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Remarks on hyperbolic secant memory functions

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Abstract. Recent studies of the dynamic theory of liquids have been much influenced by Mori's formulation of the generalized Langevin equation. An essential component of this formalism is the memory function. For realistic models like a Lennard-Jones liquid it is too difficult to calculate the memory function. Recent approaches have been to propose various forms for it including the hyperbolic secant. In perhaps the most serious attempt yet, Tankeshwar and Pathak have been said to derive hyperbolic secant memory directly from the generalized Langevin equation. Here the validity and justification of this work is closely examined. Other approximate studies which have yielded hyperbolic secant memory are also examined and comparisons are made.

1. Introduction

Studies of the dynamic theory of liquids during the past two decades have been much influenced by Mori's formulation of the generalized Langevin equation (GLE) [1]. An essential component of the GLE is the memory function. If it is known, the GLE allows one to obtain the relaxation function, e.g. the single-particle velocity autocorrelation, from which transport properties like the diffusion constant can follow. Although there is a formal prescription for calculating the memory function itself from first principles, for models like a Lennard-Jones (LJ) liquid it is prohibitively difficult. Many have thus proposed various forms for it including hyperbolic secant, most of which have little physical justification. Sech memory has drawn the attention of several workers in this field and beyond as it has some attractive features [2–5]. It would be of great interest if one could even approximately demonstrate its existence in a model.

In perhaps the most serious attempt yet, Tankeshwar and Pathak (TP) [6], using two significant approximations, have recently been said to derive sech memory from the GLE directly. It is an approach quite the opposite of the usual. If their approximations are valid, one could say that sech memory does exist—if approximately—in a model where they are justified. TP's approximations, however, do not refer to any specific model and appear general, although intended for a LJ liquid, on which they have contributed several articles [4].

What is remarkable is that sech memory is an exact solution of the GLE for a certain class of models [5, 7]. That is, it cannot be a general solution but only a particular solution of limited applicability. It is thus natural to examine TP's method of solution closely, especially their two great approximations, to see what they might imply.

TP reduce an already approximated version of the GLE via another approximation termed an *ansatz* (to be referred to as TP's *ansatz*). This results in sech memory. This *ansatz* also yields a constraint in the form of a 'universal' constant, which is roughly realized

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in a LJ liquid. TP take it to mean that their *ansatz* is justified and sech memory exists in this liquid.

There are two issues at hand. Firstly, TP's *ansatz* as noted is *not* applied to the GLE. Hence, it is necessary to know first the validity of their first approximation by which the GLE is changed. Secondly, there is a question of uniqueness of TP's method, and also a question of sufficiency of TP's constraint, in letting sech memory be attributed to a LJ liquid without reservation. The purpose of this work is to address these issues. In addition, we shall examine other derivations of sech memory and related ones to see their validity and limitations. We will attempt to find connections between these efforts and TP's work.

2. Sech memory

According to Mori [8], the time evolution of the dynamical variable A (e.g. the velocity of a single particle in a liquid) may be regarded as a vector in a d-dimension Hilbert space S. Let $M_{k+1}(t)$ be the memory function in the k-subspace of S, with $M_k(0) = \Delta_k > 0$ if $0 \leqslant k \leqslant d-1$, $\Delta_0 \equiv 1$ and $\Delta_d \equiv 0$. The scalar version of the GLE in the k-subspace S_k is

$$\dot{m}_k(t) + \Delta_{k+1} \int_0^t m_{k+1}(t-t') m_k(t')\, \mathrm{d}t' = 0 \qquad 0 \leqslant k \leqslant d-1 \tag{1}$$

where $m_k(t) = M_k(t)/\Delta_k$ and $m_0(t) = (A(t), A)/(A, A)$, where the inner product means the Kubo scalar product. It will be insightful to work with a general case as given above. It indicates the existence of a hierarchy of the memory functions, $m_1, m_2, \ldots, m_{d-1}$, each of which refers to the time evolution in each subspace S_k, $0 \leqslant k \leqslant d-1$, and $S_0 \equiv S$. The subspace S_k has $d-k$ dimensions, and the structure is denoted by Δ_p, $p \geqslant k$. There is less information contained in it than in any one of its superspaces. Since $A(t) = \exp(\mathrm{i}Ht)A\exp(-\mathrm{i}Ht), \overline{h} = 1$, where H is a model's Hamiltonian, the structure of S_k is realized through the dimensionality d and the recurrants Δ_ks by a model.

It is clear that if $d \to \infty$, equation (1) cannot be solved without input from a model since there are two unknown functions for every equation. If $d < \infty$, it can be solved and there are only periodic solutions. These solutions are excluded by TP, meaning that theirs is for $d = \infty$.

Following TP [6], we can transform (1) into another equation, now involving m_k and m_{k+2}, as follows. By differentiating (1) once and using (1) once more therein, noting that $m_k(t) = 0$ if $t < 0$, we can obtain

$$\ddot{m}_k(t) + \Delta_{k+1} m_k(t) + \Delta_{k+2} \int_0^t m_{k+2}(t-t') \dot{m}_k(t')\, \mathrm{d}t' = 0 \qquad 0 \leqslant k \leqslant d-1. \tag{2}$$

This is still exact, just like (1), although no more solvable independently of H if $d \to \infty$. It does have certain advantages since it introduces two constants explicitly. For example, if $\Delta_{k+2} = 0$ but $\Delta_{k+1} \neq 0$, i.e. $k = d-2$, then $m_k(t) = \cos at$, $a^2 = \Delta_{k+1}$. If $t \to 0$, to order t^2 one cannot distinguish it from, e.g., $\exp(-a^2t^2/2)$ or sech at. Also, equation (2) relates time evolution in the subspaces of even or odd dimensions—not mixed as in (1). If $k = 1$, we recover TP's form. Our derivation of (2) is direct. It is not necessary to use Laplace transforms.

TP [6] propose to solve (2) when $d \to \infty$ but without reference to H by introducing an approximation and an *ansatz*. First, for the integral term of (2), they let

$$\int_0^t m_{k+2}(t-t') \dot{m}_k(t')\, \mathrm{d}t' = m_{k+2}(t) \int_0^t \dot{m}_k(t)\, \mathrm{d}t \tag{3}$$

to be referred to as TP's approximation. It is as if $t \gg t'$ in m_{k+2} in the lhs of (3)—as if t and t' have macro- and microscopic time-scales, respectively. The validity and implications of this approximation will be discussed later. By use of (3) in (2), it follows that

$$\ddot{m}_k(t) + \Delta_{k+1} Q(t) m_k(t) = 0 \tag{4a}$$

where

$$Q(t) = 1 - x(m_{k+2}(t)/m_k(t))(1 - m_k(t)) \qquad x \equiv \Delta_{k+2}/\Delta_{k+1}. \tag{4b}$$

This is now purely a differential equation, but still with two unknown functions, and hence not solvable.

To overcome the inherent difficulty, due to the hierarchic nature of the memory functions of an ∞-dimensional Hilbert space, TP propose an *ansatz*. If generalized, it corresponds to

$$m_{k+2}(t) = 2x^{-1} m_k(t)(1 + m_k(t)). \tag{5}$$

The above is, we believe, the simplest generalization of TP's *ansatz* in the k-subspace, recovering theirs if $k = 1$. The significance of TP's *ansatz* and our generalized form will also be discussed later. Now eliminating m_{k+2} in (4b) by using (5), we obtain

$$\ddot{m}_k(t) + \Delta_{k+1}(2m_k^2(t) - 1) m_k(t) = 0. \tag{6}$$

The above now contains only one constant, the other being constrained by (5). As shown by TP, the above is solved by

$$m_k(t) = \operatorname{sech} at \qquad a^2 = \Delta_{k+1}. \tag{7}$$

This solution recalls a similar one due to Balucani *et al* [9]. But is it really a solution of (1), if approximately? If so, how approximately? If $t = 0$ in (5),

$$x = \Delta_{k+2}/\Delta_{k+1} = 4 \tag{8}$$

to be referred to as TP's constraint. This must be independent of any physical parameters (e.g. temperature, at least explicitly), a pure number. Now setting $k = 1$ (to follow TP's argument), we see that TP's *ansatz* implies $x(k = 1) = \Delta_3/\Delta_2$, requiring the ratio of these two recurrants be 4. If this constant is realized in a model, TP argue that their *ansatz* is justified for that model. They further argue that for that model sech memory is a valid solution of (1).

Even if TP's constraint is realized, this kind of justification is clearly questionable being dependent on two independent steps. Nevertheless, TP adduce values for Δ_3/Δ_2 in a LJ liquid. If sech memory is an exact solution of (1) in the $k = 1$ subspace, there exist as we shall see in the next section some other special constants. Are they—or at least some of them—also realized in the same liquid in the same manner? It would seem that sech memory cannot be attributed to a LJ liquid without additional evidence provided by them.

3. LJ liquids and sech memory

We have shown previously that in the k-subspace, $m_k(t) = \operatorname{sech} at$, $a^2 = \Delta_{k+1}$, is an exact solution of (1) for $d \to \infty$ if

$$\Delta_{p+1} = (p - k + 1)^2 \qquad p \geqslant k \tag{9}$$

in some dimensionless units [7]. If $k = 1$, we obtain $\Delta_3/\Delta_2 = 4$, which corresponds to TP's constraint in the k-subspace. But there are also $\Delta_4/\Delta_2 = 9$, $\Delta_5/\Delta_2 = 16$, etc, which *together* form the signature of sech memory in that ($k = 1$)-subspace. One or two such constants are insufficient to denote sech memory.

Table 1. Δ_k/Δ_2 versus $T, k = 3$, 4 and 5, reproduced from [10], table 1. T is the reduced temperature. For high temperatures, $\Delta_3/\Delta_2 \approx 3.7$, $\Delta_4/\Delta_2 \approx 38$, $\Delta_5/\Delta_2 \approx 118$ (also $\Delta_4/\Delta_3 \approx 10.2$, $\Delta_5/\Delta_4 \approx 3.1$).

	T	Δ_3/Δ_2	Δ_4/Δ_2	Δ_5/Δ_2
1	0.72	3.184	19.92	433.7
2	0.77	3.374	16.98	344.7
3	1.10	3.261	11.01	167.3
4	1.43	3.306	9.06	94.40
5	1.45	3.319	9.21	91.24
6	1.57	3.284	8.83	75.96
7	4.66	3.703	35.19	127.8
8	4.76	3.698	40.73	116.4
9	5.02	3.667	37.61	122.3
10	5.08	3.619	32.95	126.6
11	5.12	3.712	43.39	107.9
12	5.26	3.686	40.09	108.7

TP have sought this first constant $\Delta_3/\Delta_2 = 4$ in a LJ liquid, in particular in the work of Lee and Chung [10] who have obtained several Δs for this liquid. In that work values of $\Delta_2 - \Delta_5$ are given as a function of the reduced density in the range 0.30–0.85 and as a function of the reduced temperature in the range 0.7–5.3. These calculated Δs do not appear to be sensitive to the density, at least in this range. Hence, we have arranged them according to the temperature (ignoring the density altogether) as shown in table 1. Observe that they divide into roughly two groups—those of low and high temperatures (rows 1–6 and rows 7–12, respectively). The third column shows Δ_3/Δ_2. Their values range from 3.18 to 3.71 as stated by TP, indicating a strong temperature dependence. At low temperatures the average value for Δ_3/Δ_2 is approximately 3.28 and at high temperatures it is 3.68. Clearly TP's constraint is close only to the high-temperature values.

Although TP's theory allows no explicit temperature dependence in their constraint, let us assume that it is applicable at least to high temperatures and see whether the other constants are as close to the corresponding sech values. The fourth and fifth columns show Δ_4/Δ_2 and Δ_5/Δ_2. For the high-temperature group, their average values are approximately 38 and 118, which are far from the sech values of 9 and 16, respectively. Observe also that at these high temperatures, $\Delta_4/\Delta_3 \approx 10.2$ and $\Delta_5/\Delta_4 \approx 3.1$, both departing considerably from TP's *ansatz* which would require them all to be 4. On the basis of this simple comparison, it is difficult to say that one is seeing sech memory in a LJ liquid even at high temperatures. We shall show below that the occurrence of $\Delta_3/\Delta_2 \approx 4$ is not uncommon. It alone does not necessarily signify sech memory.

In the literature on the GLE [5, 11, 12], there are a number of models for which Δs, also known as recurrants, have been accurately calculated. Although for some of them, Δ_3/Δ_2 (or equivalently Δ_2/Δ_1) is close to 4, hardly anyone has taken it seriously to signify sech memory (or sech relaxation). We shall first quote a few examples from other LJ models. Tognetti and co-workers [13–15] have extensively studied a LJ chain, and also a Toda chain, in which a wavevector-dependent single-particle displacement is the dynamical variable. For the LJ chain, at a wavevector $k = \pi$ and at the reduced density $\rho = 0.890$, Δ_3/Δ_2 shows a strong temperature dependence: 3.965 ($T = 0.1$), 2.552 ($T = 0.2$), 2.236 ($T = 0.3$), etc. Here T is the reduced temperature. For the Toda chain, at the zone boundary and at the reduced $T = 1.0$, Δ_3/Δ_2 shows a dependence on 'quantum coupling': 3.227 ($g = 0$), 3.295 ($g = 0.4$), 3.423 ($g = 1$). Here $g = 0$ indicates the classical regime. In both cases the values for Δ_3/Δ_2 all lie in the range of the classical LJ liquid values. It would be no more justified to conclude that sech memory is operative in them than in a LJ liquid.

For the magnetic models the picture is much clearer since many more recurrants are accurately known [5]. For example, for the transverse Ising chain at $T = \infty$ [16], in which a single spin is the dynamical variable, the following is known: $\{\Delta_p/\Delta_1\} = 4$, 7, 10.285, 12.0476, 16.660, etc, where $p = 2, 3, \ldots$. These recurrants depart rapidly from the signature of sech relaxation. For the classical XX-chain [17, 18], 18 recurrants are known: 2, 6.840, 10.190, 16.165, 26.4495, 30.6636, etc. Although they do not initially suggest sech relaxation, higher ones actually do approach it approximately.

These examples further illustrate the great difficulty in extracting the form for the relaxation or memory function even from a relatively large set of recurrants. Unless their behaviour is 'regular', attempts based on a small set of recurrants are hazardous especially for long times [12].

4. The GLE and TP's approximation

As a first step in their method, TP introduce an approximation (TP's approximation) to (1). We shall examine below its validity. In particular, we shall want to see whether it preserves certain essential properties of the equation of motion.

The GLE is formally solved via an orthogonal expansion by regarding $A(t)$ as a vector in a d-dimensional Hilbert space S [19]:

$$A(t) = \sum_{k=0}^{d-1} a_k(t) f_k \tag{10}$$

where the f_ks form a complete set of basis vectors spanning the space S, i.e. $(f_k, f_{k'}) = 0$ if $k' \neq k$, and the a_ks are projection coefficients, e.g. $a_0(t) = (A(t), A)/(A, A) = m_0(t)$. Given that $A(t)$ is a solution of the GLE, the orthogonality of these basis vectors implies that the a_ks are themselves linearly independent at any t. The converse is also true. An admissible solution for the GLE has this fundamental structural property. That is, throughout the time evolution, $A(t)$ must remain in the space S if it is to be an admissible solution.

In this formalism, $F(t)$, the random force on $A(t)$, is also a vector but in S_1, a subspace of S, i.e. $(F(t), A) = 0, t \geqslant 0$. Hence,

$$F(t) \equiv A_1(t) = \sum_{k=1}^{d-1} b_k(t) f_k$$

where $b_1(t) = m_1(t)$. Since $A(t)$ and $F(t)$ are two different physical quantities, it is necessary that $b_k \not\sim a_k$. With respect to the time evolution of A_1 taking place in the subspace S_1, there is a random force on it also, say $A_2(t)$. It is a vector in S_2, a subspace of S_1. It follows that

$$A_2(t) = \sum_{k=2}^{d-1} c_k(t) f_k$$

where, e.g., $c_2(t) = m_2(t)$ and $c_k \not\sim b_k \not\sim a_k$. One can continue this process of construction indefinitely if d is infinitely large. To be admissible, these vectors $A_1, A_2, \ldots$ must also remain within their own spaces $S_1, S_2, \ldots$ throughout the time evolution. The hierarchic nature of the memory functions derives from the structural relationship of these subspaces.

We can now see whether these vectors remain in the same spaces during the course of time evolution if TP's approximation is applied. The projection coefficients are related by a convolution [19]:

$$a_k(t) = \int_0^t b_k(t')a_0(t-t')\,\mathrm{d}t' \qquad k \geqslant 1. \tag{11}$$

If TP's approximation (3) is imposed on $a_0(t-t')$ under the integral sign above, equation (11) becomes

$$a_k(t) = \left(\int_0^{t\to\infty} b_k(t')\,\mathrm{d}t'\right) a_0(t) = B_k a_0(t) \qquad k \geqslant 1 \tag{12}$$

where B_k is a constant. The upper limit in (12) may be made to grow since $t \gg t'$ is implied by TP's approximation. According to (12), the a_ks are now not linearly independent. That is, the f_ks ($k \geqslant 0$) are not orthogonal vectors spanning the space S. (If TP's approximation were made on b_k in (11), we would obtain the non-allowed $b_k \sim a_k$.)

The same is true in every subspace. For example, $b_k \sim b_1$, under TP's approximation. Hence, the f_ks ($k \geqslant 1$) are not orthogonal vectors spanning S_1. One can thus conclude that the GLE under TP's approximation produces solutions $A(t), A_1(t), \ldots$ which do not remain in the original Hilbert spaces $S, S_1, \ldots$ as the time evolves. It was this argument which was used to rule out exponential decay for the relaxation function [20].

TP argue that their approximation can be used in higher memory functions, i.e. in higher subspaces, apparently to justify its use on m_3, but not on m_1 or m_2. But because the memory functions are all hierarchically linked (see (1)), the approximation is transmitted to the lower ones—to m_2, then m_1 and finally to m_0. It cannot be contained in one subspace alone. To see this, let us introduce TP's approximation in the subspace $S_k, k \geqslant 1$. Then the basis vectors for this subspace $f_k, f_{k+1}, \ldots$ are no longer mutually orthogonal as shown above. Now the superspace S_{k-1} is spanned by $f_{k-1}, f_k, f_{k+1}, \ldots$. Since f_k and f_{k+1} are also basis vectors in S_k, $(f_{k+1}, f_k) \neq 0$. Given the general property $(\dot{f}_k, f_k) = 0$ and the recurrence relation [19] $f_{k+1} = \dot{f}_k + \Delta_k f_{k-1}$, we are led to $(f_k, f_{k-1}) \neq 0$. One can then show that $(f_{k-1}, f_{k-2}) \neq 0$ and by continuation no basis vectors in all other superspaces are orthogonal, which contradicts (10). TP's approximation is simply not a valid approximation for the GLE in any subspace.

Let us now turn to TP's *ansatz*, borrowed from the mode-coupling theory of critical phenomena. Near its critical point, a liquid behaves anomalously owing to the existence of dominant large-scale modes. Here mode coupling can be a significant factor in the dynamic critical behaviour of the liquid. But far from the critical point—the domain of our present interest—it is difficult to envisage that mode coupling is as significant.

For critical dynamics Götze introduced an *ansatz* [21] which if generalized to the k-subspace has the following form:

$$m_{k+2}(t) = am_k(t)(1 + bm_k(t)) \tag{13}$$

where a and b are some coupling constants. The above form is at best only heuristically understood in terms of the two undetermined constants. TP adopt (13) unchanged but only at the special values $a = 2x^{-1}$ and $b = 1$ for their *ansatz*. We have shown in appendix A that if slightly different sets of values are used, one can obtain quite different memory functions from (4*a*). Thus, even on the grounds of critical dynamics, it is no simple matter to find justification for TP's *ansatz*. As already shown in section 3, TP's *ex post facto* justification in a normal LJ liquid falls short of the mark.

It does seem curious that an approximated equation of motion, together with this *ansatz*, should yield sech memory, an admissible solution of the exact equation of motion. We will show in appendix A that another *ansatz*—but not based on the mode-coupling theory—can yield the same sech memory. Hence, if it is merely to produce sech memory, TP's *ansatz* holds no special place.

5. Discussion

TP's approximation places their solution for $A(t)$ outside of its original Hilbert space. As a result, its random force $F(t)$ need not even be orthogonal to $A(t = 0)$. Their *ansatz* has had the fortuitous effect of restoring the solution to its original space (see appendix B). This kind of approach is evidently spurious. We have also shown (see appendix A) that their way of obtaining sech memory is not unique. In addition, by extension we have obtained other solutions for the memory, all of which are devoid of physical significance since the *ansatz* applied is arbitrary.

TP pin the justification of their *ansatz* on finding their constraint $x(k = 1) = \Delta_3/\Delta_2 = 4$ in a LJ liquid. We have shown that there are other constants in the same liquid which do not support sech memory at all. One might perhaps argue that since TP's method is inexact, the signature of sech memory, which is an exact solution of (1), should not apply. An alternative derived from (5) offers no relief. Here TP's constraint implies that $\Delta_{p+1} = 4^p$, $p \geqslant k$ in the k-subspace. Setting $k = 1$, we find that Δ_4/Δ_2 and Δ_5/Δ_2 lend no more support to TP's cause. Actually it is known that if $\Delta_{p+1} = y^p$, $|y| > 1$, $p \geqslant 1$, equation (1) does not have a solution [22, 23].

One might still argue that TP's *ansatz* is intended strictly for the $(k = 1)$-subspace only. As such, only the constraint $x(k = 1) = \Delta_3/\Delta_2 = 4$ is meaningful; TP contend that it is close to the LJ liquid values 3.18–3.71. We have shown that this constraint is recoverable from the recurrants for sech memory in the $(k = 1)$-subspace (see equation (9)). We have also shown that under another *ansatz* (A8), we can obtain a new constraint, $x = 3$, and a new memory function, the hyperbolic secant squared. The new constraint $x(k = 1) = \Delta_3/\Delta_2 = 3$ is just as exactly recoverable from $\Delta_{p+1} = p(p + 1)$, $p \geqslant k = 1$, the recurrants for this new memory function in the $(k = 1)$-subspace [7]. Also it is close to the LJ liquid values. In fact, it is closer at low temperatures than TP's while less so at higher temperatures. Thus, even if restricted just to the constraint alone, a LJ liquid offers no unambiguous support for TP's *ansatz* nor—by their logic—sech memory in this liquid. Another *ansatz* and another memory function would do just as well.

Others have mishandled the GLE or its equivalent, the Heisenberg equation of motion, to produce e.g. Lorentzian dynamic structure factors in Hermitian models [24]. In these instances the errors are traceable to mixing up Hilbert spaces as TP did [25, 26]. Via approximations like TP's, the GLE can be reduced to the much studied Langevin equation. As is well known, the solutions are exponentially damped functions [27]. They are of course inadmissible for the GLE [20].

There are correct ways to solve the GLE approximately. We shall illustrate a simple example in hydrodynamics, one due to Tsekov and Radoev [28, 29] (the TR model). As an approximation, let $m_{k+1}(t) = m_k(t) \equiv m(t)$ in (1), i.e. $\Delta_k = \Delta$, $k \geqslant 0$. We then obtain one of the simplest admissible solutions for (1): $m(t) = 2J_1(t)/t$, where J_1 is the Bessel function and $\Delta = 1/4$ for simplicity. Although an exactly realizable solution, it is still useful for showing a correct way of approximating (1).

To solve (1) approximately but correctly, it is necessary to ensure that the conditions like $m_k(t = 0) = 1, \dot{m}_k(t = 0) = 0$ are unaffected by the approximation. The TR model does so, being an exact solution. In standard classical approximations, one is already in the regime where $t \gg t_0, t_0 > 0$, so the behaviour at small times is often overlooked [27].

In appendix B we illustrate another method due to Balucani *et al* [9]. By this approximation method, a variety of admissible solutions are obtained including TP's solution. It is thus possible to obtain sech memory properly if approximately. But these approximate solutions are not driven by the structure of the recurrants Δ_k. Hence one cannot connect them to any models.

We have already demonstrated that given (9), sech memory is an exact solution of the GLE. Hence, equation (9) uniquely implies sech memory. The possible existence of sech memory is interesting—but still more interesting is in what model it might exist. This point has been addressed already [7].

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Appendix A. The *ansatze*, sech memory, etc

In this appendix we shall show that sech memory can be derived perhaps more simply via another *ansatz* together with TP's approximation. If (1) is differentiated once,

$$\ddot{m}_k(t) + \Delta_{k+1} m_{k+1}(t) + \Delta_{k+1} \int_0^t m_{k+1}(t-t')\dot{m}_k(t')\,\mathrm{d}t' = 0 \qquad k \geqslant 0. \tag{A1}$$

If TP's approximation is applied to m_{k+1} under the integral sign above, we obtain

$$\ddot{m}_k(t) + \Delta_{k+1} m_{k+1}(t) m_k(t) = 0 \tag{A2}$$

which involves one constant. Although much simpler than equation (4a), it is still not solvable since there are still two unknown functions in it. Following TP, we consider an *ansatz*

$$m_{k+1}(t) = 2m_k^2(t) - 1 \tag{A3}$$

evidently unrelated to (5). The substitution for m_{k+1} in (A2) of (A3) yields

$$\ddot{m}_k(t) + \Delta_{k+1}(2m_k^2(t) - 1)m_k(t) = 0 \tag{A4}$$

which is exactly the same as equation (6). Hence, we recover

$$m_k(t) = \operatorname{sech} \alpha t \qquad \alpha^2 = \Delta_{k+1}. \tag{A5}$$

Equation (A1) can be expressed slightly differently, such that in the second and third terms $m_k(t)$ and $m_{k+1}(t)$ are exchanged. Then, TP's approximation used for m_k, not m_{k+1} as above, still leads identically to (A2). It is immaterial whether TP's approximation is applied to a higher or lower memory function. Our *ansatz* (A3) does not give rise to a constraint involving Δ_ks in the manner of TP since there is only one constant in (A2). However, self-consistency between (A3) and (A5) implies that our generalized form (8) is a possibility.

Now if, instead of (A3), one takes the *ansatz*

$$m_{k+1}(t) = 3m_k(t) - 2 \tag{A6}$$

equation (A2) yields another admissible solution:

$$m_k(t) = \operatorname{sech}^2 \beta t \qquad \beta^2 = \Delta_{k+1}/2. \tag{A7}$$

This form of the *ansatz* can be generalized to obtain $m_k(t) = \operatorname{sech}^n \nu t$, $\nu^2 = \Delta_{k+1}/n$, $n = 1, 2, \ldots$.

These *ansatz*-driven solutions for (A2) suggest that something similar should also be found for (4a), TP's equation. To explore this possibility, instead of TP's *ansatz* (5), let

$$m_{k+2}(t) = 3x^{-1} m_k(t) \qquad x = \Delta_{k+2}/\Delta_{k+1} \tag{A8}$$

i.e. $a = 3x^{-1}$, $b = 0$ in (13). Then, equation (4a) becomes

$$\ddot{m}_k(t) + \Delta_{k+1}(3m_k(t) - 2)m_k(t) = 0. \tag{A9}$$

Thus, equation (A9) is also solved by (A7). (One can have a similar generalization.) In this case, the *ansatz* (A8) implies that $x = 3$.

If in (5) we now let

$$m_{k+2}(t) = x^{-1} m_k(t)(1 + m_k(t)) \tag{A10}$$

(i.e. $a = x^{-1}$, $b = 1$ in (13)), which differs from TP's *ansatz* only in the numerical prefactor $2 \to 1$, then (4a) becomes

$$\ddot{m}_k(t) + \Delta_{k+1} m_k^3(t) = 0. \tag{A11}$$

Equation (A10) implies a new constraint: $x = 2$. The solution for (A11) is a Jacobi elliptic function [30]. Finally, to obtain an equation for the constraint $x = 1$ (i.e. $\Delta_k = \Delta, k \geqslant 1$), it is sufficient to let

$$m_{k+2}(t) = m_k(t) \tag{A12}$$

i.e. $a = x^{-1} = 1, b = 0$ in (13). Then (4a) becomes

$$\ddot{m}_k(t) + \Delta m_k^2(t) = 0. \tag{A13}$$

The solution is a Weierstrass elliptic function [30].

Observe that the three new forms of the *ansatz* (equations (A8), (A10), and (A12)) all derive from a common origin in the mode-coupling theory of critical dynamics, just like TP's. They merely assume different special values of the coupling constants such as to allow the constraint x to range from 1 to 4. TP's *ansatz* and (A10) are very similar, yet their constraints and solutions are very dissimilar. TP's *ansatz* and (A8) are more dissimilar, yet their constraints and solutions are more similar.

These examples show that solutions for (4a) are highly sensitive not only to the forms but also to even minor details of the *ansatz*. In appendix B, the role of the *ansatz* in yielding admissible solutions is discussed.

Finally, equation (A12) implies the TR model. See section 5. The solution for (1) for the TR model is a Bessel function, which is very different from a Weierstrass elliptic function, the solution for (A13). As these two different solutions indicate, the same Hilbert space structure (e.g. $\Delta_k = \Delta, k \geqslant 1$) yields unrelated solutions depending on whether the equation of motion is exact or reduced. One must therefore be very careful not to attribute the solutions of some reduced equations to the exact equation without additional justifications.

Appendix B. The method of Balucani, Tognetti and Vallauri

Some years ago, Balucani, Tognetti and Vallauri [9] (BTV) gave an interesting approximation method of solution for the GLE. This important work appears not to have received due attention. Unlike TP's, this method is valid if handled properly. In the following we shall simplify it somewhat and obtain a variety of approximate solutions including TP's. This method also lends insight into TP's *ansatz*.

Tokuyama and Mori [31] showed that (1) can also be expressed as

$$\dot{m}_k(t) + \Delta_{k+1}\phi_{k+1}(t)m_k(t) = 0 \tag{B1}$$

where ϕ_{k+1} is some unknown modulated function. It must depend on Δ_p, $p \geqslant k+2$, but not on Δ_p, $p \leqslant k+1$. According to the recurrence relations formalism $\phi_1(t) = a_1(t)/a_0(t)$. Since this function is unknown, equation (B1) is no more solvable without input from models than equation (1). However, it admits a formal solution:

$$m_k(t) = \exp\left\{-\Delta_{k+1}\int_0^t \phi(t)\ \mathrm{d}t\right\} \tag{B2}$$

in terms of the unknown function ϕ (subscript suppressed). Recall that $m_k(0) = 1$. Equation (B2) is also suitable for obtaining approximate solutions.

Since $\dot{m}_k(t)$ is an odd function of t, according to (B1) $\phi(t)$ must also be an odd function. Also since $\dot{m}_k(t = 0) = 0$, so too $\phi(t = 0) = 0$. Approximate admissible solutions for $m_k(t)$ can be generated by choosing a $\phi(t)$ which has these properties. They are, however, necessary, not sufficient, so care must be exercised. For example, an admissible solution must also be bounded at all times.

We shall first consider a few simple examples to illustrate the method of BTV, all but one of which result in admissible solutions.

Example 1:

$$\phi(t) = t \qquad m_k(t) = \exp(-at^2) \qquad a = \Delta_{k+1}/2.$$

Example 2:

$$\phi(t) = \tanh at/a \qquad m_k(t) = \mathrm{sech}^n\, at \qquad a^2 = \Delta_{k+1}/n \qquad n = 1, 2, \ldots.$$

Example 3:

$$\phi(t) = t/(1+at^2) \qquad m_k(t) = (1+at^2)^{-n/2} \qquad a = \Delta_{k+1}/n \qquad n = 1, 2, \ldots.$$

Example 4:

$$\phi(t) = \frac{\sin at}{a(1+\cos at)} \qquad m_k(t) = 2^n(1-\cos at)^{-n}$$
$$a^2 = \Delta_{k+1}/n \qquad n = 1, 2, \ldots.$$

Observe that in example 2, the $n = 1$ case corresponds to TP's solution [6], and the $n = 2$ case corresponds to BTV's solution [9]. The solution in example 4 is not bounded at all times. Example 1 is an exact solution of (1), and also of (B1), in the k-subspace S_k if $\Delta_p = (p-k)$, $p \geqslant k+1$ [7]. Similarly, example 2 is an exact solution if $\Delta_p = (p-k)(p-k+n-1)$, $p \geqslant k+1$ and $n \geqslant 1$.

If (B1) is differentiated once,

$$\ddot{m}_k(t) + \Delta_{k+1}\mu(t)m_k(t) = 0 \tag{B3}$$

where

$$\mu(t) = \dot{\phi}(t) - \Delta_{k+1}\phi^2(t). \tag{B4}$$

From the properties of $\phi, \mu(t)$ is an even function of t and $\mu(t = 0) = 1$. They are in turn some of the necessary requirements on $\mu(t)$ for (B3) to yield admissible solutions. Equation (B3) has a similar structure to (4a) and (A2). Hence, one can understand how these 'improper' equations can be made to yield admissible solutions by means of an *ansatz*. A comparison of (A2) and (B3) shows that $m_{k+1}(t)$ in (A2) plays the role of $\mu(t)$ in (B3). Hence, if by an *ansatz* it is made to have the required properties of $\mu(t)$, equation (A2) can yield admissible solutions. The two choices, equations (A3) and (A6), are those which belong to this class. Similarly, $Q(t)$ (see equation (4b)) plays the role of $\mu(t)$. TP's *ansatz* (5) or ours (equation (A8)), i.e. $xm_{k+2}/m_k = 2(1 + m_k)$ or 3, endows $Q(t)$ with some of the necessary properties of $\mu(t)$. In these instances, the *ansatz* acts to restore the Hilbert space which had been deformed by the approximation. This is merely fortuitous since such a restoration need not take place.

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