Heisenberg, Langevin, and current equations via the recurrence relations approach

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Some years ago the Heisenberg equation of motion was formally solved by the recurrence relations approach. It is shown here that the Langevin equation represents a structural property of the recurrence relations. The Langevin equation is useful for studying the time evolution of the current. The resulting current-current correlation function is compared with Luttinger's phenomenological theory. Geometric interpretations are made for the conductivity and the dielectric function.

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I. INTRODUCTION

More than 30 years ago Mori showed that the Heisenberg equation of motion can be reformulated as an expression much resembling the classical Langevin equation for Brownian motion [1]. This work is a tour de force in formal analysis. It appeared during the time when the physics of Brownian motion had played a major role in formulating nonequilibrium statistical mechanics [2]. Thus Mori's formulation was seen as providing a basis for the phenomenological theory of Brownian motion. The new expression itself, not inappropriately, was named the generalized Langevin equation (GLE), as it is known to this day. Perhaps more significant is the influence that Brownian motion theory has exerted on Mori's GLE. The Brownian terminology, e.g., random force and memory, has gained a new foothold [3–6].

Although appealing, this Brownian analogy did not, however, help solve the GLE. It did not even lend any significant insight into the nature of time evolution implied by the equation of motion. Mori and others have introduced approximate methods of solution [1,7], but since they were based on unsupported physical arguments the validity of these methods was never clear [8]. What was evidently needed was an exact or even almost exact solution of the GLE for a nontrivial model. To our knowledge no one was able to produce such a solution.

Nearly 20 years later we proposed a method for solving the Heisenberg equation directly [9]. Since the GLE is a reformulation of the Hesienberg equation, this method should in fact also solve the GLE. The GLE has a cumbersome structure, which obscures the geometric simplicity that is inherent in the Heisenberg picture. Our method takes advantage of this simplicity.

What we have found is that a certain set of recurrence relations (RRs) underly the Heisenberg equation. Unraveling these RRs is tantamount to obtaining the time evolution according to the equation of motion. A particular time evolution is delineated by a unique trajectory in Hilbert space. These trajectories are confined to the surfaces of realized spaces that are determined by properties of the RRs. The trajectories are generally irregular. That is, the surfaces on which they lie are not smoothly shaped. Regular trajectories or smooth surfaces would indicate exact solvability of the Heisenberg equation. If a rough surface is smoothed, one is looking at an approximate time evolution solution.

Some essential physical properties such as irreversibility, slow decay, even dynamic critical behavior are embedded in the geometric properties of the realized Hilbert space [10–12]. This understanding has emerged from several exact and asymptotically exact solutions by this method, now known as the recurrence relations method.

At an earlier stage we derived the GLE starting from the Heisenberg equation using the recurrence relations method [13]. It is much simpler than Mori's original treatment. But viewed from today's perspective the derivation still suffers from the unwieldy weight of the GLE. In the RR analysis of time evolution mentioned above there are no references to any Brownian concepts. They are thus not necessary for solving the Heisenberg equation. In the same vein we shall show below that the GLE itself is simply a structural property of the RRs, useful for studying the current, for example.

As an illustration we will show how the conductivity formula due to Kubo follows quite simply. Our result may be compared with the phenomenological treatment of Luttinger [14,15]. We will also show that such physical quantities as the dielectric function may be given a geometric interpretation.

II. TIME EVOLUTION AND ORTHOGONAL EXPANSIONS

In this section we will give a brief review of the recurrence relations approach to solving the Heisenberg equation of motion. We will state several of the basic results without proof. We will also present an overview of this approach.

Consider a dynamical variable of interest, say, $A \equiv A(t=0)$. The time evolution of A is given by $A(t) = \exp(iHt)A\exp(-iHt)$, where H is the Hamiltonian ($\hbar=1$), and $t \geqslant 0$. We shall assume that H is Hermitian. We can construct a Hilbert space $\mathbf{S}$ for $A(t)$ and study the time evolution geometrically.

Let A be a vector in this space $\mathbf{S}$ pointing to some arbitrary initial direction. The time evolution of A may then be viewed as a continuous change in the direction of the vector, the length of this vector being independent of the time, i.e., $\|A(t)\| = \|A\|$, since H is assumed Hermitian, where $\|A\|$ means the norm of A. Also A is such that $0 < \|A\| < \infty$.

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If the tail of the vector is fixed, say, at the origin of **S**, the head of the vector begins to delineate a trajectory as the time evolves. This trajectory evidently depends on the dimensions d of the space and hence on A and H. Whatever d, whether finite or infinite, the trajectory defines the surface of this space and the shape of the surface characterizes the nature of the time evolution in our system.

At a time $t \geqslant 0$ we can evidently express $A(t)$ as an orthogonal expansion,

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

Here f_k are a complete set of basis vectors which span the d-dimensional space **S** of $A(t)$. These basis vectors are assumed orthogonal, that is, for $0 \leqslant k,\ k' \leqslant d-1$,

$$(f_k, f_{k'}) = 0 \quad \text{if } k' \neq k, \tag{2}$$

where the inner product is such as to realize the space **S** according to the physical requirements. The conjugate quantities $a_k(t)$ denote the magnitudes of the projection of the vector onto the basis vectors at a time t; hence they are functions of t and d.

In constructing f_k for **S** we shall exercise one degree of freedom allowed and choose $f_0 = A$. Then an important boundary condition results from Eq. (1):

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

If the inner product is taken to mean the Kubo scalar product [16], the basis vectors f_k that span the space **S** are found to satisfy a three-term recurrence relation known as the RR1 given below [16]. For $k \geqslant 0$ and $f_{-1} \equiv 0$,

$$f_{k+1} = \dot{f}_k + \Delta_k f_{k-1}, \tag{4}$$

where $\Delta_k = \|f_k\| / \|f_{k-1}\|$, $k \geqslant 1$, and for any f the ''norm'' on **S** is defined as $\|f\| = (f,f)$. We shall adopt this form of a norm on **S**, instead of the conventional one, to simplify our notation.

Observe that given the initial or basal basis vector f_0, all others simply follow one by one according to the RR1. Hence we can also obtain $\|f_k\|$ one by one and put up the frames for the structure of the space.

A realized space is what makes the orthogonalization process simple and physically based. In fact, H explicitly enters into the construction of f_k, $k \geqslant 1$, and it helps to determine the required number of f_k's or d. We avoid using the Gram-Schmidt process, whose generality makes the construction process highly impractical especially if d is indefinite [16].

It should be noted that our basis vectors f_k, $k \geqslant 1$, are not normalized. This condition makes the shape of the space, and hence the trajectory, model dependent, allowing a geometric interpretation for a physical process. In addition, the same condition makes the form of the RR2 (to be introduced below) the simplest possible.

Now the trajectory of our interest is one that is governed by the Heisenberg equation of motion,

$$\dot{A}(t) = i[H, A(t)] \equiv i\{HA(t) - A(t)H\}. \tag{5}$$

For f_k satisfying the RR1 and the trajectory constrained by Eq. (5), we find that a_k must satisfy an analogous three-term recurrence relation known as the RR2: For $k \geqslant 0$ and $a_{-1} \equiv 0$,

$$\Delta_{k+1} a_{k+1}(t) = -\dot{a}_k(t) + a_{k-1}(t). \tag{6}$$

The RR2 is realizable by Δ_k, called the *recurrants*. That is, since the recurrants are in effect the norms of the basis vectors, the RR2 reflects the geometry of the realized space for a given H. If a_0 were known, the RR2 would permit us to determine the rest also one by one. But a_0 is not known *a priori* and a_k must all be determined at once. One possible avenue is to find the congruence between a *realized* RR2 and some known three-term recurrence relation. This is an algebraic approach.

Another avenue is by the analytic theory of continued fractions. For $\mathrm{Re}\, z > 0$, let $\tilde{a}_k(z) = \mathbf{T} a_k(t)$, where **T** is the Laplace transform operator. Then, owing to Eq. (3), the RR2 splits into two terms:

$$1 = z\tilde{a}_0 + \Delta_1 \tilde{a}_1, \tag{7a}$$

$$\tilde{a}_{k-1} = z\tilde{a}_k + \Delta_{k+1}\tilde{a}_{k+1}, \quad k \geqslant 1. \tag{7b}$$

If the two are combined, we obtain the continued fraction for $\tilde{a}_0$, first obtained by Mori [1]:

$$\tilde{a}_0 = 1/z + \Delta_1/z + \Delta_2/z + \cdots. \tag{8}$$

Thus a continued fraction of this form implies the existence of a d-dimensional space defined by a set of norms or Δ_k. If this shape is sufficiently smooth, the right-hand side (rhs) of Eq. (8) may have a simple enough analytic structure to be solvable. In such a case a_0 may be determined by the inverse transform thereof and the rest of the a_k's by the RR2. This is an analytic approach.

This program has been implemented by us for several models of physical interest [17]. Many authors have discussed both the formal and physical aspects of this approach [18–27]. There now exists a large body of literature on the applications of this method [28–39] and also on applications of the results obtained by it [40–51]. Cited here are some representative examples.

III. TIME EVOLUTION IN SUBSPACE

If both sides of Eq. (7a) are divided by $\tilde{a}_0$, we have

$$1/\tilde{a}_0 = z + \Delta_1 \tilde{a}_1/\tilde{a}_0. \tag{9}$$

Let us define the ratio of the two functions appearing in Eq. (9) as

$$\tilde{a}_1/\tilde{a}_0 \equiv \tilde{b}_1. \tag{10}$$

Then comparing Eqs. (8) and (9), we immediately obtain

$$\tilde{b}_1 = 1/z + \Delta_2/z + \Delta_3/z + \cdots. \tag{11}$$

Recalling our interpretation attached to $\tilde{a}_0$ [see Eq. (8) and below], we may see $\tilde{b}_1$ as denoting the existence of a (d-l)-dimensional space, say $\mathbf{S}_1$, spanned by $f_1 f_2 \cdots f_d$. Clearly $\mathbf{S}_1$ is a subspace of $\mathbf{S} \equiv \mathbf{S}_0$ and $\tilde{b}_1$ plays the same role in $\mathbf{S}_1$ as does $\tilde{a}_0$ in $\mathbf{S}_0$. This relationship can be established as follows.

If $k=1$ in Eq. (7b) and the resulting equation is divided by $\tilde{a}_0$, we obtain with Eq. (10)

$$1 = z\tilde{b}_1 + \Delta_2 \tilde{b}_2, \tag{12}$$

where we have introduced analogously to Eq. (10)

$$\tilde{a}_2/\tilde{a}_0 = \tilde{b}_2. \tag{13}$$

Similarly we obtain

$$\tilde{b}_{k-1} = z\tilde{b}_k + \Delta_{k+1}\tilde{b}_{k+1}, \quad k \geqslant 2, \tag{14}$$

provided that

$$\tilde{a}_k/\tilde{a}_0 = \tilde{b}_k, \tag{15}$$

which can include Eqs. (10) and (13) if $k \geqslant 1$. Equations (12) and (14) together stand as the transformed RR2 in subspace $\mathbf{S}_1$ as Eqs. (7a) and (7b) are in space $\mathbf{S}_0$.

We shall now see what physical significance might be contained in the $\tilde{b}_k$ [Eq. (15)] themselves by examining $b_k(t) = \mathbf{T}^{-1}\tilde{b}_k(z)$, where $\mathbf{T}^{-1}$ is the inverse Laplace transform operator. We are assuming that the $\tilde{b}_k$'s are all finite and well behaved, so that b_k's exist. Now, as shown in Appendix A, if $z \to \infty$,

$$\tilde{a}_k(z) = z^{-k-1} + O(z^{-k-3}). \tag{16}$$

That is,

$$\tilde{b}_k(z \to \infty) = z^{-k} + O(z^{-k-2}). \tag{17}$$

Hence it follows by the inverse transform that

$$b_k(t=0) = \begin{cases} 1 & \text{if } k=1 \\ 0 & \text{if } k \geqslant 2. \end{cases} \tag{18}$$

Thus, the b_k's have boundary conditions exactly analogous to those for the a_k's, which were imposed by the choice $f_0 = A$.

Equations (18), (12), and (14) imply that for $k \geqslant 1$

$$\Delta_{k+1} b_{k+1} = -\dot{b}_k + b_{k-1}, \tag{19}$$

with $b_0 \equiv 0$. We obtain the RR2 that is operative in subspace $\mathbf{S}_1$, where the b_k's must then be the proper projection coefficients for the time evolution of, say, B. That is,

$$\sum_{k=1}^{d-1} b_k(t) f_k \equiv B(t). \tag{20}$$

But $B \equiv B(t=0) = f_1$ by Eq. (18) and $B = \dot{A}$ by RR1 given $f_0 = A$. Thus B is not arbitrary. Unlike the time evolution of $\dot{A}$, however, the time evolution of B is confined in subspace $\mathbf{S}_1$ at all times, i.e., for $t \geqslant 0$,

$$(B(t), f_0) = (B(t), A) = 0. \tag{21}$$

Recall that the initial choice $f_0 = A$ has given the boundary conditions on the a_k's and hence also on the b_k's [see Eqs. (3) and (18)]. What it all means is that the trajectory of $A(t)$ that takes place in space $\mathbf{S}_0$ may be decomposed into different components, some of which evolve in subspaces only. Indeed, this notion becomes physically relevant when we consider the current.

It is clear that there are other subspaces and we can construct them in the same manner as $\mathbf{S}_1$, e.g., $\Sigma_2^{d-1} c_k(t) f_k = C(t)$, $k \geqslant 2$. For the dynamics described by linear response theory they are not needed, however. Hence we will not discuss them here.

IV. TIME EVOLUTION OF THE CURRENT

According to the continuity equation, the current J can be related to the density fluctuations ρ at wave vector q as [15] $iq \cdot J_q(t) = -\dot{\rho}_q(t)$. Hence if $\rho_q = A$, the dynamical variable, the time evolution of $\dot{A}$ is in effect the time evolution of the current, apparently first conceived by Kubo [52]. One may thus regard the current as a structural property of the recurrence relations.

If Eq. (1) is differentiated once with respect to time,

$$\dot{A}(t) = \dot{a}(t) f_0 + \sum_{1}^{d-1} \dot{a}_k(t) f_k. \tag{22}$$

If the $\mathbf{T}$ operator is applied to Eq. (22), we obtain

$$\begin{aligned} \tilde{\dot{A}}(z) &= (z\tilde{a}_0 - 1) f_0 + z \sum \tilde{a}_k f_k \\ &= -\Delta_1 \tilde{a}_1 f_0 + (1 - \Delta_1 \tilde{a}_1) \sum \tilde{b}_k f_k, \end{aligned} \tag{23}$$

where we have applied Eq. (7a) to replace $z\tilde{a}_0$ and Eq. (15) to replace $\tilde{a}_k$. Further, with the identity $\tilde{a}_1 \tilde{b}_k = \tilde{b}_1 \tilde{a}_k$, we can write Eq. (23) as

$$\tilde{\dot{A}}(z) = \sum_1 \tilde{b}_k f_k - \tilde{\varphi}(z) \sum_0 \tilde{a}_k f_k = \tilde{B}(z) - \tilde{\varphi}(z) \tilde{A}(z), \tag{24}$$

where we have introduced $\tilde{\varphi} = \Delta_1 \tilde{b}_1$.

Finally, by applying the inverse operator $\mathbf{T}^{-1}$ to the above equation, we obtain

$$\dot{A}(t) = B(t) - \int_0^t \varphi(t') A(t-t') dt', \tag{25}$$

where $\varphi(t) = \Delta_1 b_1(t)$. Observe that $\dot{A} = B$, but $(\dot{A}(t), f_0) \neq 0$ whereas $(B(t), f_0) = 0$ as noted previously. The validity of this result may be verified by integrating Eq. (25) over the interval $(0,t)$, which should yield $A(t)-A(0)$. See Appendix D.

According to Eq. (25), the time evolution of $\dot{A}$ consists of two components, one part of the trajectory remaining entirely in subspace $\mathbf{S}_1$ and another encompassing the full space $\mathbf{S}_0$. The second part of the trajectory is one that is induced, starting at $t=0$, modulated by $\varphi(t)=\Delta_1 b_1(t)$. It represents the induced part of the current, which might be termed the diffuse current after phenomenological theories [14,52]. Thus the trajectory that is confined to the subspace at all times must represent the nondiffuse or intrinsic part of the current. Because the induced current is modulated by φ, it gives rise to a special relationship between the diffusivity and the conductivity (see the next section).

We recognize Eq. (25) as the GLE, first derived by Mori [1]. Evidently our derivation is much simpler. In our view the GLE is just a structural property of the RRs. Observe that $\dot{A}(t)\neq 0$ except possibly when $t\to\infty$ if $d=\infty$ [53]. Thus the trajectory must continuously evolve in time. It is either closed if $d<\infty$ or open if $d\to\infty$.

V. CURRENT-CURRENT CORRELATION FUNCTION

As suggested earlier, the current-current correlation function can be obtained if we let $A=\rho_q$, the electron number-density fluctuations at wave vector q, which now carry the electron charge e. By the continuity equation, $iq\cdot J_q(t)=-\dot{A}(t)$. Hence, denoting $(J_q(t),J_{-q})\equiv G_q(t)$, and suppressing q dependence wherever convenient,

$$q\cdot G(t)\cdot q\equiv \mathcal{G}(t)=(\dot{A}(t),\dot{A})=\|f_1\|\dot{a}_1(t), \tag{26}$$

where the norm of f_1 means the f sum rule, i.e., $\|f_1\|=\Delta_1\chi$, where $\chi=\|f_0\|=(A,A)$, retaining the standard notation for the static susceptibility.

One can evaluate Eq. (26) in two equivalent ways, either by means of the GLE [Eq. (25)] or by using the recurrence relations properties directly. In this section the former method is given and in Appendix C the latter. If Eq. (25) is substituted in Eq. (26), we obtain

$$\mathcal{G}(t)/\|f_1\|=b_1(t)-\int_0^t\varphi(t-t')a_1(t')dt'. \tag{27}$$

Here the integral term on the rhs vanishes at $t=0$; hence it is of an induced origin, i.e., the correlation of the diffuse current.

If the $\mathbf{T}$ operator is applied to Eq. (27), for $\mathrm{Re}\,z>0$ (i.e., $z=i\omega+\eta$, where ω is the frequency and $\eta\to+0$), we obtain

$$\tilde{\mathcal{G}}(z)/\|f_1\|=\tilde{b}_1(z)-\tilde{\varphi}(z)\tilde{a}_1(z). \tag{28}$$

Then by the identities already introduced, e.g., $\|f_1\|=\chi\Delta_1$, $\tilde{\varphi}(z)=\Delta_1\tilde{b}_1(z)$, and $\Delta_1\tilde{a}_1(z)=\tilde{\chi}(z)/\chi$, where $\tilde{\chi}(z)$ is the z-dependent susceptibility, we finally obtain

$$\tilde{\mathcal{G}}(z)=\chi\tilde{\varphi}(z)\text{-}\tilde{\chi}(z)\tilde{\varphi}(z), \tag{29}$$

where $\tilde{\chi}(z)$ may be further related to $\tilde{\varphi}(z)$ by a linear response relation corresponding to the RR2,

$$\tilde{\chi}(z)/\chi=\frac{\tilde{\varphi}(z)}{z+\tilde{\varphi}(z)}. \tag{30}$$

In general, $\tilde{\chi}(z=0)\leqslant\chi$. If $d\to\infty$ (where d is the Hilbert space dimensionality), the equality generally rules.

As noted, the convoluted term [second term of the rhs of Eq. (29)] refers to the correlation of the induced current. Hence it is to be identified with the diffusivity. Using $\tilde{\varphi}(z)=\mathcal{D}(z)$ due to Kubo [52,54], we can write Eq. (29) as

$$\tilde{\mathcal{G}}(z)=\chi\mathcal{D}(z)-\tilde{\chi}(z)\mathcal{D}(z). \tag{31}$$

One can show using Eq. (30) that $\tilde{\chi}(z\to\infty)=z^{-2}+0(z^{-4})$, which again indicates that the second term of the rhs of Eq. (31) is the diffusive term. Hence we conclude that

$$\chi\mathcal{D}(z)=\sigma\!\!\!/(z), \tag{32a}$$

where $\sigma\!\!\!/\equiv q\cdot\sigma\cdot q$, σ being the conductivity. By removing the slashes,

$$\chi D(z)=\sigma(z). \tag{32b}$$

If $z\to 0$ while the suppressed wave vector q is held finite, Eq. (32b) gives an equilibrium condition: $\sigma(0)=\chi D(0)$. By removing the slashes from Eq. (31) (allowed since these slashed variables are longitudinal), we obtain the final form,

$$\tilde{G}(z)=\sigma(z)-\frac{\sigma\!\!\!/(z)}{z+\mathcal{D}(z)}D(z). \tag{33}$$

Recall that the wave vector q has been suppressed for simplicity in all the above quantities. If $q\to 0$ while $z\neq 0$, the second term of the rhs of Eq. (33) behaves as $0(q^2)$. Hence, in this long wavelength limit, $\tilde{G}(z)=\sigma(z)$, whereupon the $z\to 0$ limit is taken. If, however, we let $z\to 0$ first in Eq. (29), which is an equilibrium limit, $\tilde{G}(z)=0$ (see also the second part of Appendix C). That of course means $\sigma(z=0)=\chi D(z=0)$, previously obtained from Eq. (32b), provided that $\tilde{\chi}(z=0)=\chi$. We have thereby recovered the two results that Luttinger deduced phenomenologically [14]. Observe also that if now $z\to\infty$ (i.e., $t\to 0$), the induced terms contribute very little. That is, $\tilde{G}(z)=\sigma(z)[1+O(z^{-2})]$.

Finally, by defining $\tilde{G}(z)/\sigma(z)=\epsilon^{-1}$, where ϵ is the dielectric function, we obtain

$$\epsilon^{-1}=1-\tilde{\chi}(z)/\chi \tag{34a}$$

$$=z\tilde{a}_0(z). \tag{34b}$$

The first relation (34a) is well known. The second relation (34b) makes it possible to give a geometric interpretation to the dielectric function. For example, the Drude dielectric function has but two dimensions in the realized Hilbert space, classifiable as a *dynamic* random phase approximation RPA [54].

By taking the inverse of Eq. (34b) it follows at once that

$$\epsilon=1+\tilde{\varphi}(z)/z \tag{35a}$$

$$=1+\tilde{\chi}^{sc}(z)/\chi, \tag{35b}$$

where $\tilde{\chi}^{SC}$ denotes the *screened* susceptibility. By comparing Eq. (35a) with Eq. (35b), we recover the standard relation that $\tilde{\chi}^{sc}(z)=\sigma(z)/z$ and also $\tilde{\chi}^{sc}(z)/\tilde{\chi}(z)=\epsilon^{-1}$, as required. For recent applications of the conductivity formula, see [55].

VI. DISCUSSION

As stated in the Introduction, we have derived the GLE by means of the RR1 and RR2 alone. Our derivation is straightforward with no reference to any Brownian concept. In this circumstance attaching the word ''random'' to $B(t)$ does not appear supportable. We might still regard $B(t)$ as a force that drives the time evolution of A, i.e., one that pulls or draws out the trajectory [56]. If, for example, $d=2$, $B(t)=B$. Thus the pulling is constant in time and $A(t)$ can only be periodic. If $d\to\infty$, the pulling force itself evolves in time and $A(t)$ can be nonperiodic.

Calling $\varphi(t)=\Delta_1 b_1(t)$ a memory function has some merit. However, this function (at least according to our exact solutions) does not show any special dependence on slow time scales, a Brownian feature often attributed to it *a priori*. In fact, $a_0(t)$ and $b_1(t)$ have rather similar behavior ordinarily if $d\to\infty$.

If $\varphi(t-t')=\Gamma\delta(t-t')$, Γ a constant, we could obtain from Eq. (25) the classical Langevin equation. But no memory functions of microscopic origin show this behavior even approximately. There is no microscopic evidence for the earlier belief that the GLE can justify the classical Langevin equation.

The formalism of the GLE itself has given rise to conjectures, some of which have not been found supportable. For example, it was thought that functions such as a_0 possess an addition property, i.e., $a_0(t-t')=a_0(t)a_0(t')$. This is not correct. The true addition property is richer (see Appendix E). Then by the RR2, $a_1(t)$ may not have an addition property, nor by the convolution relation $b_1(t)$, so the memory function also has no addition property of this type. This explains the lack of sensitivity to slow time scales noted above in the memory function.

It has also been conjectured that the basis vectors $f_{k\to\infty}$ would paint a fine picture of $A(t)$. This cannot be true. If $z\to\infty$, $\tilde{a}_k(z\to\infty)=z^{-k-1}$ (see Appendix A). Hence if $t\to 0$, $a_{k\to 0}(t)$ are important and $f_{k\to\infty}$ have little bearing on the orthogonal expansion of $A(t)$. If $t\to\infty$, all $a_k(t)$ and thus all f_k contribute significantly.

The basis vectors are in effect the normal modes of energy delocalization. They are perhaps best observed through classical models like the nearest-neighbor coupled harmonic oscillator chains [17]. If an atom in a chain is perturbed, the energy transfer process consists of f_{2k}'s, where k represents the kth atom with respect to the perturbed one. Each f_{2k} contains changes in the nearest neighbors of the kth atom only, with no reference to other atoms or the perturbed atom at $k=0$. These f_{2k}'s do not give a fine description but modes at successive positions of the chain. If N is the number of atoms in a chain, $d=N+1$. Thus in the thermodynamic limit $d\to\infty$ and irreversibility sets in as the delocalization process is continued. The mechanism of the long time behavior thus is contained in f_{2k}, $k\to\infty$.

We have demonstrated that the GLE is but a structural property of the RR1 and RR2. It is especially useful for formulating the current with the aid of the continuity equation. It leads directly to the current-current correlation function, comparable to Luttinger's theory based on a phenomenological transport equation. The conductivity is identifiable formally as the part of the trajectory for the current that remains in the subspace. The same geometric picture can be applied to the dielectric function and the associated sum rules.

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APPENDIX A: THE ASYMPTOTIC BEHAVIOR OF $\tilde{a}_k(z)$

We shall prove one by one that

$$\tilde{a}_k(z\to\infty)=z^{-k-1}-\Delta_{12\cdots k+1}z^{-k-3}+\cdots, \tag{A1}$$

where $\Delta_{12\cdots k}=\Delta_1+\Delta_2+\cdots+\Delta_k$. If $z\to\infty$, we can expand $\tilde{a}_0(z)$ using Eq. (8) as shown below:

$$\tilde{a}_0(z)=z^{-1}-\Delta_1 z^{-3}+\Delta_1\Delta_{12}z^{-5}-\Delta_1 Pz^{-7}+\Delta_1 Qz^{-9}-\cdots, \tag{A2}$$

where

$$P=\Delta_{12}^2+\Delta_2\Delta_3,$$

$$Q=\Delta_{12}^3+\Delta_2\Delta_3(\Delta_{12}+\Delta_{1234}).$$

To obtain the large z behavior of $\tilde{a}_1$, we use the relation (7a) and Eq. (A2). We obtain

$$\tilde{a}_1=z^{-2}-\Delta_{12}z^{-4}+Pz^{-6}-Qz^{-8}+\cdots. \tag{A3}$$

To obtain the large z behavior of $\tilde{a}_2$, we use $\Delta_2\tilde{a}_2=\tilde{a}_0-z\tilde{a}_1$, given by the RR2 [see Eq. (7b)]. Using the previous results (A2) and (A3), we obtain

$$\tilde{a}_2=z^{-3}-\Delta_{123}z^{-5}+(P+\Delta_3\Delta_{1234})z^{-7}-\cdots. \tag{A4}$$

Similarly, using $\Delta_3\tilde{a}_3=\tilde{a}_1-z\tilde{a}_2$ from the RR2 and Eqs. (A3) and (A4), we obtain

$$\tilde{a}_3=z^{-4}-\Delta_{1234}z^{-6}+\cdots. \tag{A5}$$

Given these results we can arrive at the general results stated in Eq. (A1).

APPENDIX B: STRUCTURAL PROPERTIES

We shall show that the RRs underlie all time evolution expressions such as the GLE [Eq. (25)]. Consider $(\dot{A}(t),f_0)$, where the inner product means the Kubo scalar product. If $\dot{A}(t)$ is given by Eq. (25), we obtain

$$\dot{a}_0(t)=-\int_0^t\varphi(t')a_0(t-t')dt'. \tag{B1}$$

If the **T** operator is applied to Eq. (B1), we obtain

$$z\tilde{a}_0 - 1 = -\tilde{\varphi}\tilde{a}_0 = -\Delta_1\tilde{a}_1, \tag{B2}$$

where we have used $\tilde{\varphi}=\Delta_1\tilde{b}_1$ and $\tilde{b}_1=\tilde{a}_1/\tilde{a}_0$. We have recovered Eq. (7a), the first of the RR2.

Consider now $(\dot{A}(t),f_1)$ again using Eq. (25). We obtain

$$z\tilde{a}_1=\tilde{b}_1-\tilde{\varphi}\tilde{a}_1. \tag{B3}$$

Hence

$$\tilde{a}_0^{-1}=z+\tilde{\varphi}. \tag{B4}$$

If both sides of Eq. (B4) are multiplied by $\tilde{a}_0$, we recover Eq. (7a) again. Similarly, $(\dot{A}(t),f_k)$ for $k\leqslant d-1$ yields Eq. (7a), showing that the basal relation for the RR2 [Eq. (7a)] alone underlies the GLE.

We see that the GLE really refers to a relationship between $\dot{a}_k$ and a_k. Since the two are connected via φ for all k, only Eq. (7a) appears. In higher relationships, such as between $\ddot{a}_k$ and a_k there would appear Eq. (7b). The RR2 underlies all these expressions for time evolution in Hermitian systems.

APPENDIX C: CONDUCTIVITY FORMULA VIA RECURSION RELATIONS

In Sec. V [see Eq. (26)] the current-current correlation function was given by $\mathcal{G}(t)=\|f_1\|\dot{a}_1(t)$. This quantity was evaluated by using the GLE to arrive at the conductivity formula. It can be evaluated more simply via the relations of the RR2, which is done here. From Eq. (26),

$$\tilde{\mathcal{G}}(z)=z\chi\Delta_1\tilde{a}_1(z). \tag{C1}$$

Using $\tilde{a}_1=\tilde{b}_1\tilde{a}_0$ and eliminating $z\tilde{a}_0$ by Eq. (7a), and also using $\Delta_1\tilde{b}_1(z)=\tilde{\varphi}(z)$, we obtain

$$\tilde{\mathcal{G}}(z)=\chi\tilde{\varphi}(z)-\tilde{\chi}(z)\tilde{\varphi}(z), \tag{C2}$$

where we have used the connection to linear response theory, $\Delta_1\tilde{a}_1(z)=\tilde{\chi}(z)/\chi$. We have thus obtained the conductivity formula (29) quite directly.

It was remarked after Eq. (33) that $\tilde{G}(z\to 0)=0$, attaining a static limit which is an equilibrium state. This can be readily seen from the Laplace-transformed continuity equation, $z\langle\rho_q\rangle+iq\cdot\langle J_q\rangle=0$. If $z\to 0$ while q is held fixed, $\langle J_q\rangle\to 0$. By linear response theory this implies that $\tilde{G}(z\to 0)=0$.

One can also obtain this behavior directly from the recurrence relations formalism. From Eq. (26),

$$\tilde{\mathcal{G}}(z=0)/\|f_1\|=\int_0^\infty \dot{a}_1(t)dt=a_1(t=\infty)-a_1(t=0). \tag{C3}$$

Now $a_1(0)=0$ [see Eq. (3)]. Also, $a_1(t=\infty)=0$ since $a_0(t)$ and all the derivatives vanish as $t\to\infty$. Exact solutions [17], e.g., $a_1=J_1(t)$, $te^{-t^2/2}$, $\tanh t/\cosh t$, satisfy this requirement. See Appendix A of [13] and also Eq. (8.10) of [52(a)]. A more general proof will be given elsewhere [53].

APPENDIX D: VALIDITY OF THE GENERALIZED LANGEVIN EQUATION

The validity of the GLE may be established if we can recover from Eq. (25)

$$\int_0^t\left(B(t')-\int_0^{t'}\varphi(t'-t'')A(t'')dt''\right)dt'=A(t)-A(0). \tag{D1}$$

To prove this result, we shall use two identities, the first given by Eq. (15) and another which follows from it. If $k\geqslant 1$,

$$\tilde{b}_k(z)=\tilde{a}_k(z)/\tilde{a}_0(z), \tag{D2}$$

$$\tilde{a}_k(z)\tilde{b}_1(z)=\tilde{b}_k(z)\tilde{a}_1(z). \tag{D3}$$

Hence, by convolution, we obtain

$$a_k(t)=\int_0^t b_k(t-t')a_0(t')dt'. \tag{D4}$$

$$\int_0^t a_k(t-t')b_1(t')dt'=\int_0^t b_k(t-t')a_1(t')dt'. \tag{D5}$$

Our idea is to eliminate the first term on the lhs of Eq. (D1) by an equivalent contained in the second term on the same side. This is accomplished by means of the above two identities (D4) and (D5).

Looking at the second integral term of Eq. (D1), we replace φ by $\Delta_1 b_1$ and resolve $A(t)$ into $a_0f_0+a_kf_k$, where a sum on $k\geqslant 1$ is implied. The two resolved terms will be treated separately. The first term gives us

$$\Delta_1\int_0^t dt'\int_0^{t'} b_1(t'-t')a_0(t')dt''\, f_0$$

$$=-\int_0^t \dot{a}_0(t)dt\, f_0=A(t=0)-a_0(t)f_0. \tag{D6}$$

In the second line we have used Eq. (D4) and $\Delta_1 a_1=-\dot{a}_0$ from RR2 [see Eq. (6)].

The second term gives

$$\Delta_1\int_0^t dt'\int_0^{t'} b_1(t'-t'')a_k(t')dt''\, f_k=-\int_0^t dt' I(t')f_k, \tag{D7}$$

where

$$I(t)=\int_0^t \dot{a}_0(t-t')b_k(t')dt'. \tag{D8}$$

Here we have used Eq. (D5) and RR2 as above in obtaining Eq. (D6).

Let

$$\psi(t)=\int_0^t a_0(t-t')b_k(t')dt'. \tag{D9}$$

Then

$$(d/dt)\psi(t)=b_k(t)+I(t). \tag{D10}$$

Substituting $I(t)$ from Eq. (D10) into Eq. (D7), we obtain immediately

$$\text{rhs of Eq. (D7)}=\int_0^t B(t)dt-a_k(t)f_k. \tag{D11}$$

If Eqs. (D6) and (D11) are now combined, we obtain the desired proof stated by Eq. (D1).

One can obtain the proof somewhat more directly by first applying the Laplace transform to Eq. (25) and then using Eqs. (D2) and (D3). After resolving the coupled terms, one can then apply the inverse transform to put the proof in the final form. The solution we have shown above does provide more details and hence perhaps is more insightful. To our knowledge, ours is the first proof of the validity of the GLE.

APPENDIX E: ADDITION PROPERTY OF $a_0(t)$

The addition property of $a_0(t)$ may be established from the stationarity of $A(t)$, i.e.,

$$(A(t),A(t'))=(A(t-t'),A), \tag{E1}$$

where $A\equiv A(t=0)$. Using Eqs. (1) and (2), we obtain at once the addition property:

$$\begin{aligned} a_0(t-t')&=\sum_{k=0}^{d-1} a_k(t)a_k(t')\|f_k\|/\|f_0\| \\ &=a_0(t)a_0(t')+\Delta_1 a_1(t)a_1(t') \\ &\quad+\Delta_1\Delta_2 a_2(t)a_2(t')+\cdots. \end{aligned} \tag{E2}$$

Observe that if $t'=0$, it yields a trivial identity with the help of Eq. (3). If $t'=t$, Eq. (E2) with Eq. (3) yields the Bessel equality [9].

We can easily test the validity of the addition property with the known admissible solutions of Eq. (5). For example, if $d=2$ (i.e., $\Delta_k=1$ and 0 if $k=1$ and $k\geqslant 2$, respectively), then $a_0(t)=\cos t$, $a_1(t)=\sin t$. This is a trivial case. If $\Delta_k=2$ and 1 if $k=1$ and $k\geqslant 2$, respectively, $a_k(t)=J_k(t)$, the Bessel function. Then Eq. (E2) yields the familiar addition property of $J_0(t)$.

We may use Eq. (E2) to obtain the addition property of other admissible functions such as $\exp(-t^2/2)$, sech t, $j_0(t)$, the spherical Bessel function, etc. The addition property of $a_0(t)$ is indeed very rich. It is even useful for establishing the addition properties of certain mathematical functions.

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