Generalized Langevin equation and recurrence relations

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The generalized Langevin equation (GLE) is a reformulation of the Heisenberg equation of motion, and hence, an exact equation. It is the basis of the memory function approach, a very widely used method for studying dynamics of classical and quantum fluids. The GLE was first derived by Mori in a very formal way. A much simpler and more physically motivated derivation was given by us some years later. In this work we provide perhaps the simplest possible derivation of the GLE. The simplicity of the derivation helps to bring out the subtleties present in this important dynamical relationship.

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I. INTRODUCTION

The generalized Langevin equation (GLE) has played an important role in contemporary studies of the time and frequency dependent behavior in many particle systems [1]. It is the basis of the very widely applied memory function approach to dynamics. The GLE was first derived by Mori [2] and an equivalent version by Zwanzig [3]. Although highly formal—it is in fact a *tour de force* in formal analysis—Mori's derivation is one that is still almost solely relied upon [4].

Several years later we gave a much simpler, more physically motivated derivation of the GLE [5]. In this paper we present yet another derivation but one that is simple enough to be regarded as almost elementary. It uses rather little of the recurrence relations formalism. The simplicity, we believe, brings out the underlying process of converting the Heisenberg equation into the GLE.

II. HEISENBERG EQUATION AND RECURRENCE RELATIONS SOLUTION

Let A be a dynamical variable at time $t=0$. Then $A(t)$, the time evolution of A, may be obtained by solving the Heisenberg equation of motion,

$$\dot{A}(t)=i[H,A(t)]\equiv i\{HA(t)-A(t)H\}, \tag{1}$$

where H the Hamiltonian is assumed to be *Hermitian*. We are concerned with $t\geqslant 0$ only. Hence, it is convenient to take $A(t)=0$ if $t<0$ as in the Laplace transform theory.

We regard $A(t)$ as a vector in a d-dimensional *realized* space S. Then one may give a formal solution of Eq. (1) in the form of an orthogonal expansion as shown below:

$$A(t)=\sum_{k=0}^{d-1} a_k(t) f_k . \tag{2}$$

Here the f_k's are a complete set of basis vectors that span the space S. That is,

$$(f_k, f_{k'})=0 \quad \text{if } k'\neq k, \tag{3}$$

where (,) denotes an inner product to be decided later. The coefficients a_k are time dependent functions representing the projection of $A(t)$ onto the basis vectors at time t. Hence, $a_k(t)=0$ also if $t<0$.

If we choose $f_0=A(t=0)\equiv A$, exercising one degree of freedom always available in an orthogonalization, there result the following boundary conditions on a_k:

$$a_k(t=0)=\begin{cases}1 & \text{if } k=0\\ 0 & \text{if } k=1,2,3,\ldots .\end{cases} \tag{4}$$

Given Eqs. (3) and (4), the recurrence relations method [6(a)] rests on the following fact. If the inner product is taken to be the Kubo scalar product [6(b)], both f_k's and a_k's satisfy certain unique recurrence relations. They are three-term recurrence relations except the basal ones which have two terms only. For deriving the GLE we mostly need the two-term ones:

$$f_1=\dot{f}_0 . \tag{5}$$

$$\Delta_1 a_1(t)=-\dot{a}_0(t), \tag{6}$$

where $\Delta_1\equiv(f_1,f_1)/(f_0,f_0)>0$, a static quantity, relating, e.g., the f sum rule to the susceptibility. If $\Delta_1=0$, $A(t)=A$, i.e., $d=1$. We assume that $(A,A)<\infty$.

The recurrence relations method is now well established. It has been applied to many problems, contributing to recent advances in nonequilibrium statistical mechanics. For some representative examples, see [7].

III. LANGEVIN EQUATION AND RECURRENCE RELATIONS FORMALISM

If Eq. (2) is differentiated with respect to time,

$$\dot{A}(t)=\dot{a}_0(t)f_0+\sum_{k=1}\dot{a}_k(t)f_k . \tag{7}$$

For Hermitian systems, the length or magnitude of this vector $A(t)$ remains constant for $t\geqslant 0$, i.e., $(A(t),A(t))=(A,A)$. Hence $A(t)$ can change only its direction as the time evolves. That is to say, $\dot{A}(t)$ has a component that remains orthogonal to $f_0=A(t=0)$ always, which may be called a *normal* component of $\dot{A}(t)$. At $t=0$, there is only the normal component. But as time evolves, there appears another component, not orthogonal to f_0, which may thus be called an *induced* component of $\dot{A}(t)$.

To show this decomposition of $\dot{A}(t)$, we introduce a second set of coefficients $b_k(t)$ for $t\geqslant 0$ [$b_k(t)=0$ if $t<0$ also], to be justified later. They are defined in a convolution relation to $a_k(t)$ as shown below. For $k\geqslant 1$,

$$a_k(t)=\int_0^t b_k(t')a_0(t-t')dt'. \tag{8}$$

If Eq. (8) is differentiated,

$$\dot{a}_k(t)=b_k(t)+\int_0^t b_k(t')\dot{a}_0(t-t')dt'. \tag{9}$$

We replace the $\dot{a}_0$ term in the above integral by Eq. (6) and rearrange it using Eq. (8) as

$$\int_0^t b_k(t')a_1(t-t')dt'=\int_0^t a_k(t')b_1(t-t')dt' \tag{10}$$

(see Appendix A). In the first and second terms on the right-hand side (rhs) of Eq. (7), we substitute Eqs. (6) and (8) with $k=1$, and Eqs. (9), (10), and (2), respectively, and finally obtain

$$\dot{A}(t)=\sum_{k=1} b_k(t)f_k-\Delta_1\int_0^t b_1(t')A(t-t')dt'. \tag{11}$$

Observe that the first term on the rhs of Eq. (11) is the normal component, orthogonal to $f_0=A$ for $t\geqslant 0$. The second term is the induced component since it vanishes when $t=0$. It is not orthogonal to f_0 for $t>0$.

IV. RECURRENCE RELATIONS

It now remains to show the boundary conditions $b_k(t=0)$. We can obtain them from Eq. (9) by setting $t=0$, i.e.,

$$b_k(t=0)=\dot{a}_k(t=0), \quad k\geqslant 1, \tag{12}$$

and by using the recurrence relation for $a_k(t)$, usually known as RR2 [6],

$$\Delta_{k+1}a_{k+1}(t)=-\dot{a}_k(t)+a_{k-1}(t), \quad k\geqslant 0, \tag{13}$$

where $a_{-1}\equiv 0$ and $\Delta_k=(f_k,f_k)/(f_{k-1},f_{k-1})$. Note that when $k=0$ in Eq. (13), we recover Eq. (6), the basal relation. Setting $t=0$ in Eq. (13) and using Eq. (4), we establish at once that

$$b_k(t=0)=\begin{cases}1 & \text{if } k=1\\ 0 & \text{if } k=2,3,\ldots\ .\end{cases} \tag{14}$$

Hence, if we define

$$\sum_{k=1}^{d-1} b_k(t)f_k\equiv B(t), \tag{15}$$

$B(t)$ is the time evolution of $B=f_1=\dot{A}(t=0)$ [see Eq. (5)], just as $A(t)$ is the time evolution of $A=f_0$. But $B(t)$ is a vector in a subspace, say S_1, spanned by $f_1,f_2,\ldots$, i.e., $(B(t),A)=0$ for $t\geqslant 0$. One can further show (see Appendix B) that $b_k(t)$ have a recurrence relation of exactly the same form (13) but operative in the subspace S_1.

Using Eq. (15), we put Eq. (11) in the final form,

$$\dot{A}(t)=B(t)-\int_0^t \varphi(t')A(t-t')dt', \tag{16}$$

where $\varphi(t)\equiv\Delta_1 b_1(t)$, sometimes known as the memory function [1]. We can show that if Eq. (16) is integrated in the interval $(0,t)$, the rhs yields $A(t)-A(0)$ [8]. Equation (16) is known as the GLE. It really is a reformulation of the Heisenberg equation (1). Hence the two are exactly equivalent.

V. CONCLUDING REMARKS

This work differs from our earlier derivation [5] in that the coefficients $\{b_k\}$ are introduced in the beginning. The derivation of the GLE is thereby made very simple. It is accomplished without the use of continued fractions. See Appendix C, where different approaches are briefly compared. The simplicity of our present approach also helps to reveal the intricacies in the hierarchy of subspaces in which the GLE is structured. As discussed below, we find that the GLE represents a spatial relationship.

Although $A(t)$ and $B(t)$ are both vectors of constant magnitude or length, they are not in the same space. We can shed some light on the relationship between the two vectors by taking an inner product of Eq. (16) with A,

$$\dot{a}_0(t)=-\Delta_1\int_0^t b_1(t')a_0(t-t')dt'. \tag{17}$$

Observe that the above is also obtained from Eq. (8) as a special case if $k=1$, therein remembering Eq. (6). The GLE thus expresses the relationship between a_0 and b_1, and hence ultimately between the two spaces S and S_1.

As b_k were defined with respect to a_k [see Eq. (8)], we can introduce another set of coefficients, say, c_k, $k\geqslant 2$, now with respect to b_k. Their space S_2 is a subspace of S_1. The relationship between these two spaces S_1 and S_2 is yet another GLE.

The above interspatial relationships are different from intraspatial ones such as between a_0 and a_1, both of the space S. This particular relationship, given by Eq. (6), is known as the (first) fluctuation dissipation formula. A second fluctuation dissipation formula can be found from the relationship between b_1 and b_2, which is about the subspace S_1. Higher ones can be found similarly, e.g., between c_2 and c_3 of the subspace S_3. Remarkably, the existence of these fluctuation dissipation formulas was already anticipated by Kubo [9].

Although Eq. (16) is purely formal, being an operator equation, the structure of the GLE makes it rather natural for studying certain physical problems. For example, if A is the charge density, $\dot{A}(t)$ is proportional to the longitudinal current by the continuity equation. According to Eq. (16), the total current is composed of the normal and induced parts. They correspond to the intrinsic and diffusive currents [10]. For another example, let A now be the number density of neutral particles. If the long time behavior of $\dot{A}(t)$ is sought, as in certain physical laws, e.g., Fick's law, then the induced part of Eq. (16) can be put readily into an asymptotic form [11]. Finally, the scalar form of the GLE (17) is a widely used dynamical equation. Many approximate theories of classical and quantum fluids have been developed based on it, known collectively as the memory function approach [4].

APPENDIX A: PROOF OF EQUATION (10), AN IDENTITY

We take advantage of the property that $a_0(t)$, $a_k(t)$, and $b_k(t)$, $k \geqslant 1$, are defined to be zero if $t<0$. Hence, the lhs of Eq. (10) may be immediately written as

$$\int_0^\infty b_k(t_1) a_1(t-t_1) dt_1 = \int_0^\infty b_k(t_1) \int_0^{t-t_1} b_1(t_2) \times a_0(t-t_1-t_2) dt_2 dt_1, \quad \text{(A1)}$$

where we have used Eq. (8) on the rhs. Now the second upper limit may also be taken to ∞, giving

$$\int_0^\infty \int_0^\infty b_1(t_2) b_k(t_1) a_0(t-t_2-t_1) dt_1 dt_2 = \int_0^\infty b_1(t_2) \int_0^{t-t_2} b_k(t_1) a_0(t-t_2-t_1) dt_1 dt_2, \quad \text{(A2)}$$

where on the lhs we have exchanged the order of integration, allowed under both limits, and on the rhs we have reduced the upper limit on t_1, allowed since $a_0(t)=0$ if $t<0$. Finally, using Eq. (8),

$$\int_0^\infty b_1(t_2) a_k(t-t_2) dt_2 = \int_0^t b_1(t_2) a_k(t-t_2) dt_2. \quad \text{(A3)}$$

QED.

One can also obtain the same result by use of the convolution theorem of the Laplace transform theory. Let $\tilde{a}_0(z)$, $\tilde{a}_k(z)$, and $\tilde{b}_k(z)$ denote the Laplace transforms of $a_0(t)$, $a_k(t)$, and $b_k(t)$, respectively. If we Laplace transform the lhs of Eq. (10), by the convolution theorem we obtain

$$\tilde{b}_k(z) \tilde{a}_1(z) = \tilde{a}_k(z) \tilde{b}_1(z), \quad \text{(A4)}$$

where on the rhs we have used

$$\tilde{a}_k(z) = \tilde{b}_k(z) \tilde{a}_0(z), \quad \text{(A5)}$$

obtained by taking the Laplace transform of the defining Eq. (8). The inverse transform of Eq. (A4) gives the desired result Eq. (A3).

APPENDIX B: RECURRENCE RELATION FOR $\{b_k\}$

An elementary way to derive the recurrence relation for $\{b_k\}$ is to apply Eq. (8) in Eq. (13). We may write Eq. (8) in an equivalent form. For $k \geqslant 1$,

$$a_k(t) = \int_0^t b_k(t-t') a_0(t') dt' \equiv \{b_k \times a_0\}. \quad \text{(B1)}$$

Then

$$\dot{a}_k(t) = b_k(0) a_0(t) + \{\dot{b}_k \times a_0\}. \quad \text{(B2)}$$

Given Eq. (14), there are two possibilities: $k \geqslant 2$ and $k=1$.

For $k \geqslant 2$, we may substitute Eqs. (B1) and (B2) in Eq. (13) and obtain

$$\Delta_{k+1} \{b_{k+1} \times a_0\} = -\{\dot{b}_k \times a_0\} + \{b_{k-1} \times a_0\}. \quad \text{(B3)}$$

Thus we obtain

$$\Delta_{k+1} b_{k+1}(t) = -\dot{b}_k(t) + b_{k-1}(t), \quad k \geqslant 2. \quad \text{(B4)}$$

For $k=1$, with $b_0 \equiv 0$,

$$\Delta_2 \{b_2 \times a_0\} = -\{\dot{b}_1 \times a_0\}. \quad \text{(B5)}$$

Hence,

$$\Delta_2 b_2(t) = -\dot{b}_1(t). \quad \text{(B6)}$$

We can combine Eqs. (B4) and (B6) to obtain the final form:

$$\Delta_{k+1} b_{k+1}(t) = -\dot{b}_k(t) + b_{k-1}(t), \quad k \geqslant 1, \quad \text{(B7)}$$

with $b_0 \equiv 0$. The above is the recurrence relation for $\{b_k(t)\}$, operative in the subspace S_1, spanned by $f_1, f_2, \ldots, f_{d-1}$.

APPENDIX C: COMPARISON OF DIFFERENT APPROACHES: AN OVERVIEW

In this Appendix, the main ideas behind Mori's and our approaches are described. This will show the progress that has led to our finding the latest derivation, which we believe is thus far the simplest and clearest. There are two essential aspects to the existing work [2,5].

The derivation of Mori is based on the Mori-Zwanzig (MZ) projection operator formalism. This is an orthogonalization process of abstract Hilbert space. It seems not to have been recognized that the MZ formalism is a reinvention of the Gram-Schmidt process.

The MZ or Gram-Schmidt process is general, but the generality also diffuses the underlying physics (e.g., subspaces and dimensionality). The resultant analysis necessarily is heavily formal. It is no surprise that the GLE on occasion has been incorrectly approximated and even improperly applied.

This approach is made all the more abstruse by the presence of continued fractions. As given, these continued fractions are not tractable, nor is it clear why they should be there. Since the GLE cannot be solved without solving the continued fractions, the GLE appeared to some to be an empty reformulation.

The recurrence relations formalism [5] removes both difficulties, the first by taking on realized spaces. Realized spaces have unique orthogonalization processes. They are generally much simpler than the Gram-Schmidt, as has been demonstrated [6(b)]. One can also trace to this realized space the origin of the continued fractions that appear in the time evolution problem.

Our earlier work [5] is in effect a reanalysis of the Heisenberg equation following Mori, modified by a new orthogonalization process. The analysis is thus greatly simplified. Also the continued fractions are made tractable—and meaningful—removing the second difficulty.

The present work recognizes the essentialness of realized *subspaces* from the outset. This idea allows us to transform the Heisenberg equation into the GLE directly. Continued fractions are not needed. It suffices to have only an elementary knowledge of the recurrence relations method.

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