Conditions for the validity of the quantum Langevin equation

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From microscopic models, a Langevin equation can, in general, be derived only as an approximation. Two possible conditions to validate this approximation are studied. One is, for a linear Langevin equation, that the frequency of the Fourier transform should be close to the natural frequency of the system. The other is by the assumption of "slow" variables. We test this method by comparison with an exactly soluble model and point out its limitations. We base our discussion on two approaches. The first is a direct, elementary treatment of Senitzky. The second is via a generalized Langevin equation as an intermediate step.

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I. INTRODUCTION

The Langevin equation is certainly only an approximation (except in the special case when the underlying equations of motion are all linear when it is an exact consequence of the Heisenberg equations of motion), and so it is of interest to find the conditions for it to be a good approximation.

The equation has been justified, starting from microscopic equations of motion, by various general arguments and in some particular models. These arguments start from the Heisenberg equations of motion for a simple (macroscopic or mesoscopic) system, described by an operator Q, interacting with an environment (or bath) with many degrees of freedom. We will assume the systems are quantum ones, but everything we say would equally apply to classical systems (replacing commutators by Poisson brackets and so on). We choose a microscopic model in which the interaction is bilinear in the environment variables. This is the simplest change from the (trivial) linear case and is necessary if the environment is fermionic.

We will concentrate on two approaches. The first is due to Senitzky [1]. It uses only elementary quantum mechanics, but it is not clear for what ranges of parameters the approximations made are good ones. We argue that one region in which Senitzky's approximations may be justified is where the frequency of Q is close to the natural frequency Ω of the simple system (which therefore assumes that system to be linear). That is, if $\tilde{Q}(\omega)$ is the Fourier transform of $Q(t)$, the solution of the Langevin equation is reliable for ω close to Ω. Our approach is to regard the Langevin equation as summing an infinite subset of perturbation theory terms. The question is then, when does this subset dominate?

For an earlier discussion of Senitzky's argument, see [2]. As far as we know, textbooks do not offer a derivation as simple and direct as Senitzky's. See, for example, [3–8].

The second method of justification is indirect. First, a generalized Langevin equation is established by a projection method [9–11]. This is formally exact, but probably not useful. [It is usually restricted to the case of a linear system, equation (2.3).] In Sec. V B we point out that in the generalized Langevin equation the separation into a noise term and a dissipative term is ambiguous.

Then it is assumed that the system variables are "slow" compared to the environmental ones. It is argued that the generalized Langevin equation then simplifies greatly and becomes an ordinary Langevin equation. In Sec. V, we examine this proposal critically and test it in an exactly soluble example. For some textbook accounts, see [3,8,11–13].

It is worth noting that both the above methods work by manipulating the underlying Heisenberg equation of motion. Yet the Langevin equation in the end refers to an expectation value over some distribution function, chosen on physical grounds. Clearly, some assumptions have been made during the course of the derivations.

A paper by Cortés *et al.* [14] has a similar aim to ours but a different approach. To avoid any confusion, we explain the similarity and differences in Sec. VII.

II. THE UNDERLYING MICROSCOPIC SYSTEMS

We use the Heisenberg picture throughout.

We are concerned with attempts to deduce a Langevin equation from an underlying dynamics. This consists of a simple macroscopic or mesoscopic system interacting with an environment (sometimes called a bath). For simplicity, we take the system to have one degree of freedom, with phase space Q, P. The environment has many (microscopic) degrees of freedom q_i, p_i, with $i = 1, \ldots, N$. The Hamiltonian is

$$H = H_0(t) + H'(t), \quad H_0(t) = H_S(t) + H_E(t), \tag{2.1}$$

$$H_S = (1/2)P^2/M + V(Q),$$

$$H_E = \sum_{i=1}^{N} (1/2)\left(p_i^2/m_i + m_i\omega_i^2 q_i^2\right), \tag{2.2}$$

$$H' = -\alpha Q K(q_i, p_i)$$

(N is large). Thus we are assuming the environment to be a set of oscillators. We do not need to specify the distribution of

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the frequencies ω_i. We will sometimes take

$$V(Q) = (M/2)\Omega^2 Q^2; \tag{2.3}$$

that is, the system is an oscillator too. In this case, the resulting Langevin equation is linear. It will turn out that we are able to justify the Langevin equation for the special case (2.3) only, but it is useful to have the notation $V(Q)$ for the more general case in order to point out (Sec. IV) the difficulty that arises then. In (2.2), α designates the coupling strength. We have assumed that H' is linear in the system variables, and for simplicity we have chosen Q (not P) to appear there.

It will be useful to define operators Q_0, P_0, q_{0i}, p_{0i} to coincide with Q, P, q_i, p_i at an initial time t_0 but to vary with time according to the free ($\alpha = 0$) equations of motion. That is,

$$\begin{aligned} Q_0(t_0) &= Q(t_0), \quad P_0(t_0) = P(t_0), \\ \hbar\dot{Q}_0(t) &= i[H_{S0}, Q_0(t)], \quad \hbar\dot{P}_0(t) = i[H_{S0}, P_0(t)], \\ H_{S0} &= H_S(Q_0(t), P_0(t)), \\ q_{0i}(t_0) &= q_i(t_0), \quad p_{0i}(t_0) = p_i(t_0), \\ \hbar\dot{q}_{0i}(t) &= i[H_{E0}, q_{0i}(t)], \quad \hbar\dot{p}_{0i}(t) = i[H_{E0}, p_{0i}(t)], \\ H_{E0} &= H_E(q_{0i}(t), p_{0i}(t)). \end{aligned} \tag{2.4}$$

Note that H_{S0} and H_{E0} are each independent of t.

If the function K in (2.2) is linear, the equations of motion of the environment are linear, and these variables can be simply eliminated to produce an exact Langevin equation. No statistical distribution function appears in this Langevin equation. For these two reasons, the case of K being linear is misleadingly simple, although it is treated in many textbooks, for example, as a model of Brownian motion and of decoherence. For a comprehensive study, see [15].

The simplest nontrivial example is for K to be bilinear in q_i, p_i, and this is what we shall assume below. Note that the environment might consist of fermionic variables (such as conduction electrons), and then K would necessarily be bilinear or of higher degree. We will not treat this fermionic case explicitly, but our arguments below can easily be generalized to cover Fermi statistics.

The remaining ingredient is a statistical distribution function. In nonequilibrium statistical physics, the choice of distribution function is a matter of physical judgment. We shall mention just two possibilities. The first is simply

$$\rho = Z^{-1}\exp(-H/T), \tag{2.5}$$

the equilibrium distribution. The second is the factorized free distribution:

$$\rho_0 = Z_0^{-1}\exp(-H_0/T) = \rho_S\rho_E = \rho_S Z_E^{-1}\exp(-H_{E0}/T), \tag{2.6}$$

where H_{E0} is the time-independent energy defined in (2.4), and we need not specify ρ_S further. Units of temperature T are chosen so that Boltzmann's constant is unity, and the partition functions Z, Z_0, and Z_E are normalization factors. The use of ρ_0 is motivated by the idea that the environment is initially at equilibrium by itself, and then the system is brought into contact with it at some initial time t_0. Since we use the Heisenberg picture, density matrices are time independent, and so the factorization property (2.6) is a single condition, not one for each value of t as it would be in the Schrödinger picture. But H_{E0} and therefore also ρ_E depend implicitly on the initial time t_0. For the Hamiltonian H_E in (2.2), ρ_{E0} factorizes further:

$$\rho_{E0} = \prod_i \rho_{i0}. \tag{2.7}$$

The assumption of (2.6) means that the complete system (Q system plus environment) is not initially in thermal equilibrium.

We define expectation values, for an operator X,

$$\langle X\rangle = \mathrm{tr}(X\rho), \quad \langle X\rangle_0 = \mathrm{tr}(X\rho_0). \tag{2.8}$$

In its simplest form, the Langevin equation that one might hope to derive is usually assumed to be (for $t > t_0$)

$$M\ddot{Q}(t) + V'[Q(t)] + \alpha^2\int_{t_0}^{\infty} dt'\bar{C}(t,t')Q(t') = \alpha K_0(t), \tag{2.9}$$

defining $V' = dV/dQ$, where

$$\bar{C}(t,t') = \langle C(t,t')\rangle_0 = \langle C(t,t')\rangle_E \equiv \mathrm{tr}\{C_E(t,t')\rho_E\} \tag{2.10}$$

and

$$\begin{aligned} C(t,t') &= \theta(t-t')c(t,t'), \quad c(t,t') = -\frac{i}{\hbar}[K_0(t), K_0(t')] \\ &= C(t,t') - C(t',t), \end{aligned} \tag{2.11}$$

and $K_0 = K(q_{0i}, p_{0i})$. [In the classical case, the right-hand side of (2.11) is to be replaced by the Poisson bracket and the trace in (2.8) would be replaced by $\int\prod_i dq_i dp_i$.] Equation (2.9) shows the characteristic features of a Langevin equation: the noise K_0 and dissipation contained in the C term (non-Markovian in general, i.e., frequency dependent).

If K is linear in the environment variables, (2.9) is exact. This follows simply by solving for $q_i(t)$ (the retarded solution) in terms of Q and $q_i(t_0), p_i(t_0)$ and inserting this solution into $K(q_i, p_i)$. In this special case $C(t,t')$ is a c-number and, in fact, is not dependent on any dynamical variables, so the expectation value in (2.10) is redundant.

A typical quantity one might want to compute by using (2.9) is the correlation function,

$$S_Q(t,t') = \langle Q(t)Q(t')\rangle_0 \equiv \mathrm{tr}\{Q(t)Q(t')\rho_0\}. \tag{2.12}$$

In general, S_Q may not be a function of $(t-t')$ only. This is because ρ_0 defined in (2.7) does not commute with H' and so does not commute with the total Hamiltonian H. If t and t' are much later than t_0, the form of ρ_S may be unimportant in (2.12).

There is a general result, which is the fluctuation-dissipation theorem. Define

$$S_{K_0}(t-t') = \langle K_0(t)K_0(t')\rangle_E \equiv \mathrm{tr}\{K_0(t)K_0(t')\rho_E\} \tag{2.13}$$

(note that S_K depends only on the time difference because $\hbar\dot{K}_0 = i[H_E, K_0]$ and $[H_E, \rho_E] = 0$), and define the Fourier transform by

$$S_{K0} = \int d\omega e^{-i\omega(t-t')}\tilde{S}_K(\omega). \tag{2.14}$$

Then the relation is

$$-i\hbar\tilde{\dot{c}}(\omega) = \tanh\left(\frac{\hbar\omega}{2T}\right)[\tilde{S}_K(\omega) + \tilde{S}_K(-\omega)], \quad (2.15)$$

where $\tilde{c}$ is the Fourier transform of the expectation value of c in (2.11).

In Sec. III we review Senitzky's derivation of a Langevin equation and then derive one condition for its validity. Section IV reviews the so-called generalized Langevin equation, and Sec. V discusses how the ordinary Langevin equation might follow if Q and P are slow variables. Section VII summarizes our conclusions.

III. SENITZKY'S ARGUMENT

We first emphasize the salient features of Senitzky's [1] argument, which is quite general.

By using the Heisenberg equations of motion, for K and H_E, Senitzky derives the exact equations

$$M\ddot{Q} + V'(Q) = \alpha K, \quad (3.1)$$

$$K(t) = K_0(t) - \frac{i\alpha}{\hbar}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 U^*(t-t_1) \times [K(t_1), \dot{K}(t_2)Q(t_2)]U(t-t_1), \quad (3.2)$$

where

$$i\hbar\dot{K}(t) = [K(t), H] \equiv [K(t), H_E(t) + H_S(t) + H'(t)] = [K(t), H_E(t)], \quad (3.3)$$

$$U(t) = \exp[-it\,H_E(t_0)/\hbar] = \exp(-it\,H_{E0}/\hbar). \quad (3.4)$$

Note that it is $H_E(t)$ that comes in (3.3), not H_{E0}.

Senitzky then approximates in (3.2) K by K_0 and $U^*(t-t_1)Q(t_2)U(t-t_1)$ by $Q(t_2)$ to obtain

$$K(t) \simeq K_0(t) - \frac{i\alpha}{\hbar}\int_{t_0}^{t} dt_1 \times \int_{t_0}^{t_1} dt_2 [K_0(t), \dot{K}_0(t_2 + t - t_1)]Q(t_2). \quad (3.5)$$

Now the t_1 integration may be done to give

$$K(t) \simeq K_0(t) - \alpha\int_{t_0}^{t} dt' C(t,t')Q(t'), \quad (3.6)$$

where C is given by (2.11).

Equation (3.6) is the first stage of Senitzky's approximation. The second is to use to use the further approximation

$$C(t,t') \simeq \bar{C}(t,t'), \quad (3.7)$$

giving, together with (3.1), the Langevin equation (2.9). Note that the approximation (3.7) is needed in the classical case as well as the quantum one. Only in the linear case is (2.9) exact.

The approximations leading to (3.6) amounts to neglecting in K some, but not all, terms of order α^2. In order to discuss this, we define the power series

$$K = K_0 + \alpha K_1 + \alpha^2 K_2 + \cdots, \quad Q = Q_0 + \alpha Q_1 + \alpha^2 Q_2 + \cdots. \quad (3.8)$$

Then, for example, a neglected term containing $K_1 Q_0$ is not obviously smaller than the retained term $K_0 Q_1$ in (3.5). Thus it is far from obvious that (3.5) is a valid approximation.

A. Perturbation theory

In order to investigate the region of validity of Senitzky's first approximation (3.5), we consider an expansion of K in powers of α. The approximation picks out an infinite subset of terms. The question is, when do these terms dominate? We shall attempt to answer this question by looking at the lowest-order terms, but we believe that our argument generalizes to all orders.

The solution of the exact equation (3.2) is more easily derived directly from the original Heisenberg equations of motion (3.3) and so on. It is

$$K(t) = W^*(t)K_0(t)W(t), \quad (3.1.1)$$

where W is the solution of

$$i\hbar\dot{W}(t) = H_0'(t)W(t) = -\alpha K_0(t)Q_0(t)W(t), \quad W(t_0) = 1. \quad (3.1.2)$$

We may now compare the order α^2 term K_2 from (3.1.1) with the approximation from (3.5). To order α^2, the exact (3.1.1) gives

$$K_2(t) = -\frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \times \int_{t_0}^{t_1} dt_2 [[K_0(t), K_0(t_1)Q_0(t_1)], K_0(t_2)Q_0(t_2)]. \quad (3.1.3)$$

In order to find the approximate form of K_2 deduced from (3.5), we first find Q_1. This is derived in (3.1), with K on the right approximated by K_0. The solution of this equation may be written

$$Q_1(t) = \frac{i}{\hbar}\int_{t_0}^{t} dt'[Q_0(t), Q_0(t')]K_0(t'). \quad (3.1.4)$$

It is easy to check if V is a sum of integral powers of Q.

Inserting (3.1.4) into (3.6) gives [using (2.11)]

$$K_2(t) \simeq -\frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \times \int_{t_0}^{t_1} dt_2 [K_0(t), K_0(t_1)]K_0(t_2)[Q_0(t_1), Q_0(t_2)]. \quad (3.1.5)$$

The difference between (3.1.3) and (3.1.5) is

$$-\frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 [[K_0(t), K_0(t_1)], K_0(t_2)]Q_0(t_2)Q_0(t_1). \quad (3.1.6)$$

In general, (3.1.5) and (3.1.6) are of the same order. It is clear that the Langevin equation sums a subset of the terms in (3.1.1). The question is, what are the conditions for this subset to dominate over the other terms, such as (3.1.6)? We are able to propose an answer to this question, but only for the case

where the system is an oscillator, that is, assuming (2.3). Then the free equation for $Q(t)$ has a Green's function,

$$G(t) = \theta(t)(M\Omega)^{-1}\sin(\Omega t), \tag{3.1.7}$$

and

$$\theta(t-t')[Q_0(t), Q_0(t')] = -i\hbar G(t-t'). \tag{3.1.8}$$

The Fourier transform of (3.1.7) is

$$\tilde{G}(\omega) = -\frac{1}{(2\pi M)}\frac{1}{(\omega+i\epsilon)^2-\Omega^2}. \tag{3.1.9}$$

The structure of (3.1.5), but not of (3.1.6), allows for the pole in (3.1.9) at $\omega = \Omega$ to appear in suitable functions of ω. But to complete this argument, we must include Senitzky's second approximation, and to do this we need a more detailed model for K, which is the subject of the next section.

B. A model interaction

In this section we will take $t_0 = -\infty$. We discuss later what changes if t_0 is finite.

In order to test Senitzky's argument, we take the simplest model we can think of, which is not completely linear. We take K in (2.2) to be bilinear in the environmental variables. If we have in mind a model for Brownian motion, then the simple case when K is linear might be thought of as representing the emission of a phonon by the Brownian particle. In our bilinear generalization, phonons scatter off the particle. Of course, these are only crude models.

Define annihilation operators by

$$a_i(t) = \frac{ip_i(t) + m_i\omega_i q_i(t)}{\sqrt{2m_i\omega_i}}, \quad a_i(t) = \exp(-i\omega_i t)a_i. \tag{3.2.1}$$

Then we take

$$K = \hat{K} - \langle\hat{K}\rangle_E, \quad \hat{K}(t) = L^{-1}\sum_{i,j=1}^{N}(\omega_i\omega_j)^{1/2}a_i^*(t)b_{ij}a_j(t), \tag{3.2.2}$$

where b_{ij} are dimensionless numbers and L is a parameter with dimensions of length, which we shall not specify further (but which might represent, for example, a lattice spacing). With K defined as in (3.2.2), α in (2.2) is dimensionless.

Our formalism could easily be extended to the case when the environment contained fermions and a_i in (3.2.1) were fermionic annihilation operators.

We shall concentrate on c, the odd part of C in (2.11). From (3.2.2),

$$c(t,t') = \sum_{ij}(\omega_i\omega_j)^{1/2}X_{ij}(t,t')a_i^*a_j, \tag{3.2.3}$$

where

$$X_{ij}(t,t') = -iL^{-2}\sum_k \omega_k b_{ik}b_{kj}[\exp\{i(\omega_i-\omega_k)t + i(\omega_k-\omega_j)t'\} - (i\leftrightarrow j)]. \tag{3.2.4}$$

From (3.2.3) and (3.2.4),

$$\bar{c}(t-t') \equiv \langle c(t,t')\rangle_E = \sum_i X_{ii}w(\omega_i), \tag{3.2.5}$$

where

$$X_{ii}(t-t') = -2L^{-2}\sum_k \omega_k b_{ik}b_{ki}\sin[(\omega_k-\omega_i)(t-t')] \tag{3.2.6}$$

and

$$w(\omega) = \hbar\omega[\exp(\hbar\omega/T)-1]^{-1}. \tag{3.2.7}$$

The classical (high-temperature) limit of $w(\omega)$ is T, and the low-temperature limit is $\hbar\omega\exp(-\hbar\omega/T)$.

We first discuss Senitzky's second approximation (3.7) and return to (3.5) later. So we begin by assuming (3.6) and combine it with (3.1) to give

$$M\ddot{Q} + M\Omega^2 Q + \frac{\alpha^2}{2}\int_{-\infty}^{t}dt'\{C(t,t')Q(t') + Q(t')C(t,t')\} = \alpha K_0(t). \tag{3.2.8}$$

We have symmetrized the order of the operators in the integrand in order to make it explicitly Hermitian. Since $[C,Q] = O(\alpha)$, this involves only higher-order terms in the integrand.

We will formally solve (3.2.8) as a power series in α and then compare the terms in this series, with and without the use of (3.7). Of course, the Langevin equation sums an infinite number of orders of α, but approximations that fail term by term in the power series are unlikely to succeed for the complete series.

In order to be definite, we assume we are using the Langevin equation in order to calculate the Q-noise correlation function (2.12). It is this assumption that gives a physical motivation for using ρ_0 as the distribution function. Up to this point, there was no reason to prefer ρ_0 in the approximation (3.7).

Through order α^4, we get

$$\begin{aligned}S_Q(t-t') = {}& \langle Q_0(t)Q_0(t')\rangle_0 \\ &+\alpha^2\int dt_1dt_2G(t-t_1)G(t'-t_2)\langle K_0(t_1)K_0(t_2)\rangle_0 \\ &+\frac{\alpha^4}{2}\int dt_1dt_2dt_3t_4G(t'-t_4)G(t-t_1)G(t_2-t_3) \\ &\times\langle\{C(t_1,t_2)K_0(t_3)+K_0(t_3)C(t_1,t_2)\}K_0(t_4)\rangle_0 \\ &+(\text{H.c. with } t\leftrightarrow t').\end{aligned} \tag{3.2.9}$$

Note that, using $t_0 = -\infty$, S_Q turns out to depend only on $t-t'$, although this is not obvious from the definition (2.12). If the approximation (2.7) were valid, we should be able to approximate the expectation value at the end of (3.2.9) by

$$\langle C(t_1,t_2)K_0(t_3)K_0(t_4)\rangle \simeq \bar{C}(t_1-t_2)\langle K_0(t_3)K_0(t_4)\rangle \tag{3.2.10}$$

and so on. So this is what we now check, using (3.2.3) and (3.2.4).

To evaluate the expectation value in (3.2.10), we need [using (3.2.2)]

$$\sum_{ijklmn}X_{ij}b_{kl}b_{mn}\mathrm{tr}\left(a_i^*a_ja_k^*a_la_m^*a_n\prod_r\rho_{r0}\right). \tag{3.2.11}$$

This receives nonzero contributions from the following values:

$$\begin{aligned}&\text{(a)}: \quad i=j, k=n, l=m;\\ &\text{(b)}: \quad i=l, k=n, j=m;\\ &\text{(c)}: \quad i=n, j=k, l=m,\end{aligned} \tag{3.2.12}$$

where in each case we assume there are no other equalities. There are also contributions such as $i=j=k=n, l=m$, but for large N these are negligible compared to (3.2.12).

The contribution to (3.2.11) from region (a) in (3.2.12) gives the right-hand side of (3.2.10); so the question is, when are the contributions from regions (b) and (c) small compared to that from (a)?

The Fourier transform of (3.2.9) has the form

$$i\alpha^4[\tilde{G}(\omega)]^2\sum_{ijkl}[W_a+W_b+W_c]+\text{H.c.}, \tag{3.2.13}$$

where W_a, W_b, W_c come from the ranges in (3.2.12):

$$\begin{aligned}W_a &= \tilde{G}(\omega)w(\omega_j)w(\omega_l)b_{kl}b_{lk}b_{ij}b_{ji}(\omega-\omega_i+\omega_j+i\epsilon)^{-1}\\ &\quad\times\delta(\omega-\omega_k+\omega_l)-(\omega_{i,j,k,l}\to-\omega_{i,j,k,l}), \quad (3.2.14a)\\ W_b &= \tilde{G}(\omega_i-\omega_k)w(\omega_j)w(\omega_l)b_{ij}b_{jl}b_{lk}b_{ki}(\omega-\omega_i+\omega_j+i\epsilon)^{-1}\\ &\quad\times\delta(\omega-\omega_l+\omega_j)-(\omega_{i,j,k,l}\to-\omega_{i,j,k,l}), \quad (3.2.14b)\\ W_c &= \tilde{G}(\omega_j-\omega_l)w(\omega_j)w(\omega_l)b_{ij}b_{jl}b_{lk}b_{ki}(\omega-\omega_i+\omega_j+i\epsilon)^{-1}\\ &\quad\times\delta(\omega-\omega_k+\omega_l)-(\omega_{i,j,k,l}\to-\omega_{i,j,k,l}), \quad (3.2.14c)\end{aligned}$$

Here $\tilde{G}$ is defined in (3.1.9) and has a pole where its argument is equal to the natural frequency Ω. There are three such poles at $\omega=\Omega$ in (3.2.13) from (3.2.14a), whereas from the other two terms there are only two poles. Thus W_a, and therefore the approximation of (3.2.10) by (3.2.9), may be good for values of ω sufficiently near Ω. Otherwise, we can see no reason why W_a, W_b, and W_c should not be comparable.

The structure of the terms in equations (3.2.14) is illustrated in Fig. 1. The generalization to all orders of α is that the Langevin equation sums "bubble graphs," that is, graphs like the first one in Fig. 1, with a sequence of bubbles like the one marked X in Fig. 1, connected by Q propagators. These graphs have the maximum number of poles at $\omega=\Omega$.

We now turn to the first approximations made in Senitzky's argument, the replacement of (3.2) by (3.5). To order α^2, this implied neglecting (3.1.6) compared to (3.1.5). If we work out the contribution of (3.1.5) to (3.2.9), we need, instead of (3.2.10),

$$\langle[C(t_1,t_2),K_0(t_3)]K_0(t_4)\rangle_0. \tag{3.2.15}$$

A contribution such as (3.2.14a) is zero because $[\tilde{C}(t_1,t_2),K_0(t_3)]=0$. Thus (3.1.5) has parts with three poles at $\omega=\Omega$, but (3.1.6) does not, so near this pole both Senitzky's approximations (3.5) and (3.7) are justified.

If t_0 is finite, there are no poles at $\omega=\Omega$. However, in the Fourier transform of (3.2.9), times less than t_0 do not contribute much if

$$\omega|t_0|\gg 1. \tag{3.2.16}$$

Thus we expect the would-be poles at $\omega=\Omega$ to be large provided that $|t_0|$ is large enough to satisfy (3.2.16).

IV. NONLINEAR Q SYSTEMS

Most of our arguments above have assumed that the simple system is an oscillator, as in (2.3), with a well-defined natural frequency Ω, so that we can recognize the poles (3.1.9). But we may ask if the arguments extend to the more general potential $V(Q)$ in (2.2) when the equation of motion for Q is nonlinear. Then a simple Green's function such as (3.1.9) does not exist. However, when working to first order, there is Eq. (3.1.4), where $\theta(t-t')[Q_0(t),Q_0(t')]$ looks a bit like a Green's function, though, in general, it is an operator and is a function of t and t' separately.

Let us consider an example like (3.2.9). For a nonlinear system, each Green's function $G(t-t')$ is replaced by the operator $i\theta(t-t')[Q_0(t),Q_0(t')]/\hbar$. We have to take the expectation value of the products of these commutators using ρ_S in (2.6). In order to make the same sort of argument as we did with the propagator poles (3.1.9), two things are needed: the expectation values of products of commutators should approximately factorize into products of expectation values $\langle Q_0(t)Q_0(t')\rangle$, and the Fourier transforms of each of these should have a pole at some definite frequency. Whether or not these things happen in any useful approximation will depend upon the potential $V(Q)$.

As the simplest example, take a product of two commutators, as would occur in the first line of (3.2.9). In the nonlinear case, the product of two Green's functions $G(t-t_1)G(t'-t_2)$ would be replaced by

$$\begin{aligned}&-(1/\hbar^2)\theta(t-t_1)\theta(t'-t_2)\text{tr}\{[Q_0(t),Q_0(t_1)]\\ &\quad\times[Q_0(t'),Q_0(t_2)]\rho_S\}.\end{aligned} \tag{4.1}$$

Let us assume that H_S has a discrete set of energy eigenstates $|\alpha\rangle$ with energy E_α and take the simplest case where ρ_S corresponds to the (pure) ground state $|0\rangle$. Then (4.1) has contributions

$$\begin{aligned}&-(1/\hbar^2)\theta(t-t_1)\theta(t'-t_2)\sum_{\alpha,\beta,\gamma}(\langle 0|Q_0(t)|\alpha\rangle\langle\alpha|Q_0(t_1)|\beta\rangle\\ &\quad\times\langle\beta|Q_0(t')|\gamma\rangle\langle\gamma|Q_0(t_2)|0\rangle-(t\leftrightarrow t_1)-(t'\leftrightarrow t_2)\\ &\quad+(t,t'\leftrightarrow t_1,t_2)).\end{aligned} \tag{4.2}$$

We will get the required behavior if there is a significant contribution to (4.2) from $|\beta\rangle=|0\rangle$ and $|\alpha\rangle=|\gamma\rangle$ for some $|\alpha\rangle$. If this happens, the time dependence of (4.2) is

$$\begin{aligned}&\theta(t-t_1)\theta(t'-t_2)\sin\{(t-t_1)(E_\alpha-E_0)/\hbar\}\\ &\quad\times\sin\{(t'-t_2)(E_\alpha-E_0)/\hbar\},\end{aligned} \tag{4.3}$$

and then the Fourier transform has poles at the frequency

$$\Omega_{0\alpha}\equiv(E_\alpha-E_0)/\hbar, \tag{4.4}$$

which looks like what one gets from (3.1.7). But, of course, as well as (4.3), there will be other contributions to (4.2), which are not functions of just the two variables $(t-t_1)$ and $(t'-t_2)$. So there is, in general, no reason to expect (4.4) to dominate.

A heuristic quantum Langevin equation has been used for a system involving a shunted Josephson junction [3,16–20]. Then Q is the Josephson angle, and

$$V(Q)=-IQ-I_0\cos(Q), \tag{4.5}$$

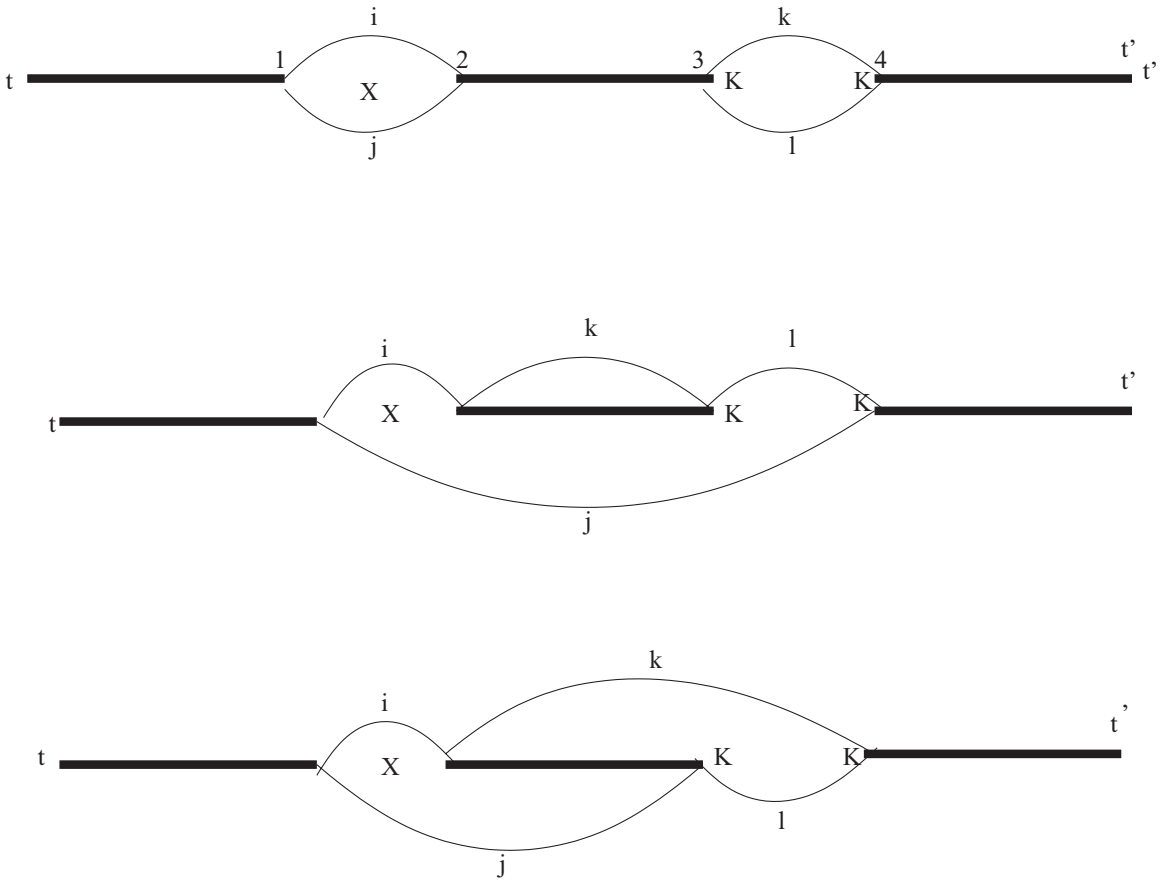

FIG. 1. Graphs symbolizing the terms in (3.2.14). Thick lines represent the Q propagator (3.1.9). Thin lines indicate the pairings in (3.2.12). The X represents the commutator c in (2.11). The vertices are labeled according to the values of the times in (3.2.9).

with the constant coefficients satisfying $I > I_0$. In this potential, there are no discrete quantum states, so the above considerations are irrelevant. What is more, in the classical motion $\dot{Q}$ increases indefinitely, but when the damping due to the Langevin equation is included, the motion is, in general, qualitatively very different. So it is not possible to use an expansion in powers of the interaction strength α (except perhaps for a short time interval after the initial time t_0). So in this case we are not able to study the validity of the approximations leading to the Langevin equation.

Thus we are unable to find any conditions that would validate Senitzky's approximations for a general potential $V(Q)$.

V. Generalized Langevin equations

Another route to a Langevin equation is via a generalized Langevin equation, constructed with the aid of projection operators, followed by the assumption that Q and P are slow variables (see, for example, [8–11,21]).

A more recent and powerful approach, equivalent to the original formulation of Mori [10] and Zwanzig [9,11], is the recurrence relation method from Lee [22,23]. For our purposes, there seems to be no advantage in working with this formalism.

A. Projection operators

In the dynamics defined in (2.1) and (2.2), we will assume that Q and P are slow (or "relevant") and q_i and p_i are "fast" variables. We need a projection operation, projecting onto the slow subspace. This entails a scalar product between operators, which we will choose to define as (for Hermitian operators A and B)

$$(A,B)_0 = (1/2)\langle (AB + BA)\rangle_0 \equiv (1/2)\mathrm{tr}\{(AB + BA)\rho_0\}. \tag{5.1.1}$$

This is symmetric, which is convenient. Some authors [8] use the more complicated Mori product. For simplicity, we do not take this course.

We have defined (5.1.1) using ρ_0, defined in (2.6). A disadvantage of (5.1.1) is that

$$(A,[H,B])_0 \neq -([H,A],B)_0. \tag{5.1.2}$$

Another possibility, which does not have this disadvantage, is to use the equilibrium distribution ρ. We will adopt this second choice in Sec. V C and then drop the suffixes 0 in (5.1.1)

From now on, for simplicity, we will set $t_0 = 0$.

Given (5.1.1), the projection operation onto the slow subspace is defined to be, for any operator X,

$$\mathcal{P}_0 X = \frac{(X,Q(0))_0}{(Q(0),Q(0))_0} Q(0) + \frac{(X,P(0))_0}{(P(0),P(0))_0} P(0), \tag{5.1.3}$$

and the complementary projection is $(1 - \mathcal{P}_0)$. It seems to be normal to define $\mathcal{P}_0$ in terms of Q,P at the initial time, and we have emphasized this in (5.1.3). In general, a different

choice of time would define a different projector. Note that $(Q(0),P(0))=0$ because of invariance under time reversal.

Obviously,

$$\mathcal{P}_0 Q^2(0) \neq Q(0), \tag{5.1.4}$$

and for this reason the method may not be appropriate except in the linear case (2.3) (see Sec. 8.2 of [11]). Also

$$\mathcal{P}_0 Q(t) \neq Q(t) \quad (t \neq 0). \tag{5.1.5}$$

For this reason, the projection method may be more appropriate in the Schrödinger picture, as in the derivation of the master equation. But, for the linear case, we do have

$$\mathcal{P}_0 Q_0(t) = Q_0(t), \tag{5.1.6}$$

and

$$\begin{aligned} \mathcal{P}_0 g(q_{0i}(t),p_{0i}(t)) &= 0, \\ \mathcal{P}_0\{Q_0(t)g(q_{0i}(t),p_{0i}(t))\} &= Q_0(t)\langle g(q_{0i}(t),p_{0i}(t))\rangle_0, \end{aligned} \tag{5.1.7}$$

etc., where g is any function. These equations would not be true if we had defined $\mathcal{P}$ in terms of ρ rather than $\mathcal{P}_0$ in terms of ρ_0.

B. Generalized Langevin equation

We need also to define the Liouville operator $\mathcal{L}$, acting on an operator X, by

$$\mathcal{L}X = i[H,X]. \tag{5.2.1}$$

From the Heisenberg equations of motion, the generalized Langevin equation is deduced (see, for example, [11]):

$$M\dot{Q}(t) = P(t), \tag{5.2.2}$$

$$\dot{P}(t) + M\Omega^2 Q(t) - \alpha\Lambda_{KQ}Q(t) - \alpha\Lambda_{KP}P(t) + \int_0^t dt'\{J_Q(t-t')Q(t') + J_P(t-t')P(t')\} = F(t), \tag{5.2.3}$$

where

$$F(t) = \exp\{t(1-\mathcal{P}_0)\mathcal{L}\}(1-\mathcal{P}_0)\mathcal{L}P(0), \tag{5.2.4}$$

with the property that

$$\mathcal{P}_0 F(t) = 0, \tag{5.2.5}$$

$$\begin{aligned} \Lambda_{KQ} &\equiv (K(0),Q(0))_0/(Q(0),Q(0))_0, \\ \Lambda_{KP} &\equiv (K(0),P(0))_0/(P(0),P(0))_0, \end{aligned} \tag{5.2.6}$$

and

$$\begin{aligned} J_Q(t) &= -(\mathcal{L}F(t),Q(0))_0/(Q(0),Q(0))_0, \\ J_P(t) &= -(\mathcal{L}F(t),P(0))_0/(P(0),P(0))_0. \end{aligned} \tag{5.2.7}$$

The quantities in (5.2.6) are, in fact, zero as we are using ρ_0 in this section, but the corresponding quantities in Sec. V C (using ρ) are not both zero.

One should note that (5.2.3) is an exact consequence of the Heisenberg equations of motion, and yet it contains a reference to the choice of ρ_0 in (5.1.1). Any apparent dependence on ρ_0 must cancel between the terms in (5.2.3). This, of course, may no longer be true if any approximations are made to (5.2.3).

In (5.2.3), it is usual to think of F as being some generalized noise and the J term as representing some (in general, non-Markovian) friction. For this interpretation, we would hope that

$$\langle F(t)\rangle_0 = 0. \tag{5.2.8}$$

We cannot prove this in general or even that $\langle F(t)\rangle_0$ is time independent. (But in this respect, see Sec. 8.3 of [11].)

It may shed some light on (5.2.3) to expand F and J through second order in α. Let

$$F(t) = \alpha F_1(t) + \alpha^2 F_2(t) + \cdots. \tag{5.2.9}$$

In (5.2.4),

$$\begin{aligned} (1-\mathcal{P}_0)\mathcal{L}P(0) &= (1-\mathcal{P}_0)\{-M\Omega^2 Q(0) + \alpha K(0)\} \\ &= (1-\mathcal{P}_0)K_0(0) + O(\alpha^2) \\ &= K_0(0) + O(\alpha^2), \end{aligned} \tag{5.2.10}$$

and so, from (5.2.4) and (5.2.7), to first order

$$F_1(t) = \exp\{t(1-\mathcal{P}_0)\mathcal{L}\}K_0(0). \tag{5.2.11}$$

Since we are working to first order in α here, we can neglect H' in $\mathcal{L}$ and get

$$(1-\mathcal{P}_0)\mathcal{L}K_0(0) \simeq (1-\mathcal{P}_0)\dot{K}_0(0) = \dot{K}_0(0) \tag{5.2.12}$$

[using (5.1.7)] and similarly for higher derivatives. Therefore

$$F_1(t) = \exp(t\mathcal{L})K_0(0) + O(\alpha^2) = K_0(t) + O(\alpha^2). \tag{5.2.13}$$

Inserting (5.2.13) into (5.2.7), we find a contribution [using (2.2)]

$$\begin{aligned} J_Q(t) &\simeq -(i/\hbar)\alpha([H',K_0(t)],Q)_0/(Q,Q)_0 \\ &= -(i/\hbar)\alpha^2\langle[K_0(t),K_0(0)]\rangle_0, \\ J_P(t) &\simeq 0, \end{aligned} \tag{5.2.14}$$

which, working through second order, is all we need.

We can now infer F_2 in (5.2.9). The generalized Langevin equation (5.2.3) is exact, and our expansion through second order in α must be exact to that order. But the Langevin equation (3.1) with (3.6) is also exact through second order (because the terms neglected in going from (3.1.3) to (3.1.4) were higher than the second). So (5.2.3) must be the same as (3.6) when (5.2.13) and (5.2.14) are inserted. This requires that

$$F_2(t) = (i/\hbar)\int_0^t dt'\{[K_0(t),K_0(t')] - \langle[K_0(t),K_0(t')]\rangle_0\}Q_0(t'). \tag{5.2.15}$$

We may check that this satisfies (5.2.5).

Thus we see that the "noise" term (5.2.15) corrects the approximate friction term (5.2.14) so as to give the correct (through order α^2) friction term in (3.6). The interpretation of F as noise may be open to question.

C. The slow variable approximation

It has been proposed to derive an ordinary Langevin equation from the generalized one (5.2.3) as an approximation

assuming that, in our example, Q and P are slow variables. We will express this assumption in the form

$$\dot{Q} = O(\Omega)Q, \quad \dot{P} = O(\Omega)P, \tag{5.3.1}$$

where Ω is small. Presumably, this means that $\Omega \ll \bar{\omega}$, where $\bar{\omega}$ is some sort of typical value of ω_i in (2.2).

We will follow the argument as presented in Sec. 8.6 of [11]. First, we must depart from the choice ρ_0, which we have made up to now, and use the equilibrium distribution ρ as in [11]. Then, since $[H,\rho] = 0$,

$$(X,\mathcal{L}Y) = -(\mathcal{L}X,Y). \tag{5.3.2}$$

This allows (5.2.7) to be written in the form

$$\begin{aligned} J_P(t) &= (I(t)F(0),F(0))/(P(0),P(0)), \\ J_Q(t) &= (1/M)(I(t)F(0),(1-\mathcal{P})P)/(Q(0),Q(0)) = 0, \end{aligned} \tag{5.3.3}$$

where

$$I(t) = \exp\{t(1-\mathcal{P})\mathcal{L}\} \tag{5.3.4}$$

and

$$\begin{aligned} F(0) &= (1-\mathcal{P})\mathcal{L}P(0) = (1-\mathcal{P})[-\Omega^2 Q(0) + \alpha K(0)] \\ &= \alpha(1-\mathcal{P})K(0) = \alpha K(0) - \alpha^2(c_{KQ}/c_{QQ})Q(0), \end{aligned} \tag{5.3.5}$$

where we define the functions of temperature

$$c_{QQ} = (Q(0),Q(0)), \quad \alpha c_{KQ} = (K(0),Q(0)). \tag{5.3.6}$$

There is now (using ρ) a nonzero contribution from (5.2.6),

$$\Lambda_{KQ} = \alpha c_{KQ}/c_{QQ}, \quad \Lambda_{KP} = 0, \tag{5.3.7}$$

the latter being a consequence of time-reversal invariance (and the symmetry of the scalar product).

Note that here, because we have chosen the equilibrium distribution ρ and therefore can use (5.3.2), $J_Q = 0$ and $J_P \neq 0$, whereas in the approximation used in (5.2.13) (having chosen ρ_0) it was the other way around.

For any X [using (5.3.2)],

$$\mathcal{P}\mathcal{L}X = -\frac{(X,\mathcal{L}Q(0))}{(Q(0),Q(0))}Q(0) - \frac{(X,\mathcal{L}P(0))}{(P(0),P(0))}P(0), \tag{5.3.8}$$

and if (5.3.1) is equivalent to

$$\mathcal{L}Q = O(\Omega)Q, \quad \mathcal{L}P = O(\Omega)P, \tag{5.3.9}$$

it follows that (5.3.8) is $O(\Omega)$; then it is argued that we may approximate (5.3.4) by

$$I(t) \simeq \exp\{t\mathcal{L}\}. \tag{5.3.10}$$

In this approximation,

$$F(t) \simeq \exp(t\mathcal{L})F(0) = \alpha K(t) - \alpha^2(c_{KQ}/c_{QQ})Q(t) \tag{5.3.11}$$

and

$$\begin{aligned} c_{PP}J_P(t) \simeq{}& \alpha^2(K(t),K(0)) - \alpha^3(c_{KQ}/c_{QQ})\{(K(t),Q(0)) \\ &+ (Q(t),K(0))\} + \alpha^4(c_{KQ}/c_{QQ})^2(Q(t),Q(0)). \end{aligned} \tag{5.3.12}$$

The last term in (5.3.11) [but not in (5.3.12)] is canceled by (5.3.7).

The approximations (5.3.11) and (5.3.12) are to be inserted into (5.2.2) to get the hoped-for Langevin equation. We will now make some remarks about this slow approximation.

(a) Because of the dependence on $Q(t)$ on the right-hand sides of (5.3.11) and (5.3.12), the resulting equation has a different form from an ordinary Langevin equation.

(b) If we retain the term $\alpha K(t)$ on the right of (5.3.11) but discard everything else in (5.3.11) and (5.3.12), the resulting equation (5.2.3) would reduce to just the original Heisenberg equation of motion (3.1), not a Langevin equation at all.

(c) Since $\mathcal{L}P = -\Omega^2 Q + \alpha K$, the assumption (5.3.9) seems to require that α as well as Ω be small.

(d) We can test the slow approximation in the special case when K is a linear function,

$$K = \sum c_i q_i, \tag{5.3.13}$$

when the ordinary Langevin equation is well known and is, in fact, exact. This equation may be written in the form (5.2.3) with

$$\begin{aligned} J_Q &= 0, \quad J_P(t) = \alpha^2(1/M)\sum(c_i/m_i\omega_i)^2\cos(\omega_i t) \\ &= \alpha^2(MT)^{-1}\mathrm{tr}\{K_0(t)K_0(0)\rho_E\}, \\ F(t) &= \alpha K_0(t) - \alpha^2 Q(0)\sum(c_i/m_i\omega_i)^2\cos(\omega_i t), \end{aligned} \tag{5.3.14}$$

where we have used the notation of (2.6).

Let us see if we can get (5.3.14) from (5.3.11) and (5.3.12) in any approximation. The nearest we can get is to write (5.3.11) and (5.3.12) as

$$\begin{aligned} F(t) &= \alpha K_0(T) + O(\alpha^2), \\ J_P(t) &= \alpha^2(1/MT)\langle K_0(t)K_0(0)\rangle_0 + O(\alpha^3). \end{aligned} \tag{5.3.15}$$

This does reproduce (5.3.14) *except* for the $Q(0)$ term at the end of (5.3.14), which has to be considered as being of the neglected orders.

This example confirms our expectation in point (c) that α as well as Ω has to be regarded as small. But even then the slow approximation seems to be incapable of reproducing the whole of the correct result (5.3.14) including the $Q(0)$ term.

It is worth remarking that the Langevin equation for linear model (5.3.13) can alternatively be written in the form (5.2.3) with $J_P = 0$ and $J_Q \neq 0$, and then there is no $Q(0)$ term, but the slow approximation to the generalized Langevin equation forces the alternative form with $J_Q = 0$.

Finally, we note that if we are prepared to neglect higher powers of α on the right-hand sides, we can immediately make Senitzky's approximation (3.5), for example, without going via the generalized Langevin equation.

We conclude that the slow approximation to the generalized Langevin equation is not straightforward.

VI. COMPARISON WITH RELATED WORK

Reference [14] has a similar aim to ours: to derive a Langevin equation when the quantity K in (2.2) is nonlinear. Also, perturbation theory in α is employed in [14] and also in this paper. But the two arguments are not the same. In [14]

weak coupling is assumed, and q_i (but not Q) are expanded to first order in α in order to obtain the "fluctuation" to first order and the "dissipation" to second order. The steps in the argument in [14] are easily seen in Senitzky's [1] treatment. The weak-coupling assumption justifies Senitzky's approximation of (3.2) by (3.5). Then the difference neglected in (3.7),

$$C(t.t') - \bar{C}(t,t'),$$

is claimed to be a fluctuation term and therefore (being of order α^2) is neglected. Thus the method of [14] is restricted to small α (but makes no restrictions on the frequency).

In contrast, in this paper, we use perturbation theory only as a means of identifying the infinite set of graphs that dominates for frequency ω close to the natural frequency Ω. We do not assume that the coupling strength α is weak.

VII. CONCLUSIONS

Although the Langevin equation (for a simple system interacting with a large environment) is often used, not very much attention has been given to judging its validity. We have critically examined two possible methods for doing this, with particular attention given to the quantum case.

The first is a direct approach from Senitzky [1]. He made approximations whose validity is not obvious in general. We identify one region in which the method may be justified, and that is where the measured frequency is close to the natural frequency of the free system. This condition cannot be formulated when the system is nonlinear, although there are important examples where this is the case.

The second approach (which also requires the system to be a linear one) seems to be completely different (see, for example, [11]). It proceeds by using a projection operator to a generalized Langevin equation, which, like the recurrence relation formalism [22], is an exact consequence of the Heisenberg equations of motion. In Sec. V B, we argued that the identification of the noise and dissipation terms is ambiguous in the generalized equation.

Then we studied the assumption that the system variables are slow compared to the environmental ones. This leads to an equation that looks like an ordinary Langevin equation. We examine the steps going into this derivation, particularly by comparison with the model in which all the equations of motion are linear, for which the Langevin equation is easily established and is exact. We argue that the slow approximation necessarily entails neglecting also terms of higher order in the coupling strength α as well as in the frequency ratio. But even then the correct Langevin equation requires a selective choice of orders of α.

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