\mathcal{D}$:

$$\mathcal{D} = \int_0^\infty \mathcal{K}(t) e^{-\mathcal{D}t} dt . \tag{4.15}$$

By development of the time-ordered exponential appearing in Eq. (4.10) in a Taylor series of the interaction term $\mathcal{L}_1$, we obtain the following expression for $\mathcal{D}$:

$$\mathcal{D} = \int_0^\infty \left[\sum_{n=1}^\infty \mathcal{K}_{2n}(t) \right] e^{-\mathcal{D}t} dt , \tag{4.16}$$

where $\mathcal{K}_{2n}(t)$ denotes the contribution of $2n$th order to the expansion of $\mathcal{K}(t)$. Note that in the case here under study the odd expansion contributions vanish.

At the lowest nonvanishing order, namely the second order, the exponential on the rhs of Eq. (4.16) does not contribute. We thus obtain

$$\mathcal{D}_2 = \int_0^\infty \mathcal{K}_2(t) dt , \tag{4.17}$$

where

$$\mathcal{K}_2(t-\tau) = \frac{1}{\rho_{\text{eq}}(b)} P\mathcal{L}_1(t) Q\mathcal{L}_1(\tau) P . \tag{4.18}$$

By using Eqs. (4.8), Eq. (4.18) becomes

$$\mathcal{K}_2(t) = \frac{1}{\rho_{\text{eq}}(b)} P\mathcal{L}_1 e^{\mathcal{L}_b t}\mathcal{L}_1 P . \tag{4.19}$$

By adopting for $\mathcal{L}_1$ appearing on the left the expression of Eq. (4.5) and for the one on the right the expression of Eq. (4.6), using the first of the properties of Eq. (4.8) and the assumption that the equilibrium distribution $\rho_{\text{eq}}(b)$ is canonical, namely,

$$\rho_{\text{eq}}(b) \propto e^{-H_b/k_B T} , \tag{4.20}$$

we obtain

$$\mathcal{D}_2 = \frac{\partial}{\partial v}\left[\frac{\partial}{\partial v} + \frac{Mv}{k_B T} \right] \times \int_0^\infty dt \int db \frac{k}{M}(R_1 - R_0) \times e^{\mathcal{L}_b t} \frac{k}{M}(R_1 - R_0)\rho_{\text{eq}}(b) . \tag{4.21}$$

This can immediately be rewritten in the more appealing way as

$$\mathcal{D}_2 = \frac{\partial}{\partial v}\left[\frac{\partial}{\partial v} + \frac{Mv}{k_B T} \right] \int_0^\infty dt \langle F(0)F(t) \rangle_{\text{eq}} , \tag{4.22}$$

where

$$F(t) = \frac{k}{M}[R_1(t) - R_0(t)] \tag{4.23}$$

denotes the acceleration of the Brownian particle.

The explicit expression of the next nonvanishing order is

$$\mathcal{D}_4 = \int_0^\infty dt [\mathcal{K}_4(t) + \mathcal{K}_2(t) e^{-\mathcal{D}_2 t}] . \tag{4.24}$$

This, by expansion of the exponential $\exp(-\mathcal{D}_2 t)$ up to the first order in $\mathcal{D}_2$, becomes

$$\mathcal{D}_4 = \mathcal{D}_2 + \mathcal{D}_2 \left[\frac{d\hat{\mathcal{K}}_2(z)}{dz} \right]_{z=0} + \hat{\mathcal{K}}_4(z=0) . \tag{4.25}$$

Thus we must evaluate the contribution at the fourth order to the memory kernel $\mathcal{K}$. To do that it is convenient to express the Liouvillian $\mathcal{L}$ in terms of creation and annihilation operators. As to the particle of interest, they can be defined as follows. Let us consider the dimensionless variable

$$y \equiv \frac{v}{(\langle v^2 \rangle_{\text{eq}})^{1/2}} \tag{4.26}$$

with

$$\langle v^2\rangle_{eq}=k_BT/M\ . \tag{4.27}$$

It is straightforward to show[21] that the operators

$$a_-\equiv y+\frac{\partial}{\partial y}\ ,\qquad a_+\equiv-\frac{\partial}{\partial y} \tag{4.28}$$

fulfill the important conditions

$$[a_-,a_+]=1\ , \tag{4.29}$$

$$\mathcal{L}_{FP}=\frac{\partial}{\partial v}\left[\langle v^2\rangle_{eq}\frac{\partial}{\partial v}+v\right]=-a_+a_-\ . \tag{4.30}$$

The Fokker-Planck operator $\mathcal{L}_{FP}$ is characterized by the eigenvalues $-n$ (n means a positive integer) corresponding to the right eigenstates

$$|n\rangle=\frac{1}{(2\pi)^{1/4}\sqrt{n!}}e^{-y^2/2}\mathrm{He}_n(y) \tag{4.31}$$

and the corresponding left ones,

$$\langle\tilde{n}|=\frac{1}{(2\pi)^{1/4}\sqrt{n!}}\mathrm{He}_n(y)\ . \tag{4.32}$$

The symbol $\mathrm{He}_n(y)$ denotes a function related to the Hermite polynomial $H_n(y)$ by the relation[22]

$$\mathrm{He}_n(y)=2^{-n/2}H_n\left[\frac{y}{\sqrt{2}}\right]\ . \tag{4.33}$$

The creation and annihilation operators for the velocity of the particle of interest can thus be written as follows:

$$a_+=\sum_{n=0}^{\infty}\sqrt{n+1}|n+1\rangle\langle\tilde{n}|\ ,\qquad a_-=\sum_{n=1}^{\infty}\sqrt{n}\,|n-1\rangle\langle\tilde{n}|\ . \tag{4.34}$$

If we apply the same approach to the bath variables

$$A^i_-\equiv\frac{R_i}{(\langle R_i^2\rangle_{eq})^{1/2}}+(\langle R_i^2\rangle_{eq})^{1/2}\frac{\partial}{\partial R_i}\ ,\quad A^i_+\equiv-(\langle R_i^2\rangle_{eq})^{1/2}\frac{\partial}{\partial R_i}\ ,\quad b^i_+\equiv-(\langle v_i^2\rangle_{eq})^{1/2}\frac{\partial}{\partial v_i}\ ,\quad b^i_-\equiv\frac{v_i}{(\langle v_i^2\rangle_{eq})^{1/2}}+(\langle v_i^2\rangle_{eq})^{1/2}\frac{\partial}{\partial v_i}\ , \tag{4.35}$$

with an obvious meaning of the notations, according to which $a_+=b^0_+$ and $a_-=b^0_-$, we can express the interation term $\mathcal{L}_1$ and the bath operator $\mathcal{L}_b$ as follows:

$$\mathcal{L}_1=\frac{\Omega}{\sqrt{2}}[(A^0_+-A^1_+)a_--(A^0_--A^1_-)a_+]\ , \tag{4.36}$$

$$\mathcal{L}_b=\frac{\omega_0}{2}\sum_{\substack{i=-\infty\\ i\neq 0}}^{+\infty}[(A^i_+-A^{i+1}_+)b^i_--(A^i_--A^{i+1}_i)b^i_+]\ . \tag{4.37}$$

Due to the canonical assumption on the bath,

$$A^i_-\rho_{eq}(b)=b^i_-\rho_{eq}(b)=0\quad\text{for any } i\ . \tag{4.38}$$

This leads us to adopt the Fock notation, according to which the bath equilibrium distribution can be written as follows:

$$\rho_{eq}(b)=|0,0,\ldots\rangle\ . \tag{4.39}$$

By adopting the definitions

$$A_+\equiv A^0_+-A^1_+,\quad A_-\equiv A^0_--A^1_-\ , \tag{4.40}$$

we have

$$\mathcal{L}_1=\frac{\Omega}{\sqrt{2}}(A_+a_--A_-a_+)\ . \tag{4.41}$$

From Eqs. (4.41), (4.17), and (4.19) and using the property, stemming from Eq. (4.38), that on the right side only bath creation operators can appear (remember that on the left side only bath annihilation operators can appear[20]), we obtain

$$\mathcal{D}_2=\alpha a_+a_-\ , \tag{4.42}$$

where

$$\alpha=-\frac{\Omega^2}{2}\int_0^\infty dt\int db\ A_-(t)A_+(0)\rho_{eq}(b)\ . \tag{4.42'}$$

From our remarks above, it is evident that the calculation of $\mathcal{H}_4$ will lead us to the general structure

$$\mathcal{D}_4=\alpha a_+a_-+\beta a_+a_-^3+\eta a_+a_-a_+a_-+\delta a_+^2a_-^2+\epsilon a_+^3a_-\ . \tag{4.43}$$

By taking into account that the operators $\mathcal{L}$ and $\mathcal{L}_b$ keep the excitation number unchanged, we are immediately led to

$$\beta=\epsilon=0\ . \tag{4.44}$$

Then, by using the commutation rule of Eq. (4.29), we get from Eq. (4.43)

$$\mathcal{D}_4=(\alpha+\eta)a_+a_-+(\alpha+\delta)a_+^2a_-^2\ . \tag{4.45}$$

The second contribution on the rhs of this equation would lead to the breakdown of the Fokker-Planck structure. However, the calculation of η and δ leads to the important result

$$\delta=-\eta\ . \tag{4.46}$$

It is convenient to illustrate again the calculation which leads to this important result,[21] because this will make it possible to stress the close connection between it and the transformation to the Friedrichs basis set of the preceding section. This will serve the purpose of illustrating that the projection-perturbative approach to the Fokker-

Planck equation is intimately connected to the ideas of Prigogine subdynamics and to the time evolution of the state $|S\rangle$, leading to exact exponential decay.

From the calculation rules outlined above, we have

$$\eta=-\frac{\Omega^2}{2}\alpha\left|\frac{d}{dz}\int_0^\infty dt\, e^{-zt}\int db\; A_-(t)A_+(0)\rho_{\rm eq}(b)\right|_{z=0}, \tag{4.47}$$

$$\delta=\frac{\Omega^4}{4}\int db\int_0^\infty dt_0\,A_-(t_0)\times\int_0^{t_0}dt_1\,A_-(t_1)Q\times\int_0^{t_1}dt_2\,A_+(t_2)A_+(0)\rho_{\rm eq}(b)\ . \tag{4.48}$$

To evaluate the important parameters α, η, and δ, we must consider a finite number of particles and make a transformation to the normal modes representation. This means, that using the general definition $\{A_j\}=\{v_i,R_i\}$, the transformation

$$A_i=\sum_j U_{ij}\tilde{A}_j \tag{4.49}$$

must be used, with the new variable $\tilde{A}_j$ fulfilling the relation

$$\mathcal{L}_b\tilde{A}_j=\Lambda_j\tilde{A}_j\ . \tag{4.50}$$

This immediately leads to

$$\tilde{A}_j e^{\mathcal{L}_b t}=\tilde{A}_j e^{-\lambda_j t}\ . \tag{4.51}$$

From this and applying the calculation rules outlined above, we obtain

$$\alpha=-\frac{\Omega^2}{2}\sum_j\frac{(U_{0j}-U_{1j})(U_{j0}^{-1}-U_{j1}^{-1})}{\Lambda_j} \tag{4.52}$$

and

$$\eta=-\frac{\Omega^4}{4}\sum_{j,k}\frac{(U_{0j}-U_{1j})(U_{j0}^{-1}-U_{j1}^{-1})(U_{0k}-U_{1k})(U_{k0}^{-1}-U_{k1}^{-1})}{\Lambda_j\Lambda_k^2}\ . \tag{4.53}$$

The calculation of δ is carried off along the same lines and it heavily relies on the property

$$e^{\mathcal{L}_b t}\frac{\partial}{\partial\tilde{A}_j}=e^{-\Lambda_j t}\frac{\partial}{\partial\tilde{A}_j}e^{\mathcal{L}_b t}\ . \tag{4.54}$$

which is, in turn, derived from Eqs. (4.49) and (4.50). Furthermore, use must be made of the general integration property

$$\int_0^\infty dt_0\int_0^{t_0}dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{n-1}}dt_n\exp\left[-\sum_{i=0}^n\lambda_i t_i\right]=[\lambda_0(\lambda_0+\lambda_1)\cdots(\lambda_0+\lambda_1+\cdots+\lambda_n)]^{-1}\quad(\text{if }\lambda_i>0\text{ for any }i)\ . \tag{4.55}$$

The final result is precisely Eq. (4.46). Note that the calculation of the parameters α, η, and δ was carried out by assuming that $e^{-\Lambda_j t}\rightarrow 0$ for $t\rightarrow\infty$. The next step consists of showing that the parameter $\alpha+\eta$ coincides with the expansion up to the fourth order of the parameter $-iz$, the exact value of which is given by Eq. (3.38).

To carry out this demonstration, we remark first of all that the normal modes $\xi_i^{\mp}$, introduced in the preceding section, correspond to the variables $\tilde{A}_j$ above. Then we must establish a relation among the normal modes $\xi_i^{\pm}$ and the coordinates v_i and R_i. Furthermore, we must connect the eigenvalues Λ_i above with the diagonal elements of the Friedrichs matrix $\underline{A}$ of Eq. (3.26). Using Eqs. (3.8)–(3.10), (3.15), and (3.20), we immediately obtain

$$\xi_i^{\mp}=\sum_{l=1}^{2N}T_{il}v_l\mp i\omega_i\sum_{l=1}^{2N}T_{il}q_l\mp\frac{i\epsilon_i}{m\omega_i}x\ . \tag{4.56}$$

By inversion of the definitions of Eq. (4.1), we derive

$$q_l=x+\sum_{k=1}^{l}R_k\ . \tag{4.57}$$

By substituting this expression into Eq. (4.56) we find that the coefficient of x is

$$\mp i\left[\omega_i\sum_{l=1}^{2N}T_{il}+\frac{\epsilon_i}{m\omega_i}\right],$$

and this, using Eqs. (3.12), (3.13), and (3.9), is proven to vanish for any i. Thus we obtain

$$\xi_i^{\mp}=\sum_{l=1}^{2N}T_{il}v_l\mp i\omega_i\sum_{l=1}^{2N}R_l\left[\sum_{k=1}^{2N}T_{ik}\right]\ . \tag{4.58}$$

From the orthogonality properties of the $\xi_i^{\pm}$ resulting from Eqs. (3.22) and (3.23), and from the orthogonality properties of the coordinates $\{v_i,R_i\}$ [see Eqs. (4.1) and (2.1)] and carrying out the proper normalizations, we obtain the following unitary transformation:

$$\bar{\xi}_i^{\mp}=\sum_{l=1}^{2N}\frac{T_{il}}{\sqrt{2}}\bar{v}_l\mp i\frac{\omega_i\sqrt{2}}{\omega_0}\sum_{l=1}^{2N}\bar{R}_l\left[\sum_{k=1}^{2N}T_{ik}\right], \tag{4.59}$$

the bars denoting indeed that the variables are properly normalized. Note that the coefficients of this transformation coincide with the parameters U_{ij}^{-1}. From Eq. (4.59) we find, for the transformation coefficients of interest, the following relations:

$$U_{j0}^{-1}=U_{0j}=0\ ,\qquad U_{lj}^{*}=U_{jl}^{-1}=\mp i\frac{\omega_i}{\omega_0}\sqrt{2}\sum_{l=1}^{2N}T_{il}\ . \tag{4.60}$$

Let us introduce for the eigenvalues Λ_j the following, more detailed definition:

$$\mathcal{L}_b \xi_j^{\mp} = \Lambda_j^{\mp} \xi_j^{\mp} . \tag{4.61}$$

From the matrix $\underline{A}$ of Eq. (3.26) and from Eq. (3.25) we have

$$\Lambda_j^{\mp} = \pm i\omega . \tag{4.62}$$

This expression must be properly modified. To be consistent with the assumption above, $e^{-\Lambda_j t} \to 0$ for $t \to \infty$ we must replace Eq. (4.62) with

$$\Lambda_j^{\mp} = \pm i(\omega_j \mp i\epsilon), \quad \epsilon > 0 . \tag{4.63}$$

Then the calculation of α and η is made by replacing the sums of Eqs. (4.52) and (4.53) with integrals over dw. By using Eq. (3.34) and the property

$$|U_{jl}^{-1}(w)|^2 = \frac{4}{2N+1}\left[1 - \frac{w^2}{\omega_0^2}\right] . \tag{4.64}$$

which is easily obtained from Eqs. (3.9), (3.13), and (4.60), we have the final result

$$\begin{aligned} \alpha &= -\mu\omega_0 , \\ \eta &= -\mu^2\omega_0 , \end{aligned} \tag{4.65}$$

which is precisely what we wanted to demonstrate, as it may easily be checked by expanding up to the fourth order the parameter $-\lambda$ of Eq. (2.16).

The procedure adopted in Ref. 11 to get a fully renormalized drift coefficient within the Fokker-Planck description is satisfactorily supported by the above results. To make this paper as self-contained as possible, so as to get a general and unifying picture, we would like to briefly review those results.

Let us consider again Eq. (4.9) with the memory kernel given by Eq. (4.10). Rather than expanding the time-ordered exponential in a Taylor power series (this would lead to the perturbation treatment given, explicitly illustrated up to the fourth order) we make a proper ansatz on it. This ansatz is equivalent to assuming that

$$T \exp\left[Q \int_\tau^t \mathcal{L}_1(t')dt'\right] = e^{\mathcal{D}(t-\tau)} . \tag{4.66}$$

Let us substitute this expression into Eq. (4.10) and this, in turn, into Eq. (4.15). By taking into account that $\mathcal{D}$ is an operator acting only on v and therefore commuting with $\mathcal{L}_b$, from Eq. (4.15) we obtain

$$\mathcal{D} = \frac{1}{\rho_{\rm eq}(b)} \int_0^\infty P\mathcal{L}_1 e^{\mathcal{L}_b t} e^{\mathcal{D}t} \mathcal{L}_1 e^{-\mathcal{D}t} \rho_{\rm eq}(b) dt . \tag{4.67}$$

By defining the superoperator $\mathcal{D}^X$ acting on a generic operator $\mathcal{A}$ as

$$\mathcal{D}^X \mathcal{A} \equiv [\mathcal{D}, \mathcal{A}] \tag{4.68}$$

and exploiting the identity[19-21]

$$e^{\mathcal{D}t}\mathcal{L}_1 e^{-\mathcal{D}t} = e^{\mathcal{D}^X t}\mathcal{L}_1 , \tag{4.69}$$

we obtain

$$\mathcal{D} = \frac{1}{\rho_{\rm eq}(b)} \int_0^\infty P\mathcal{L}_1 e^{\mathcal{L}_b t} e^{\mathcal{D}^X t} \mathcal{L}_1 \rho_{\rm eq}(b) dt . \tag{4.70}$$

Since the higher-order contributions (at least those at the fourth order evaluated above) do not change the Fokker-Planck structure, we find it to be reasonable to assume that the Fokker-Planck operator is characterized by the following form:

$$\mathcal{D} = \frac{k_B T}{M}\gamma \frac{\partial}{\partial v}\left[\frac{\partial}{\partial v} + \frac{Mv}{k_B T}\right] . \tag{4.71}$$

In other words, the implicit equation of Eq. (4.70) must only serve the purpose of determining the unknown damping parameter γ.

Note that

$$e^{\mathcal{D}^X t}\mathcal{L}_1 = \cosh(\gamma t)\mathcal{L}_1 + \sinh(\gamma t)\left\{\mathcal{L}_1 + \frac{2k_B T}{M}\frac{\partial}{\partial v}\left[\left[\frac{\partial}{\partial R_1} + \frac{kR_1}{k_B T}\right] - \left[\frac{\partial}{\partial R_0} + \frac{kR_0}{k_B T}\right]\right]\right\} \tag{4.72}$$

and

$$\left[\left[\frac{\partial}{\partial R_1} + \frac{kR_1}{k_B T}\right] - \left[\frac{\partial}{\partial R_0} + \frac{kR_0}{k_B T}\right]\right]\rho_{\rm eq}(b) = 0 . \tag{4.73}$$

By using Eqs. (4.72) and (4.73), from Eqs. (4.71) and (4.70) we then obtain

$$\mathcal{D} = \frac{1}{\rho_{\rm eq}(b)} \int_0^\infty P\mathcal{L}_1 e^{\mathcal{L}_b t} e^{\gamma t} \mathcal{L}_1 \rho_{\rm eq}(b) dt . \tag{4.74}$$

We now follow the same approach as that which has led us to Eq. (4.21). The final result is the following implicit equation for the parameter γ:

$$\gamma = \left[\frac{k_B T}{M}\right]^{-1} \times \int_0^\infty dt \left\langle \frac{k}{M}(R_1 - R_0) e^{\mathcal{L}_b t} \frac{k}{M}(R_1 - R_0) \right\rangle e^{\gamma t} . \tag{4.75}$$

From Eq. (4.75) we see that this approach leads to

$$\gamma = \lambda , \tag{4.76}$$

which means that we recover within the Fokker-Planck description precisely the same fully renormalized transport coefficient as that derived from the generalized Langevin equation of Sec. II [remember the Der relation of Eq. (2.15)]. To completely account for this important result, let us remark that Eq. (2.15) can be written as

$$\lambda=\int_0^\infty \frac{\langle f_1|e^{-(1-P_0)\mathcal{L}t}|f_1\rangle}{\langle f_0|f_0\rangle} e^{\lambda t}dt \ , \tag{4.77}$$

where

$$|f_0\rangle=|v\rangle \ ,$$
$$|f_1\rangle=-(1-P_0)\mathcal{L}|f_0\rangle=\frac{k}{M}(R_1-R_0) \ , \tag{4.78}$$
$$P_0=\frac{|v\rangle\langle v|}{\langle v|v\rangle} \ .$$

We have, furthermore,

$$-(1-P_0)\mathcal{L}=-\mathcal{L}_b+\frac{k}{M}(R_1-R_0)\frac{\partial}{\partial v} \ . \tag{4.79}$$

When the rhs of Eq. (4.79) is applied to $|f_1\rangle$ the second term of it vanishes. Then we must take into account that in Eq. (4.75) the operator $\exp(\mathcal{L}_b t)$ must be applied on the left. Thus γ is immediately proved to be equal to λ.

We can conclude this section by saying that we have shown mainly via a perturbation approach that the damping γ characterizing the Fokker-Planck equation of Eq. (4.71) coincides with the renormalized drift coefficient λ of the preceding section. A completely exhaustive demonstration would imply that the equality $\gamma=\lambda$ is proved at all the orders in μ. This is beyond our current capabilities and, via a perturbation calculation up to the fourth order in $\mathcal{L}_1$ we could only show that this is true up to the second order in μ. It is plausible that Eq. (4.76) is satisfied at any order in μ.

Thus, rigorously speaking, even the validity of the ansatz of Eq. (4.66) would seem to be rigorously proved only up to the fourth order. Note that this ansatz allows us to relate the Fokker-Planck equation to the same renormalized drift coefficient as that provided by the Langevin picture of the preceding section. Since the Fokker-Planck picture has to be rigorously equivalent to the Langevin picture, this ansatz is fully legitimate. In other words, we can say that the expansion of the time-ordered exponential of Eq. (4.66), if it were really carried out at all the orders, would lead us to conclude that Eq. (4.76) is an exact relation. As a more convincing argument in favor of the fact that this ansatz is exact, we must stress the interesting result of the Appendix. There we show that a natural extension of that ansatz to the non-Markovian case leads to a Fokker-Planck equation coinciding with that of Refs. 23–26. Note that the derivation of this latter Fokker-Planck equation only relies on the assumption that v is Gaussian.[23–26] Since this statistical property is certainly fulfilled by our microscopic system and our ansatz leads to a Fokker-Planck equation coinciding with that of Refs. 23–26, we can conclude that our ansatz is exact in the linear case.

V. CONCLUDING REMARKS

From a formal point of view, an element of interest of this paper is given by our fully renormalized Fokker-Planck equation. Note that Eq. (4.15) is well known in the literature concerning the generalized master equations.[27] A first discussion of it was given by Baus.[27(a)] A wide use of it was done within the context of subdynamics.[27(b)] However, the replacement of the time-ordered exponential with the time evolution driven by the Fokker-Planck operator itself, especially in the fully non-Markovian case dealt with in the Appendix—see Eq. (A3)—seems to be an element of novelty in the present paper.

As a more substantial result of this work, we have shown that the Fokker-Planck equation corresponds to the dynamics of a dressed state $|S\rangle$. The derivation of the Fokker-Planck equation illustrated in Sec. IV is perturbative in nature and it is equivalent to determining the "energy" of the "dressed" state via a perturbation approach on the discrete basis set. The next step should be to show that the state $|S\rangle$ has a real physical meaning and the experimental effect of measurement aiming at detecting the dynamical properties of the state $|e\rangle$ has actually the effect of building up the state $|S\rangle$ so that the correlation function really detected is not

$$\Phi_0(t)=\langle e|e(t)\rangle/\langle e|e\rangle \ . \tag{5.1}$$

Rather than that, the experiment should be proved to provide information on

$$\Phi_0(t)_S=\frac{\langle e|S(t)\rangle}{\langle S|S\rangle} \ . \tag{5.2}$$

This is precisely the point of view of Prigogine and coworkers.[8(a),18] We established an exciting connection between the Prigogine subdynamics and the problem of preparation. The Fokker-Planck equation provided by the projection method corresponds to studying the time evolution of the system initially prepared in the state $|S\rangle$. According to the central ideas of the subdynamics of Prigogine the space spanned by $|S\rangle$ is totally orthogonal to the nonexponential decay state.

We believe that a satisfactory discussion of this aspect should rely on a revision of the linear-response theory.[28] A central aspect of the Kubo linear-response theory[28] is that the response to an external perturbation can be expressed in terms of the bare correlation function of Eq. (5.1). This is why the recursion method of Lee[1] is expressed in terms of the Kubo scalar product. On the other hand, it has been remarked[29] that to meet the van Kampen criticism[30] of the Kubo linear-response theory, it would be convenient to operate the perturbation treatment of external excitation after carrying out a contraction over the "bath" variables. This, in our opinion, should lead to a response expressed in terms of the "dressed" rather than the "bare" correlation function of the variable of interest. This aspect will be the subject of a further investigation. It must be remarked that this issue is related to those discussed in the work of Ghirardi *et al.*,[31] concerning the role of the interaction with an experimental apparatus. The measurement process itself should be responsible for the decay process to become rigorously exponential, even if this is seemingly forbidden by rigorous theoretical constraints.

A further element of interest of the present paper rests on the consequences that these results bear on the derivation of a Fokker-Planck equation for a nonrigorously Markovian process. Some years ago this was a subject of great interest,[23–26] and the last few years have seen a revival of interest on this problem.[11,32–34] Adelman and Fox[23–25] discussed an approach to building up the Fokker-Planck equation for a non-Markovian system which heavily relies on the Gaussian assumption and the knowledge of the correlation function of the variable of interest. Ferrario and Grigolini[35] showed that the same result can be obtained via contraction from a multidimensional Markov equation. According to the alternative approach illustrated in Sec. IV and derived from that of Refs. 19–21, which, in turn, is based on the Zwanzig projection method,[36] the Fokker-Planck equation to be associated with the Hamiltonian of Eq. (2.1) reads

$$\frac{\partial}{\partial t}\sigma(v;t)=\lambda\left[\frac{\partial}{\partial v}v+\frac{k_BT}{M}\frac{\partial^2}{\partial v^2}\right]\sigma(v;t)\ . \tag{5.3}$$

In terms of the notation of this paper, the Fokker-Planck equation of Refs. 23–26 would lead to

$$\frac{\partial}{\partial t}\sigma(v;t)=-\frac{\dot{\Phi}_0(t)}{\Phi_0(t)}\left[\frac{\partial}{\partial v}v+\frac{k_BT}{M}\frac{\partial^2}{\partial v^2}\right]\sigma(v;t)\ . \tag{5.4}$$

In many cases, where the memory kernel of the generalized Langevin equation is derived using phenomenological arguments,[11] the two Fokker-Planck equations above are easily proven to lead to the same result. This is so because in these cases we have

$$\lim_{t\to\infty}\frac{\dot{\Phi}_0(t)}{\Phi_0(t)}=-\lambda\ . \tag{5.5}$$

In the asymptotic limit $t\to\infty$ Eq. (2.14) is shown (see Ref. 17) to read

$$\Phi_0(t)=\frac{(1-\mu)}{(1-2\mu)}\exp\left[-\frac{\mu\omega_0 t}{\sqrt{1-2\mu}}\right]+\frac{\mu}{(1-\mu)^2}\left[\frac{2}{\pi(\omega_0 t)^3}\right]^{1/2}\sin\left[\omega_0 t-\frac{\pi}{4}\right]\ . \tag{5.6}$$

This means that in the long-time region this correlation function is basically a harmonic function of time with an amplitude slowly decreasing upon increase of time; i.e., the second term on the rhs of Eq. (5.6). Therefore, this asymptotic limit cannot fulfill the condition of Eq. (5.5). As shown in the Appendix, this discrepancy stems from the fact that Eq. (5.3) has been obtained by replacing the upper limit of time integration in Eq. (4.14) with ∞ and a suitable use of analytical continuation. This shows that this assumption plays a fundamental role in recovering a result in line with the Prigogine subdynamics. If this assumption is not made, our renormalization procedure is shown to be compatible with the Fokker-Planck equation of Adelman and Fox.[23–26]

As the problem of the correct Fokker-Planck equation to be associated to a non-Markovian process, we can conclude this paper by remaking that we can divide non-Markovian processes into the following two major classes.

(a) Strongly non-Markovian processes. If the motion of the variable of interest significantly depends on the coupling with some macroscopic and very slow variables, the approach which led us to Eq. (5.3) cannot be followed. This agrees with the point of view of van Kampen and Oppenheim,[32] who say that their treatment of the Brownian motion as a problem of eliminating fast variables ignores the slow hydrodynamic modes of the fluid. The coupling between the variable velocity v and the slow hydrodynamic modes would result indeed in a strongly non-Markovian process. In this case, as pointed out in Ref. 23, the only practicable way would seem that of using the fully non-Markovian Fokker-Planck equation of Eq. (5.4). It must be stressed that an irretrievably non-Markovian behavior, triggered by the dynamics around an inverted parabola, has recently been met in the field of colored noise.[33,34] This is another case, where the approximation in terms of an effective Markovian process, namely, the major assumption behind Eq. (5.3), is not admitted.

(b) Weakly non-Markovian processes. The model studied in the present paper with a very small parameter μ belongs to this class. In this case, the long-time deviations from a rigorous exponential decay are shown in this paper to be closely related to those in the very-short-time regime. In other words, monitoring the deviation from the exponential decay in the long-time regime would be virtually equivalent to providing a detailed microscopic picture. This raises some fundamental questions concerning the dependence of the dynamics of the system of interest on the interaction with a measurement apparatus. Thus, intriguing aspects of the Fokker-Planck equation (5.4), such as the appearance of a divergent transport coefficient in the long-time region, would be fully cured by adopting Eq. (5.3), which is completely equivalent to accepting the major suggestion of the Prigogine subdynamics.

APPENDIX

Our aim is to write Eq. (4.9) under the following form:

$$\frac{\partial}{\partial t}\sigma(v;t)=\eta(t)\mathcal{L}_{FP}\sigma(v;t)\ . \tag{A1}$$

The operator $\mathcal{L}_{FP}$ is defined in Eq. (4.30). Let us now extend the ansatz of Eq. (4.66), thought of as applying to the time-independent operator

$$\mathcal{D}=\gamma\mathcal{L}_{FP}=\lim_{t\to\infty}\eta(t)\mathcal{L}_{FP}\ , \tag{A2}$$

to the case of a time-dependent operator. Thus we obtain the obvious generalization

$$T\exp\left[Q\int_\tau^t\mathcal{L}_1(t')dt'\right]=\exp\left[\mathcal{L}_{FP}\int_\tau^t\eta(t')dt'\right]\ . \tag{A3}$$

By substituting Eq. (A3) into Eq. (4.9) and taking Eq. (4.10) into account, we obtain

$$\eta(t)\mathcal{L}_{\mathrm{FP}}=\frac{1}{\rho_{\mathrm{eq}}(b)}\int_0^t P\mathcal{L}_1 e^{\mathcal{L}_b(t-\tau)}\exp\left[\mathcal{L}_{\mathrm{FP}}\int_\tau^t \eta(t')dt'\right]\mathcal{L}_1\rho_{\mathrm{eq}}(b)\sigma(\tau)d\tau$$
$$=\frac{1}{\rho_{\mathrm{eq}}(b)}\int_0^t P\mathcal{L}_1 e^{\mathcal{L}_b\tau}\exp\left[\mathcal{L}_{\mathrm{FP}}\int_{t-\tau}^t \eta(t')dt'\right]\mathcal{L}_1\rho_{\mathrm{eq}}(b)\sigma(t-\tau)d\tau\ . \quad \text{(A4)}$$

The counterpart of Eq. (4.13) becomes

$$\sigma(t-\tau)=\exp\left[\mathcal{L}_{\mathrm{FP}}\int_t^{t-\tau}\eta(t')dt'\right]\sigma(t)\ . \quad \text{(A5)}$$

Using Eq. (A5), from Eq. (A4) we have

$$\eta(t)\mathcal{L}_{\mathrm{FP}}=\frac{1}{\rho_{\mathrm{eq}}(b)}\int_0^t P\mathcal{L}_1 e^{\mathcal{L}_b\tau}\exp\left[\mathcal{L}_{\mathrm{FP}}\int_{t-\tau}^t \eta(t')dt'\right]\mathcal{L}_1\exp\left[-\mathcal{L}_{\mathrm{FP}}\int_{t-\tau}^t \eta(t')dt'\right]\rho_{\mathrm{eq}}(b)d\tau\ . \quad \text{(A6)}$$

This equation is obviously the counterpart of Eq. (4.67) and for $t\to\infty$ it coincides with Eq. (4.67) if the condition of Eq. (A2) holds. In such a case, we have

$$\exp(\pm\mathcal{D}\tau)=\exp\left[\pm\mathcal{L}_{\mathrm{FP}}\int_{t-\tau}^t \eta(t')dt'\right]\ , \quad \text{(A7)}$$

which then leads to Eq. (4.67). By suitably adapting to this time-dependent case the way we followed in Sec. IV from Eqs. (4.68) to (4.74), we get the counterpart of Eq. (4.75), which reads

$$\eta(t)=\left[\frac{k_B T}{M}\right]^{-1}\int_0^t d\tau\left\langle \frac{k}{M}(R_1-R_0)e^{\mathcal{L}_b\tau}\frac{k}{M}(R_1-R_0)\right\rangle \times\exp\left[\int_{t-\tau}^t \eta(t')dt'\right]\ . \quad \text{(A8)}$$

By using Eqs. (2.7), (2.8), (4.77), and (4.78), from Eq. (A8) we obtain

$$\eta(t)=\Delta_1^2\int_0^t d\tau\,\Phi_1(\tau)\exp\left[\int_{t-\tau}^t \eta(t')dt'\right]\ , \quad \text{(A9)}$$

which, via the change of variable $\tau\to t-\tau$, becomes

$$\eta(t)=\Delta_1^2\int_0^t d\tau\,\Phi_1(t-\tau)\exp\left[\int_\tau^t \eta(t')dt'\right]\ . \quad \text{(A10)}$$

Let us see under which condition the solution of Eq. (A10) is given by

$$\eta(t)=-\frac{\dot{\Phi}_0(t)}{\Phi_0(t)}\ . \quad \text{(A11)}$$

By replacing Eq. (A11) into the rhs of Eq. (A10) we obtain

$$\eta(t)=\Delta_1^2\int_0^t d\tau\,\Phi_1(t-\tau)\left|\frac{\Phi_0(\tau)}{\Phi_0(t)}\right|$$
$$=\Delta_1^2\int_0^t d\tau\,\Phi_1(t)\left|\frac{\Phi_0(t-\tau)}{\Phi_0(t)}\right|\ . \quad \text{(A12)}$$

From Eq. (A12), supplemented by Eq. (2.7), we see that Eq. (A11) provides a solution to Eq. (A9) under the condition that $\Phi_0(t)$ is positive for any value of t [remember that $\Phi_0(0)=1$].

We thus see that our Fokker-Planck equation, obtained from Eq. (4.9) without replacing the upper limit of time integration t with ∞ and supplemented by the ansatz of Eq. (A3), coincides with that of Refs. 23–26, under the limiting condition that $\Phi_0(t)$ is always positive. Actually, it seems that this is also a condition for the Fokker-Planck equation proposed by Adelman[23] and Fox[24,25] to hold. Should $\Phi_0(t)$ assume a negative value at a certain time t, continuity arguments would imply that at a certain earlier time $\Phi_0(t)$ would vanish, thereby producing a divergent value of $\eta(t)$. The corresponding Fokker-Planck equation, being a partial-derivative equation, would correspondingly become meaningless after the divergence point. We can thus conclude that the region of validity of our Fokker-Planck equation is the same as that of Adelman and Fox, and the two Fokker-Planck equations coincide.

In the special case where the limit of $\eta(t)$ for $t\to\infty$ exists and it is positive, the rhs of Eq. (A9) becomes coincidence with Eq. (2.15) and divergent. This divergence must be cured with the adoption of the same procedure of analytic continuation as that used in Sec. II, which resulted in the fully renormalized damping of Eq. (2.16). If the $\eta(t)$ function defined by Eq. (A10) does not admit a definite limit for $t\to\infty$, as it happens in the special Hamiltonian case studied in this paper, the Fokker-Planck equation of Eq. (5.4) has an unclear meaning, whereas that of Eq. (5.3), corresponding to the dynamics of the dressed variable S, can be used without any drawbacks.

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