Universality of modal time correlation functions in medium scale

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The universality of modal time correlation functions in the medium-scale

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We investigate the universality of modal time correlation functions by using a closure equation for the normalized dimensionless time correlation function. As a candidate for a new universal function for turbulence we propose a solution to the closure equation in the case of the critical value of the wavenumber, at which the decay form of the time correlation function changes from exponential to oscillatory exponential. The solution is compared with the normalized dimensionless time correlation functions obtained from numerical results for one-dimensional turbulence, such as the Kuramoto-Sivashinsky equation and that obtained from the direct interaction approximation for three-dimensional Navier-Stokes turbulence. As a result of the comparison, we adduce evidence to show that the normalized dimensionless time correlation function is universal in the case of the critical value of the wavenumber.

1. Introduction

Universality is one of the most interesting and important concepts required for understanding chaotic motion such as turbulent flow, and in a broader sense is an idea fundamental to physics in general. Universality implies that large-scale properties are independent of their governing equations, e.g. the dynamic renormalization-group method predicts the dynamic exponent $z = 3/2$ for both the noisy Burgers equation,1,2) which is also called the KPZ equation, and the Kuramoto-Sivashinsky (KS) equation.3,4) This universality is related to the slowly varying motion of large-scale properties; however, we are interested in the non-slowly varying motion of medium-scale properties in the present paper. In other words, the dynamic exponent is related to the exponent of the asymptotic decay form of the total time correlation function as $t \to \infty$,5) while we investigate the universality of the modal time correlation function throughout the entire domain $0 \leq t < \infty$ in the medium-scale, corresponding to the critical value of the wavenumber. Considering an arbitrary physical quantity $u(x,t)$ and its Fourier coefficient $\hat{u}_n(t)$, the total and modal time correlation functions are expressed by

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\langle u(x, t)u(x, 0) \rangle \) and \( \langle \hat{u}_n(t)\hat{u}_n^*(0) \rangle \), respectively, for one-dimensional steady homogeneous turbulence. Here, the asterisk * and the angular brackets \( \langle \cdot \rangle \) denote the complex conjugation and the ensemble average, respectively. It is important to note that we focus on the time correlation functions in the medium-scale, corresponding to the critical value of the wavenumber.

It may seem unlikely that a physical quantity in a non-limiting case such as the medium-scale holds universality. In this sense, this is a unique point of the present paper. To understand the relation between medium-scale quantities and universality, it is important to realize that the functional form of the normalized dimensionless time correlation function in the medium-scale is almost independent of the wavenumber, but qualitatively changes from exponential to oscillatory exponential at the critical value of the wavenumber.

The present paper is organized as follows. In Sec. II, we investigate whether the normalized dimensionless time correlation function for one-dimensional turbulence holds universality by comparing numerical results of the KS equation and also by comparing solutions of a closure equation for the time correlation function. In Sec. III, we propose a functional form of the universal time correlation function, as well as the corresponding power spectrum which is derived from the closure equation and compare them with the numerical results of the KS equation. Conclusions are drawn in Sec. IV.

2. Normalized dimensionless time correlation function \( Q_n(T) \)

2.1 Numerical results for the KS equation

We use the KS equation

\[ u_t + uu_x + u_{xx} + u_{xxxx} = 0 \quad (2.1) \]

to describe typical one-dimensional turbulence. This was originally proposed as a model for instabilities on interfaces and flame fronts\(^6\) and phase turbulence in chemical reactions,\(^7\) employing the periodic boundary condition \( u(x, t) = u(x + L, t) \). In this case the spatial period \( L \) is chosen to be 500, which is sufficiently large for the equation to produce chaotic motion. The KS equation (2.1) is invariant under time-transformations, space-transformations, and parity; hence, its statistical solution is considered to possess the corresponding symmetries.\(^8\)

The Fourier coefficient \( \hat{u}_n(t) \) of \( u(x, t) \) is defined as

\[ \hat{u}_n(t) = \int_0^L u(x, t)e^{-ik_nx}dx, \quad k_n = \frac{2n\pi}{L}. \]

The modal time correlation function \( \tilde{U}_n(t) \) is expressed as

\[ \tilde{U}_n(t) = \langle \hat{u}_n(t)\hat{u}_n^*(0) \rangle. \quad (2.2) \]
Only the modal time correlation function is treated in the present paper, and thus ‘modal’ is dropped from this point forward. A method of numerical calculation for the statistical quantities, such as the time correlation function, is given in detail in previous papers.\(^9,10\)

It is obvious that the functional form of the time correlation function \(\tilde{U}_n(t)\) in (2.2) depends greatly on the wavenumber \(k_n\), and hence we consider the normalized dimensionless time correlation function \(Q_n(T)\), defined as

\[
Q_n(T) = U_n(T \tau_n^{(n)}),
\]

to determine the universal time correlation function. Here the normalized time correlation function \(U_n(t)\) and the integral time scale \(\tau_n^{(n)}\) are defined as

\[
U_n(t) = \frac{\tilde{U}_n(t)}{\tilde{U}_n(0)} \quad \text{and} \quad \tau_n^{(n)} = \int_0^\infty U_n(t)dt.
\]

Figure 1 shows the normalized dimensionless time correlation functions \(Q_n(T)\) for the KS equation in eight cases of \(k_n\). The difference between the four curves for \(1.26 \leq k_n \leq 2.01\) is seemingly almost negligible, which suggests that the normalized dimensionless time correlation function \(Q_n(T)\) can be ‘universal’ for large wavenumbers. We examine \(Q_n(T)\) in detail by using a closure equation and obtain the result that \(Q_n(T)\) does not hold universality in the following subsection.

\[\text{Fig. 1.} \quad \text{Normalized dimensionless time correlation functions for the KS equation in eight cases of } k_n = 2\pi n/L, \; n = 20j, (j = 1, 2, \ldots, 8): \text{dashed line, } 0.25 \leq k_n \leq 1.01; \text{solid line, } 1.26 \leq k_n \leq 2.01.\]
2.2 Analytical and numerical results for a closure equation

Okamura and Mori\textsuperscript{11)} derived a closure equation, called the SA equation,

\[ \frac{dQ_n(T)}{dT} = -\int_0^{T/\tau_n} Q_n(S) Q_n(T - \tilde{\tau}_n S) dS, \quad (2.3) \]

which is the time evolution equation of the normalized dimensionless time correlation function \( Q_n(T) \) for one-dimensional turbulence under four assumptions: statistical steadiness, statistical homogeneity, statistical parity invariance, and ‘similarity’ between the time correlation function \( U_n(t) \) and the memory function \( \Gamma_n(t) \),

\[ U_n\left(T\tau_n^{(n)}\right) = \frac{\Gamma_n\left(T\tau_n^{(n)}\right)}{\Gamma_n(0)}. \]

Here the parameter \( \tilde{\tau}_n \) is defined as

\[ \tilde{\tau}_n = \frac{\tau_n^{(x)}}{\tau_n^{(\mu)}}, \quad 0 \leq \tilde{\tau}_n \leq 1, \]

where the integral time scale \( \tau_n^{(x)} \) is defined as

\[ \tau_n^{(x)} = \frac{1}{\Gamma_n(0)} \int_0^{\infty} \Gamma_n(t) dt. \]

Note that \( \tilde{\tau}_n \) depends on the wavenumber \( k_n \). The initial condition for (2.3) is chosen to be

\[ Q_n(0) = 1, \quad (2.4) \]

which is equivalent to the integral condition

\[ \int_0^{\infty} Q_n(T) dT = 1, \quad (2.5) \]

because the integration of (2.3) over \( T \) from 0 to \( \infty \) yields

\[ Q_n(0) = \left( \int_0^{\infty} Q_n(T) dT \right)^2 \]

under \( Q_n(\infty) = 0 \).

The SA equation (2.3) holds a kind of universality because it is derived considering general one-dimensional turbulence. However, its solution depends on the wavenumber. Figure 2 shows six normalized dimensionless time correlation functions \( Q_n(T) \) obtained numerically from the SA equation (2.3) for \( \tilde{\tau}_n = 0.2 j, \ (j = 0, 1, \ldots, 5) \). At a small value of \( T \) such as \( T = 0.5 \), \( Q_n(T) \) becomes smaller as \( \tilde{\tau}_n \) decreases. The solid curves correspond to the three cases of \( 0.4 \leq \tilde{\tau}_n \leq 0.8 \) and the dashed curves indicate the other three. The SA equation (2.3) has two exact solutions:\textsuperscript{11)}

\[ Q_n(T) = e^{-T} \quad \text{for} \quad \tilde{\tau}_n = 0, \]
and
\[ Q_n(T) = \frac{1}{T} J_1(2T) \quad \text{for} \quad \tilde{\tau}_n = 1, \]
where \( J_1(T) \) is the Bessel function of the first kind. Figure 2 confirms that \( Q_n(T) \) depends significantly on the parameter \( \tilde{\tau}_n \), and hence the normalized dimensionless time correlation function \( Q_n(T) \) does not hold universality.

![Fig. 2. Six normalized dimensionless time correlation functions obtained numerically from the SA equation for \( \tilde{\tau}_n = 0.2j, (j = 0, 1, \ldots, 5) \): dashed line, \( 0 \leq \tilde{\tau}_n \leq 0.2 \) and \( \tilde{\tau}_n = 1 \); solid line, \( 0.4 \leq \tilde{\tau}_n \leq 0.8 \).](image)

We now discuss the reason why \( Q_n(T) \) is likely to be a ‘universal’ function, considering the numerical results of the KS equation in the preceding subsection. Figure 3 shows the dependence of \( \tilde{\tau}_n \) on \( k_n \) for the KS equation. Solid curves in Fig. 1 are the time correlation functions for a parameter region of \( 1.26 \leq k_n \leq 2.01 \), which corresponds to that of \( 0.53 \leq \tilde{\tau}_n \leq 0.62 \), implying the weak dependence of \( \tilde{\tau}_n \) on \( k_n \) for \( 1.26 \leq k_n \leq 2.01 \), while Fig. 2 indicates that the functional form \( Q_n(T) \) is nearly independent of \( \tilde{\tau}_n \) for \( 0.53 \leq \tilde{\tau}_n \leq 0.62 \). Hence, the numerical results of the KS equation suggest that \( Q_n(T) \) is a ‘universal’ function. It is important to note that the dependence of \( \tilde{\tau}_n \) on \( k_n \) shown in Fig. 3 is not correct for \( k_n \leq 0.2 \) because, in numerical simulations, the whole domain \( 0 \leq T \leq T_m \) of \( Q_n(T) \) must be a finite length, such as \( T_m = 40 \), and hence it is impossible to numerically evaluate the integral time scale \( \tau_n^{(a)} \approx 40 \), which corresponds to the case of a small wavenumber. The correct asymptotic behavior is that \( \tilde{\tau}_n \to 0 \) as \( k_n \to 0 \).
3. Universal time correlation function \( Q(T) \)

3.1 One-dimensional turbulence

Figure 2 shows that the time correlation function decays exponentially in the case of small \( \bar{\tau}_n \) but exhibits an oscillatory exponential decay in the case of large \( \bar{\tau}_n \).\(^{11}\) Hence, it is reasoned that the time correlation function exhibits neither exponential nor oscillatory exponential decay for some value of \( \bar{\tau}_n \). This is called the critical value, denoted by \( \bar{\tau}_c \).

First, we seek the time correlation function \( Q_n(T) \) in the case of the critical value \( \bar{\tau}_c \) by solving the SA equation (2.3) analytically. We obtain the following three approximate solutions:

\[
Q(T) = (1 + 2T)e^{-2T} \quad \text{for} \quad \bar{\tau}_c = 0.36, \quad (3.1)
\]
\[
Q(T) = \frac{\beta}{2}(1 + \beta T)e^{-\beta T} \quad \text{for} \quad \bar{\tau}_c = 0.36, \quad (3.2)
\]
\[
Q(T) = (0.92 + 2.5T)e^{-2.1T} + 0.082e^{-7.0T} \quad \text{for} \quad \bar{\tau}_c = 0.38, \quad (3.3)
\]

where \( \beta = 2.05 \) and \( Q(T) \) denotes \( Q_n(T) \) in the case of the corresponding critical value \( \bar{\tau}_c \). The derivation of these solutions is given in the appendix. Three time correlation functions (3.1)–(3.3) are candidates for the universal function and we shall choose one of them as the universal function hereinafter.
Second, we compare the time correlation functions $Q(T)$ in (3.1)–(3.3) obtained analytically with the time correlation function $Q_{SA}(T)$ obtained numerically from the SA equation (2.3). The critical value $\tilde{\tau}_c$ evaluated from the numerical result of the SA equation is approximately 0.38, which is consistent with that in (3.3), but different from those in (3.1) and (3.2) by 5%. Figure 4 shows the differences $\delta Q_1(T)$ between $Q(T)$ in (3.1)–(3.3) and $Q_{SA}(T)$, where

$$\delta Q_1(T) = Q(T) - Q_{SA}(T).$$

The broken line shows that the maximum difference between $Q(T)$ in (3.1) and $Q_{SA}(T)$ is about 0.02, and the total difference $\Delta_1(10)$ is $2.7 \times 10^{-2}$ for $0 \leq T \leq 10$, where

$$\Delta_j(T_m) = \int_0^{T_m} |\delta Q_j(T)| \,dT, \quad j = 1, 2, 3.$$

The dashed-dotted line shows that the maximum difference between $Q(T)$ in (3.2) and $Q_{SA}(T)$ is about 0.025, and the total difference $\Delta_1(10)$ is $1.8 \times 10^{-2}$. This total difference is smaller than that of $2.7 \times 10^{-2}$ for (3.1), but in practice, (3.1) is more useful than (3.2), considering the whole functional form especially when evaluating its value for $T \approx 0$. The solid line shows that the maximum difference between $Q(T)$ in (3.3) and $Q_{SA}(T)$ is much smaller than those in other two cases, and the total difference $\Delta_1(10)$ is $2.5 \times 10^{-3}$. Again, (3.1) is more useful and appropriate to the universal function than (3.3) because of its simplicity. The tiny discrepancy between $Q(T)$ in (3.1) and $Q_{SA}(T)$ shown in Fig. 4 proves that a Padé approximant (A·5) with just a few terms is sufficiently accurate in this case, and hence (3.1) is a simple but fairly reliable solution to the SA equation (2.3) for the critical value $\tilde{\tau}_c$.

Finally, we consider the normalized dimensionless time correlation function $Q_{KS}(T)$ for the KS equation in the case of the critical value $\tilde{\tau}_c$. Figure 5 shows the difference $\delta Q_2(T)$ between $Q_{SA}(T)$ obtained numerically from the SA equation (2.3) and $Q_{KS}(T)$ obtained numerically from the KS equation (2.1) for the critical value $\tilde{\tau}_c = 0.38$, where

$$\delta Q_2(T) = Q_{SA}(T) - Q_{KS}(T).$$

The maximum difference between $Q_{SA}(T)$ and $Q_{KS}(T)$ is about 0.01, and the total difference $\Delta_2(3)$ is $1.3 \times 10^{-2}$. As we can see from Fig. 3, this critical value of $\tilde{\tau}_c = 0.38$ corresponds to $k_n = 0.13$ for the KS equation. Note that the difference $\delta Q_2(T)$ does not approaches zero as $T$ increases.
Fig. 4. Three differences $\delta Q_1(T)$ between $Q(T)$ and $Q_{SA}(T)$: broken line, (3.1); dashed-dotted line, (3.2); solid line, (3.3).

Fig. 5. Difference $\delta Q_2(T)$ between $Q_{SA}(T)$ and $Q_{KS}(T)$.

3.2 Three-dimensional Navier-Stokes turbulence

We now compare the time correlation function for the SA equation in the case of the critical value $\bar{\tau}$ with that of homogeneous isotropic turbulence. The latter is obtained from
the direct interaction approximation (DIA),\textsuperscript{12}) which is consistent with numerical results of the Navier-Stokes equation (e.g. Fig. 1 of Gotoh and Kaneda\textsuperscript{13}) and also reproduces the Kolmogorov energy spectrum. It is important to note that all modal time correlation functions for three-dimensional homogeneous isotropic turbulence are merged into a single function under normalization and non-dimensionality.

Figure 6(a) shows the normalized dimensionless time correlation functions obtained numerically from the DIA in three-dimensional Navier-Stokes turbulence and the SA equation (2.3) in the case of the critical value $\tilde{\tau}_c$. Figure 6(b) shows the difference $\delta Q_3(T)$ between $Q_{\text{DIA}}(T)$ obtained numerically from the DIA equation and $Q_{\text{SA}}(T)$ obtained numerically from the SA equation (2.3), where

$$\delta Q_3(T) = Q_{\text{DIA}}(T) - Q_{\text{SA}}(T).$$

The maximum difference between $Q_{\text{DIA}}(T)$ and $Q_{\text{SA}}(T)$ is about 0.025, and the total difference $\Delta_3(3)$ is $2.9 \times 10^{-2}$. The time correlation function obtained from the SA equation is quite consistent with that from three-dimensional Navier-Stokes turbulence although these are different kinds of turbulence. Hence, the normalized dimensionless time correlation function for the SA equation in the case of the critical value $\tilde{\tau}_c$ is considered to be the universal function for turbulence. Because of the tiny discrepancy between the time correlation functions $Q_{\text{SA}}(T)$ and $Q(T)$ in (3.1) as shown in Fig. 4, it is useful to consider (3.1) as the universal function. Note that the time correlation function (3.1), derived from the general one-dimensional turbulence equation, is consistent with that in three-dimensional Navier-Stokes turbulence. This independence of dimensionality suggests that (3.1) has a fundamental physical nature.

### 3.3 Power spectrum

We consider the power spectrum $I(\Omega)$, which is given by the Wiener-Khintchine theorem\textsuperscript{14})

$$I(\Omega) = \frac{1}{\pi} \int_0^{\infty} Q(T) \cos \Omega T \, dT.$$  

The power spectra corresponding to the universal time correlation functions (3.1) and (3.3) are

$$I(\Omega) = \frac{1}{\pi} \frac{1}{[1 + (\Omega/2)^2]^2}$$

(3.4)

and

$$I(\Omega) = \frac{1}{\pi} \frac{1 + b_n^{(2)} \Omega^2}{(1 + a \Omega^2)^2(1 + \beta \Omega^2)},$$

(3.5)
Fig. 6. (a) Normalized dimensionless time correlation functions $Q_{\text{DIA}}(T)$ obtained from the DIA (solid line) and $Q_{\text{SA}}(T)$ obtained from the SA equation (2.3) (broken line). (b) Difference $\delta Q_3(T)$ between $Q_{\text{DIA}}(T)$ and $Q_{\text{SA}}(T)$.

respectively, where

$$\alpha = 0.220248, \quad \beta = 0.02026252, \quad b_n^{(2)} = -0.00278301.$$  

Figure 7 shows the difference $\delta I(\Omega)$ between $I(\Omega)$ in (3.4) and (3.5) and $I_{\text{KS}}(\Omega)$ obtained
numerically from the KS equation (2.1), where

$$\delta I(\Omega) = I(\Omega) - I_{KS}(\Omega).$$

The solid line shows that the maximum difference between $I(\Omega)$ in (3.4) and $I_{KS}(\Omega)$ is about 0.006, while the broken line shows that the maximum difference between $I(\Omega)$ in (3.5) and $I_{KS}(\Omega)$ is about 0.005. This indicates that (3.5) is slightly better than (3.4), but the former is suitable for the universal power spectrum because of its simplicity. The important thing is, however, that both spectra do not approach zero as $\Omega$ increases, which means that the following asymptotic form obtained from (3.4) and (3.5) is not appropriate:

$$I(\Omega) \rightarrow \Omega^{-4} \text{ as } \Omega \rightarrow \infty.$$ 

Instead, the exponential spectrum $a e^{-b\Omega}$ is consistent with the numerical result for large values of $\Omega$ as indicated in Fig. 7 of Okamura and Mori.\(^{11}\) However, the universal power spectrum (3.4) is more suitable than the exponential spectrum for the entire domain $0 \leq \Omega < \infty$. Note that both (3.4) and (3.5) become Lorentzian for $\Omega \rightarrow 0$.

![Graph showing the differences between $I(\Omega)$ and $I_{KS}(\Omega)$](image)

**Fig. 7.** Two differences $\delta I(\Omega)$ between $I(\Omega)$ and $I_{KS}(\Omega)$: solid line, (3.4); broken line, (3.5).

### 4. Conclusion

We conclude that the normalized dimensionless time correlation function

$$Q(T) = (1 + 2T)e^{-2T}$$

(4.1)
and the corresponding power spectrum

\[ I(\Omega) = \frac{1}{\pi \left[ 1 + (\Omega/2)^2 \right]^2} \]

are universal for one- and three-dimensional turbulence.

This time correlation function is useful for one-dimensional turbulence because the functional form of the normalized dimensionless time correlation function \( Q_n(T) \) is almost independent of the wavenumber especially in the medium-scale; thus, the universal time correlation function (4.1) is satisfied for some range of wavenumber in the medium-scale, and its functional form is simple.

For three-dimensional turbulence, the normalized dimensionless time correlation function derived from the DIA is independent of the wavenumber and is the universal function itself. However, the DIA equation is complicated,\(^{12} \) and hence there is probably no analytic solution, exact or approximate. The universal time correlation function (4.1) is expressed in a simple functional form. Furthermore, the difference between them is tiny as shown in Fig. 6; hence, (4.1) is even useful for evaluating the time correlation function for three-dimensional turbulence.

Appendix: Solutions to the SA equation (2.3)

A.1 Derivation of (3.2)

The Fourier-Laplace transformation of (2.3) yields

\[ \hat{Q}_n(\Omega)\hat{Q}_n(\Omega\tilde{n}) + i\Omega\hat{Q}_n(\Omega) - 1 = 0, \quad (A\cdot1) \]

where

\[ \hat{Q}_n(\Omega) = \int_0^\infty Q_n(T)e^{-\Omega T}dT. \quad (A\cdot2) \]

The initial condition (2.4) corresponds to

\[ \int_0^\infty \Re[\hat{Q}_n(\Omega)]d\Omega = \frac{\pi}{2}, \quad (A\cdot3) \]

while the integral condition (2.5) corresponds to

\[ \hat{Q}_n(0) = 1. \quad (A\cdot4) \]

Similarly to the relation between (2.4) and (2.5), (A·3) is equivalent to (A·4). We now assume that the solution to (A·1) under (A·4) has the form of a Padé approximant as follows:\(^{11,15} \)

\[ \hat{Q}_n(\Omega) = \frac{1}{1 + a_n(2)\Omega^2 + a_n(4)\Omega^4} + i\frac{b_n^{(1)}\Omega}{1 + c_n(2)\Omega^2 + c_n(4)\Omega^4}, \quad (A\cdot5) \]
It is important to note that (A·5) is different from (15) in the previous paper. The previous paper treats the limiting case of \( \Omega \to 0 \) (or \( T \to \infty \)), while the present paper considers the whole domain \( 0 \leq \Omega < \infty \) and thus \( \hat{Q}_n(\Omega) \) must satisfy the relation
\[
|\hat{Q}_n(\Omega)| = o\left(\frac{1}{\Omega^2}\right) \quad \text{for} \quad \Omega \to \infty
\]
to guarantee the condition
\[
\frac{dQ_n(T)}{dT} = 0 \quad \text{for} \quad T = 0.
\]
Substituting (A·5) into (A·1) and expanding the result as a power series to fifth order at \( \Omega = 0 \), we obtain the coefficients as functions of \( \tilde{\tau}_n \):
\[
da_n^{(2)} = \frac{1}{(\tilde{\tau}_n + 1)^2 (\tilde{\tau}_n^2 + 1)}, \tag{A·6}
\]
\[
da_n^{(4)} = \frac{\tilde{\tau}_n^2 (\tilde{\tau}_n^2 + \tilde{\tau}_n + 1)}{(\tilde{\tau}_n + 1)^4 (\tilde{\tau}_n^2 + 1)^2 (\tilde{\tau}_n^4 - \tilde{\tau}_n + 1)(\tilde{\tau}_n^4 + 1)}, \tag{A·7}
\]
\[
b_n^{(1)} = -\frac{1}{\tilde{\tau}_n + 1},
\]
\[
c_n^{(2)} = \frac{1 - \tilde{\tau}_n}{\tilde{\tau}_n^6 + \tilde{\tau}_n^5 + \tilde{\tau}_n^4 + 2\tilde{\tau}_n^3 + \tilde{\tau}_n^2 + \tilde{\tau}_n + 1},
\]
\[
c_n^{(4)} = \frac{\tilde{\tau}_n^3 (\tilde{\tau}_n^8 - 2\tilde{\tau}_n^7 + \tilde{\tau}_n^6 + \tilde{\tau}_n^4 + \tilde{\tau}_n^4 - \tilde{\tau}_n^2 + 1)}{D_n},
\]
where
\[
D_n = (\tilde{\tau}_n + 1)^4 (\tilde{\tau}_n^2 + 1)^2 (\tilde{\tau}_n^4 - \tilde{\tau}_n + 1)(\tilde{\tau}_n^4 + 1)
\]
\times \left(\tilde{\tau}_n^4 - \tilde{\tau}_n^3 + \tilde{\tau}_n^2 - \tilde{\tau}_n + 1\right).
\]
Using (A·5) and the inverse transform of (A·2), we obtain the time correlation function
\[
Q_n(T) = \frac{2}{\pi} \int_0^\infty \frac{1}{1 + a_n^{(2)}\Omega^2 + a_n^{(4)}\Omega^4} \cos(\Omega T) d\Omega. \tag{A·8}
\]
The time correlation functions \( Q_n(T) \) exhibit exponential decay for small values of \( \tilde{\tau}_n \) and oscillatory exponential decay for large values. We expect the critical time correlation function to occur at the transition between these decay types. The condition is that \( 1 + a_n^{(2)} x + a_n^{(4)} x^2 = 0 \) has a double root, that is
\[
\left(a_n^{(2)}\right)^2 - 4a_n^{(4)} = 0, \tag{A·9}
\]
where \( a_n^{(2)} \) and \( a_n^{(4)} \) are given in (A·6) and (A·7). The condition (A·9) yields the critical value
\[
\tilde{\tau}_c \approx 0.361931.
\]
We can thus evaluate the integral (A·8) with the residue theorem in the case of the critical value as follows:

\[
Q(T) = \frac{\beta}{2}(1 + \beta T)e^{-\beta T} \quad \text{for} \quad \beta \approx 2.04833,
\]

(A·10)

where \(Q(T)\) denotes \(Q_n(T)\) in the case of the critical value \(\tilde{c}\).

It is important to note that (A·10) does not satisfy the initial condition (2.4) but the integral condition (2.5), because

\[
Q(0) = 1.02417 > 1,
\]

(A·11)

indicating that \(Q(0)\) is larger than 1 by 2%.

A.2 Derivation of (3.1)

We modify (A·10) slightly into

\[
Q(T) = (1 + 2T)e^{-2T} \quad \text{for} \quad \tilde{c} \approx 0.361931,
\]

in order to satisfy both the initial condition (2.4) and the integral condition (2.5).

A.3 Derivation of (3.3)

We seek a higher order solution \(Q(T)\) to reduce the deviation of \(Q(0)\) from 1 in (A·11) and assume that the solution to (A·1) under (A·4) has the form of a Padé approximant

\[
\hat{Q}_n(\Omega) = \frac{1 + b_n^{(2)} \Omega^2}{1 + a_n^{(2)} \Omega^2 + a_n^{(4)} \Omega^4 + a_n^{(6)} \Omega^6} + i \frac{b_n^{(1)} \Omega + b_n^{(3)} \Omega^3}{1 + c_n^{(2)} \Omega^2 + c_n^{(4)} \Omega^4 + c_n^{(6)} \Omega^6}.
\]

(A·12)

Substituting (A·12) into (A·1) and expanding the result as a power series to ninth order at \(\Omega = 0\), we obtain the coefficients as functions of \(\tilde{c}_n\), the concrete functional forms of which are omitted due to their complexity. Using (A·12) and the inverse transform of (A·2), we obtain the time correlation function

\[
Q_n(T) = \frac{2}{\pi} \int_0^\infty \frac{1 + b_n^{(2)} \Omega^2}{1 + a_n^{(2)} \Omega^2 + a_n^{(4)} \Omega^4 + a_n^{(6)} \Omega^6} \cos(\Omega T)d\Omega.
\]

(A·13)

Now we seek the critical solution between the exponential decay forms with and without oscillation. The condition is that \(1 + a_n^{(2)} x + a_n^{(4)} x^2 + a_n^{(6)} x^3 = 0\) has a double root, that is

\[
4A_n^3 + 27B_n^2 = 0,
\]

(A·14)

where

\[
A_n = \frac{a_n^{(2)}}{a_n^{(6)}} - \frac{(a_n^{(4)})^2}{3(a_n^{(6)})^2}, \quad B_n = \frac{2(a_n^{(4)})^3}{27(a_n^{(6)})^3} - \frac{a_n^{(2)} a_n^{(4)}}{3(a_n^{(6)})^2} + \frac{1}{a_n^{(6)}}.
\]
The condition (A·14) yields the critical value

$$\tilde{\tau}_c \approx 0.375178.$$ 

We can thus evaluate the integral (A·13) with the residue theorem in the case of the critical value as follows:

$$Q(T) = (0.917752 + 2.53177T)e^{-2.1308T} + 0.082032e^{-7.0251T},$$

indicating that

$$Q(0) = 0.999775 < 1$$

and that $Q(0)$ is smaller than 1 by only 0.02%. 

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References


