Convergents to Infinite Series in Turbulence Theory*

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Padé approximants to the irreducible diagram expansions are proposed as a possible source of convergent sequences of approximations to turbulence correlation functions. The approximants are used to close off infinite-series integral equations, which then must be solved for the correlation functions. Alternatively, they are applied to an explicit expansion about the direct-interaction, or random-coupling, approximation. Good results are obtained for an exactly soluble test problem, the random oscillator, which has served to exhibit inadequacies of some previous approximation schemes for turbulence.

1. INTRODUCTION

The Navier-Stokes equation leads to an expansion of the correlation functions of a turbulent velocity field about the zeroth-order values which represent linear, viscous decay. The effective expansion parameter is a characteristic Reynolds number. If the velocity field has an initial multivariate-Gaussian distribution, or is maintained by Gaussian driving forces, the coefficients of each power of Reynolds number are functionals of the zeroth-order covariance and response tensors of the velocity field. The convergence properties of the Reynolds number expansion are not established, but the radius of convergence is probably zero.[1] An important feature of the turbulence problem is that large Reynolds numbers are common, and infinite Reynolds number is a physically interesting limit.

The dynamical equations for correlation functions of a turbulent velocity field are formally similar to those of some nonlinear quantized fields, the Reynolds number expansion corresponding to expansion in powers of the coupling constant. There are analogous diagram representations, and the power series in the turbulence problem can be partially summed, to all orders, so that only irreducible diagrams and the exact, rather than zeroth-order, correlation and response functions appear in the coefficients.[2,3] The irreducible expansions appear still to be divergent.[1]

The problem of obtaining sequences of systematically better approximation sequences for the correlation functions is unsolved, and care is required even to obtain a first approximation, above the linear level, which remains internally consistent at large Reynolds numbers. Reference 2 deals with a set of closed integral equations, the direct-interaction approximation, which involve only the covariance and mean-response tensors, and retain only all iterated bubble diagrams. These equations are exact to second order in Reynolds number, and remain internally consistent at all Reynolds numbers because they happen to describe exactly a model dynamical system, called the random-coupling model. The model representation assures energy conservation, realizability of the covariance tensor, and other consistency properties. The author has since tried unsuccessfully to construct an explicit sequence of higher model systems, each expressible by closed integral equations, whose dynamics would systematically draw closer to the exact dynamics.

The present paper proposes Padé approximants to the irreducible expansions as a possible road to convergent approximation sequences for turbulence correlations. Padé approximants have been studied extensively and applied to a number of problems of statistical physics.[4,5] In physical applications, the quantity of interest typically is expanded in a power series in a perturbation parameter, and approximations to the power series are selected from the associated Padé table. The latter is an array of rational functions whose power-series expansions reproduce the series of interest, up to finite orders.

The straightforward extension to turbulence theory is to construct Padé approximants to the Reynolds number expansion. The analysis, to follow, of an exactly soluble test problem suggests that this fails at high Reynolds numbers. Instead, the present paper introduces Padé approximants to the irreducible diagram expansion and uses them to form sequences of approximate integral equations, which then must be solved for the correlation and response functions. The lowest integral equation in the sequence is the direct-interaction approximation. This procedure is found to work for the test problem, and thereby distinguishes itself from other systematic approximation schemes that have been proposed for turbulence. However, no theory of convergence properties is attempted, and so far, only a little of what happens with actual turbulence problems is known.

2. RANDOM OSCILLATOR

Let $y(t)$ obey

$$(d/dt+\nu)y(t)=-ia\lambda y(t), \quad y(0)=1, \tag{1}$$

where ν is a non-negative damping parameter, a is a constant which has a Gaussian distribution over an ensemble, with $\langle a^2\rangle=1$, and λ is an ordering parameter, to be set equal to 1 after the manipulations are finished. This random oscillator has been studied extensively, and it serves to display inadequacies of several schemes for obtaining approximation sequences for turbulence.[2] Equation (1) leads to primitive and irreducible diagram expansions homologous to those of turbulent convection by a prescribed Gaussian velocity field, and of quantum-mechanical scattering in a random potential field.[2] Although (1) is linear in the dynamical variable, like convection in a prescribed field, it

is nonlinear in stochastic quantities, and this is sufficient to bring out some essential difficulties also present in the full, nonlinear turbulence problem.

Consider the mean response function $g(t) = \langle y(t) \rangle$. The exact solution is $g(t) = \exp(-\nu t - \lambda^2 t^2/2)$. The perturbation or reducible expansion for $g(t)$ in powers of λ can be expressed in the form

$$(d/dt + \nu)g(t) = h(t) \equiv -\langle ia\lambda y(t) \rangle, \tag{2}$$

$$h(t) = \sum_{n=1}^{\infty} (-1)^n R_{2n} \lambda^{2n} q(*q)^{2n-1}, \tag{3}$$

where $q(t) = \exp(-\nu t)$ is the response function for $\lambda = 0$, $*$ denotes convolution, and $R_{2n} = \langle a^{2n} \rangle = 2n!/n!2^n$ is the number of diagrams with $2n$ vertices in an associated graphical representation. Equation (3) can be reformed as an irreducible expansion

$$h(t) = \sum_{n=1}^{\infty} (-1)^n \lambda^{2n} S_{2n} g(*g)^{2n-1}, \tag{4}$$

where S_{2n} is the number of diagrams without self-energy parts.[2] Equations (2) and (4) give an infinite-series integral equation, from which (without appeal to diagrams) S_{2n} can be found by recursion in terms of the S_{2m} for $m < n$ and the R_{2m} for $m \leq n$. The first few S_{2n} are 1, 1, 4, 27, 248, 2830, 382 32, and 593 859.

The Laplace transforms of (2)–(4) are

$$(p + \nu)G(p) = 1 + H(p), \tag{5}$$

$$H(p) = \sum_{n=1}^{\infty} (-1)^n \lambda^{2n} R_{2n} [\gamma(p)]^{2n}, \tag{6}$$

$$H(p) = \sum_{n=1}^{\infty} (-1)^n \lambda^{2n} S_{2n} [G(p)]^{2n}, \tag{7}$$

where $\gamma = (p + \nu)^{-1}$. Both (6) and (7) are divergent series for any values of λ, γ, and G, and hence they give divergent infinite-series equations for $G(p)$ when used in (5). In particular, this is true for the response time $G(0) = \int_0^\infty g(t)dt$, which is the simplest integral parameter of the system. Nonconvergence of (6) follows immediately from the formula for R_{2n}. The ratios S_{2n}/R_{2n} are 1, 0.3333, 0.2667, 0.2571, 0.2624, 0.2723, 0.2830, 0.2930, ... This suggests that S_{2n}/R_{2n} approaches a nonzero value ≤ 1 as $n \to \infty$, a conclusion also indicated by the topology of the diagram expansion.[1]

The divergence of (6) also can be inferred from the integral representation

$$G(p) = \gamma(p) + \sum_{n=1}^{\infty} (-1)^n \lambda^{2n} R_{2n} [\gamma(p)]^{2n+1}, \tag{8}$$

$$= \int_{-\infty}^{\infty} [P(a)/(\nu + p + ia\lambda)]\, da, \tag{9}$$

where $P(a) = (2\pi)^{-1/2} \exp(-a^2/2)$ is the probability distribution of a. Equation (9) follows directly from the Laplace transform of (1). For given ν and p, there is a continuous distribution of poles along the line $\lambda = i(\nu + p)/a$ $(-\infty \leq a \leq \infty)$ in the complex λ plane, and, consequently, zero radius of convergence in λ.

3. PADÉ APPROXIMANTS TO THE PERTURBATION SERIES

The Padé approximants (r, s) to a power series

$$f = \sum_{n=0}^{\infty} a_n (\lambda^2)^n$$

are[4,5]

$$f_{r,s} = \sum_{m=0}^{s} b_m \lambda^{2m} \Big/ \Big(\sum_{n=0}^{r} c_n \lambda^{2n} \Big), \quad c_0 = 1, \tag{10}$$

where the b's and c's are chosen to reproduce the series through terms in $(\lambda^2)^{r+s}$. If f has a representation of the type (9), a Padé approximant replaces the continuous distribution of poles by a finite set of discrete poles in such fashion that suitably defined moments of the distribution are correct up to some finite order. The conditions under which the Padé approximants converge to f as r and s increase are known only in special cases.[4,5]

There is an intimate relation between Padé approximants and continued fractions.[4] If the explicit values of the R_{2n} are used, (8) has the continued-fraction representation

$$G(p) = \cfrac{\gamma}{1} + \cfrac{\lambda^2\gamma^2}{1} + \cfrac{2\lambda^2\gamma^2}{1} + \cfrac{3\lambda^2\gamma^2}{1} + \cfrac{4\lambda^2\gamma^2}{1} + \cdots, \tag{11}$$

where γ denotes $\gamma(p)$. The Padé approximants (r, r) and $(r+1, r)$, $r = 0, 1, 2, \ldots$, are, respectively, the even and odd approximants of the continued fraction

$$G_{0,0} = \gamma, \quad G_{1,0} = \gamma/(1 + \lambda^2\gamma^2),$$

$$G_{1,1} = \gamma/[1 + \lambda^2\gamma^2/(1 + 2\lambda^2\gamma^2)] = \gamma(1 + 2\lambda^2\gamma^2)/(1 + 3\lambda^2\gamma^2),$$

$$G_{2,1} = \gamma(1 + 5\lambda^2\gamma^2)/(1 + 6\lambda^2\gamma^2 + 3\lambda^4\gamma^4), \ldots . \tag{12}$$

Equation (11) is a special case of Gauss's continued fraction, whose convergence properties are known.[4] The Padé sequences (r, r) and $(r+1, r)$ converge to the exact $G(p)$, as $r \to \infty$, for all $\lambda\gamma$ except $\lambda\gamma$ pure imaginary. Suppose that the approximants are used to evaluate the spectral density $\rho(\omega) = \mathrm{Re}\, G(-i\omega)$, ω real. If $\nu > 0$, the approximants obtained by taking the real part of (12) converge for all ω. But, for fixed ν, the convergence becomes worse as ω increases, and, for $\nu = 0$, there is divergence at all ω. In the latter case, the exact $\rho(\omega)$ is $(\pi/2)^{1/2}\lambda^{-1}\exp(-\omega^2/2\lambda^2)$. For $\omega = 0$, we have $\gamma = \nu^{-1}$, and, as $\nu \to 0$, all the even and odd approximants tend to zero and ∞, respectively. Thus the Padé approximants to the perturbation expansion fail to yield convergents to $G(0)$ in the limit $\nu \to 0$, which is analogous to the high-Reynolds-number limit in turbulence dynamics.

Although the approximants do not converge at any ω, if $\nu = 0$, manipulation of (12) shows that they constitute approximations for $\rho(\omega)$ in the form of finite sums of δ functions, such that the moments $\int_{-\infty}^{\infty} \omega^{2q} \rho(\omega) d\omega$ are correct for $q \leq r + s$. Thus

$$\rho_{0,0}(\omega)=\pi\delta(\omega),\quad \rho_{1,0}(\omega)=\tfrac{1}{2}\pi[\delta(\omega-\lambda)+\delta(\omega+\lambda)],$$
$$\rho_{1,1}(\omega)=\tfrac{2}{3}\pi\delta(\omega)+\tfrac{1}{6}\pi[\delta(\omega-\lambda\sqrt{3})+\delta(\omega+\lambda\sqrt{3})],\ \ldots . \tag{13}$$

These approximations to $\rho(\omega)$ are identical with the cumulant-discard approximations (truncations of the expansion in cumulants) discussed in Ref. 2.

4. PADÉ APPROXIMATIONS TO THE IRREDUCIBLE EXPANSIONS

Equation (7) defines a functional dependence of H on λ and G which is invariant either to change in the value of ν or to replacement of ν by a complex function $\nu(p)$. Since these changes do alter the value of G, we argue that the functional relation $H=H[\lambda,G]$ is a more fundamental characterization of the stochastic dynamical coupling $-ia\lambda y(t)$ than is the explicit expansion (6) of H in powers of λ. Therefore, we consider Pade approximations to $H[\lambda,G]$, with G regarded temporarily as an independent quantity rather than a function of λ.

On this basis, (7) has the continued fraction representation

$$H[\lambda,G(p)]=-\lambda^2F[\lambda,G(p)],$$
$$F[\lambda,G]=\frac{G^2\,|}{|\,1}+\frac{\lambda^2G^2\,|}{|\,1}+\frac{3\lambda^2G^2\,|}{|\,1}+\frac{11\lambda^2G^2/3\,|}{|\,1}+\frac{167\lambda^2G^2/33\,|}{|\,1}+\cdots, \tag{14}$$

where the numerical values of the S_{2n} have been used. The approximants of the continued fraction are the Padé approximants of (7):

$$F_{0,0}=G^2,\quad F_{1,0}=G^2/(1+\lambda^2G^2),$$
$$F_{1,1}=G^2(1+3\lambda^2G^2)/(1+4\lambda^2G^2),$$
$$F_{2,1}=G^2(3+20\lambda^2G^2)/(3+23\lambda^2G^2+11\lambda^4G^4),\ldots . \tag{15}$$

Again consider the case $\nu=0$, $p=0,\lambda=1$, for which Pade approximation to the perturbation expansion failed. The exact $G(0)$ is $(\pi/2)^{1/2}$, and, from (5), $H(0)=1$. If this value of $G(0)$ is used in (15), the successive approximants are $F_{0,0}=1.57080$, $F_{1,0}=0.61102$, $F_{1,1}=1.23202$, $F_{2,1}=0.81576$, $F_{2,2}=1.11706$, $F_{3,2}=0.90216$, $F_{3,3}=1.06560$, ..., which suggests that there is convergence to the correct value $F=1$. To make clearer the contrast to the perturbation expansion, (6) can be written as a continued fraction like (14):

$$-\lambda^{-2}H=\frac{\gamma^2|}{|\,1}+\frac{3\lambda^2\gamma^2\,|}{|\,1}+\frac{2\lambda^2\gamma^2\,|}{|\,1}+\frac{5\lambda^2\gamma^2\,|}{|\,1}+\frac{4\lambda^2\gamma^2\,|}{|\,1}+\cdots, \tag{16}$$

The essential difference between (14) and (16) is not in the numerical coefficients but rather that $\gamma=\infty$ in (16) while G is finite in (14), for $p=0$, $\nu=0$.

In order to offer promise in problems where the answer is not known in advance, the Padé approximants must lead to convergents to G itself. To obtain approximants to G, we substitute the successive functional forms (15) into (5) and solve the resulting equations. The values found for $G(0)$ at $\lambda=1,\nu=0$ are $G_{0,0}=1$, $G_{1,0}=\infty$, $G_{1,1}=1.12417$, $G_{2,1}=1.53729$, $G_{2,2}=1.17963$, $G_{3,2}=1.36237$, and $G_{3,3}=1.20876$. These numbers suggest that there is convergence to the exact value $G(0)=1.25331$ and that the (r,r) and $(r+1,r)$ sequences bound the correct answer from below and above, respectively.

The behavior for $p\neq 0$, $\nu=0$, $\lambda=1$ is more complicated. The (0,0) approximation yields $pG(p)=1-[G(p)]^2$, which is identical with the random-coupling, or direct-interaction, equation.[2] The corresponding spectral density is $\rho_{0,0}(\omega)=(1-\omega^2/4)^{1/2}$ $(\omega^2\leq 4)$, $=0$ $(\omega^2>4)$. For $r>0$, the (r,r) sequence yields solutions $G_{r,r}(-i\omega)$ with finite sets of branch points along the real ω axis, so that $\rho_{r,r}(\omega)$ consists of pass bands separated by stop bands. The moments $\int_{-\infty}^{\infty}\omega^{2q}\rho(\omega)d\omega$ are given correctly for $q\leq r+s$. Figure 1 shows $\rho_{r,r}(\omega)$ for $r=0,1$, and 3, together with the exact $\rho(\omega)$. The present Pade approximations differ importantly from the perturbation-series approximations in that the δ functions of (13) are replaced by pass bands of finite width and height. We conjecture that, as $r\to\infty$, the primary band spreads to include any given ω and that $\rho_{r,r}(\omega)$ within that band converges to $\rho(\omega)$. The $(r+1,r)$ sequence has been studied through (3,2). It appears to be similar to the (r,r) sequence except that the (1,0) approximant has an integrable singularity $\rho_{1,0}(\omega)\propto|\omega|^{-1/3}$ at $\omega=0$.

The solutions $G_{r,s}(-i\omega)$ were obtained by the Newton-Raphson method, starting at $\omega=0$ and using the converged value at each ω step as the starting value for the next step. The solutions were continued through the branch points by requiring $\rho(\omega)\geq 0$ and $G(-i\omega)$ continuous. The solutions were checked by verifying the integral relation $\int_{-\infty}^{\infty}\rho(\omega)d\omega=\pi$.

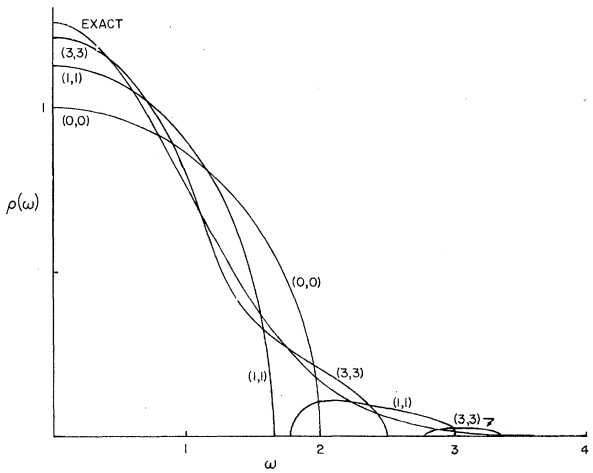

FIG. 1. Spectral density $\rho(\omega)$ from internal Padé approximations (0, 0), (1, 1), and (3, 3), compared with exact $\rho(\omega)$.

The irreducible expansion (7) can be further consolidated by introducing a vertex operator. The most compact expression of the vertex expansion is

$$H(p) = -\lambda^2 G(p)\Gamma(p), \tag{17}$$

$$\Gamma(p) = G(p) + \sum_{n=2}^{\infty} (-\lambda^2)^{n-1} V_{2n}[\Gamma(p)]^{2n-1}, \tag{18}$$

where the vertex operator is $\Gamma(p)/G(p)$, and V_{2n}, which can be found by recursion from the S_{2n}, is the number of diagrams with $2n$ vertices and without vertex parts. The first three V_{2n} are 1, 1, and 7. In analogy to what was done above with (7), we have also constructed Padé approximants to (18), regarding the latter as defining a functional relation between $G(p)$ and $\Gamma(p)$. The first two members, (0, 1) and (1, 2), of the $(r, r+1)$ sequence of such approximants are

$$\Gamma = G - \lambda^2\Gamma^3, \quad \Gamma = G - \lambda^2\Gamma^3 + \lambda^4\Gamma^5/(1 + 7\lambda^2\Gamma^2). \tag{19}$$

Each corresponding approximation to $G(p)$ is obtained by eliminating H and Γ from (5), (17), and the appropriate equation of (19). The $(r, r+1)$ approximations exhibit a band structure like that in Fig. 1, but they yield much more accurate values of $\rho(\omega)$. The error $\delta_{r,s}(\omega) = \rho_{r,s}(\omega) - \rho(\omega)$ for (0, 1) and (1, 2) is shown in Fig. 2. The (0, 1) approximation has been discussed before, in a different context.[2]

5. MODIFIED EXPLICIT λ EXPANSION

In Sec. 4, Padé approximants were used within the infinite-series equation formed by substituting (7) into (5). In this procedure, which shall be called the internal approximation scheme, the dependence of G on λ is ignored in constructing the Padé approximants and appears only upon solving the final approximation to (5). The irreducible expansion can also be used to obtain a new, fully explicit expansion of G in powers of an ordering parameter λ, where now $\lambda = 0$ corresponds to the random-coupling equation $(p+\nu)G(p) = 1 - [G(p)]^2$ rather than the unperturbed equation $(p+\nu)G(p) = 1$.

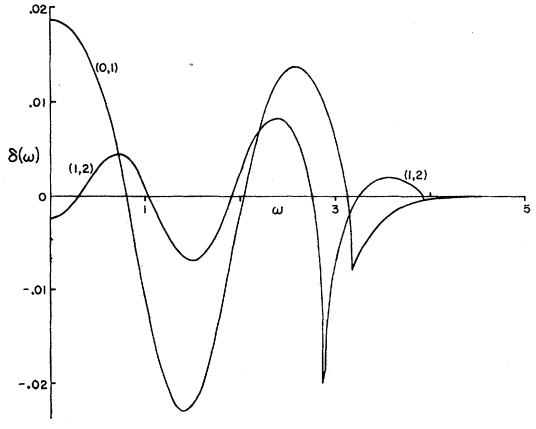

FIG. 2. Error $\delta_{r,s}(\omega) = \rho_{r,s}(\omega) - \rho(\omega)$ in the internal Padé approximations formed from the vertex expansion.

For this purpose, we consider

$$(p+\nu)G(p) = 1 + \lambda^{-2}H[\lambda, G]$$
$$= 1 - [G(p)]^2 + \sum_{n=2}^{\infty} (-1)^n \lambda^{2n-2} S_{2n}[G(p)]^{2n}, \tag{20}$$

instead of (5) and (7). Here λ is no longer interpretable as the coupling-strength parameter in an underlying amplitude equation (1) for individual realizations. Instead, it is a formal ordering parameter, which defines a weighting of the diagrams omitted in the random-coupling model. For $\lambda = 1$, (20) is identical with (5) and (7). Now we write

$$G(p) = \sum_{n=0}^{\infty} \lambda^{2n} G_n(p), \tag{21}$$

substitute into (20), collect like powers of λ, and obtain

$$(p+\nu)G_0 = 1 - S_2 G_0^2, \quad (p+\nu+2S_2G_0)G_1 = S_4 G_0^4,$$
$$(p+\nu+2S_2G_0)G_2 + S_2G_1^2 = 4S_4G_0^3G_1 - S_6G_0^6, \ldots \tag{22}$$

The random-coupling solution G_0 satisfies a nonlinear equation. Each higher G_n satisfies an equation linear in G_n, and is found to be the ratio of two polynomials in G_0.

For $\nu = 0$, (21) and (22) give for $I = G(0)$ the series

$$I = 1 + \tfrac{1}{2}\lambda^2 - \tfrac{9}{8}\lambda^4 + \tfrac{105}{16}\lambda^6 - \tfrac{7413}{128}\lambda^8 + \tfrac{169\,047}{256}\lambda^{10} - \cdots,$$

whose terms are finite, in contrast to the perturbation series for I.

Padé approximants to (21) can be set up in analogy to those for the perturbation expansion (8). For $\lambda = 1$, the (r, r) and $(r, r+1)$ approximants to I are $I_{0,0} = 1$, $I_{1,1} = 1.153\,85$, $I_{2,2} = 1.205\,86$, ..., $I_{0,1} = 1.5$, $I_{1,2} = 1.33537$, $I_{2,3} = 1.28885$, ... These two sequences appear to bound the exact value $I = 1.253\,31$ and to converge. If I is now written as

$$I = I_{0,0} + (I_{0,1} - I_{0,0}) + (I_{1,1} - I_{0,1}) + \cdots$$
$$= 1 + 0.5 - 0.346\,15 + 0.181\,52$$
$$- 0.129\,51 + 0.082\,99 - \cdots,$$

extrapolation of the latter series, by weighting with powers of an ordering parameter and taking the Padé (2, 3) approximation to the six terms shown, gives $I = 1.255\,55$, which is less than 0.2% in error.

The Padé approximants to (21), which shall be called external Padé approximants, appear to give faster convergence to I than the internal approximants of Sec. 4. However, the performance deteriorates for $p \neq 0$. The real parts of the present approximants to $G(-i\omega)$ are continuous within the range $\omega^2 \leq 4$, where the random-coupling $\rho(\omega)$ is nonzero. But for $\omega^2 > 4$, there are poles on the real ω axis, as with the Padé approximants to the original perturbation series (8).

The external Padé approximants provide an algorithm, with unknown domain of validity, for constructing direct approximations to $\int_0^\infty g(t)dt$ for any function $g(t)$ defined by a power series in t. The power series can be weighted by λ and converted to a convolution series like (2) and (4), with the S_{2n} determined by recursion from the given coefficients. Then Padè approximants to I can be constructed as above. In the present example, $g(t)$ is regular everywhere, but the algorithm works also for some examples where $g(t)$ has an essential singularity at $t=0$.

6. FORMULATION FOR TURBULENCE AND TURBULENT CONVECTION

Let the incompressible Navier-Stokes equation be written as

$$(\partial/\partial t - \nu\nabla^2)\vec{u}(\vec{x},t) = -\lambda[\vec{u}(\vec{x},t)\cdot\vec{\nabla}]\vec{u}(\vec{x},t) - \vec{\nabla}p,$$
$$\vec{\nabla}\cdot\vec{u} = 0 \qquad (23)$$

where λ, as before, is an ordering parameter, with $\lambda = 1$ at the end of the analysis. After elimination of the pressure by $\vec{\nabla}\cdot\vec{u} = 0$, $\vec{u}(\vec{x},t)$ can be expanded in powers of λ, and a suitable nondimensionalization shows that this is equivalent to expansion in powers of a characteristic Reynolds number.[1] The Reynolds number expansion can be regrouped to yield irreducible infinite-series integral equations for the covariance tensor and for the tensor that gives the ensemble-averaged response of the velocity field to infinitesimal disturbances. For isotropic turbulence, the equations corresponding to (2) and (3) are[2]

$$(\partial/\partial t + \nu k^2)G(k;t,t') = H(k;t,t'),$$
$$G(k;t',t') = 1,$$
$$H(k;t,t') = \sum_{n=1}^{\infty}\lambda^{2n}\zeta_{2n}(k;t,t'), \qquad (24)$$
$$(\partial/\partial t + \nu k^2)U(k;t,t') = S(k;t,t'),$$
$$S(k;t,t') = \sum_{n=1}^{\infty}\lambda^{2n}\xi_{2n}(k;t,t'). \qquad (25)$$

Here k is the wave number, G and U are the Fourier transforms of the defining scalars of the Green's tensor and covariance tensor, respectively, S is the Fourier transform of a triple correlation, and ζ_{2n} and ξ_{2n} are polynomial functionals of G and U. Each term in ζ_{2n} contains $2n$ factors G and n factors U, with $2n-1$ integrations over intermediate wave vector space-times, while each term in ξ_{2n} contains $2n-1$ factors G and $n+1$ factors U. The quantities H and S may also be written as vertex expansions in (complicated) analogy to (17) and (18).[1]

In a similar way, the equation

$$(\partial/\partial t - \kappa\nabla^2)\psi(x,t) = -\lambda\vec{u}(\vec{x},t)\cdot\vec{\nabla}\psi(x,t) \qquad (26)$$

for the convection of a passive scalar field ψ (of molecular diffusivity κ) by a prescribed, isotropic, multivariate-Gaussian, incompressible, velocity field leads to the irreducible expansion

$$(\partial/\partial t + \kappa k^2)G_S(k;t,t') = H_S(k;t,t'),$$
$$G_S(k;t',t') = 1,$$
$$H_S(k;t,t') = \sum_{n=1}^{\infty}\lambda^{2n}\theta_{2n}(k;t,t'). \qquad (27)$$

Here $G_S(k;t,t')$ is the Fourier transform of the average Green's function of the scalar field.[2] For $\kappa = 0$, this Green's function gives the probability density of turbulent dispersion of fluid particles from $(\vec{x}',t')$ to $(\vec{x},t)$. Each term in the polynomial functional θ_{2n} contains $2n$ factors G_S and n factors U, which is again the Fourier transform of the defining scalar of the velocity-field covariance.

Both internal and external sequences of Padé approximations to the irreducible expansions can be formed by following the example of the random oscillator, treating the series in λ^2 on the right-hand sides of (24), (25), and (27) in analogy to the series in (7). There are problems of nonuniqueness because the Padé approximants are obtained by nonlinear operations on the expansions. These problems are present already in the random oscillator example, but in the turbulence case they are linked with energy conservation and other consistency properties and thereby become very important.

The development of H and S into irreducible expansions commutes with any linear change of basis, such as the transformation from physical space $(\vec{x},t)$ to Fourier space $(\vec{k},\omega)$. This follows immediately from the characterization of the irreducible expansions in terms of collective coordinates of a collection of systems.[2] It follows that (20), and the modified explicit expansion (21) are invariant to such a change of basis. However, the Padé approximants, whether on the primitive perturbation expansion, the irreducible expansion, or the modified λ expansion, are nonlinear transformations of the series. In general, a given order of Padé approximant (r,s) gives different results when carried out in different bases, even if the sequence of approximants converges to the correct result in each basis. If the Padé approximants for the random oscillator are constructed from the time-domain expansion (2) and (3) or (2) and (4), the Laplace transforms of the results are not the same as the Padé approximants found above by working directly in the p domain. This raises the question of to what extent convergence properties in different representation are similar, and, as a matter of practical computation, which represenatations give the most satisfactory results in the lowest orders.

Each order of the irreducible expansion (25) identically satisfies conservation of kinetic energy by the nonlinear interaction: $\int\xi_{2n}(k,t,t)d^3k = 0$. This is a prime reason for giving the expansion of the triple moment S a central role rather than attempting to work directly with the expansion for U. Also, each order is individually consistent with the fluctuation-relaxation relation $U(k,t,t') = CG(k;t,t')$, $t \geq t'$, with C a constant of propor-

tionality, which characterizes the $\nu = 0$ equipartition solution.[1] If this relation is used in (24) and (25), then $\xi_{2n}(k;t,t') = C\zeta_{2n}(k;t,t')$ identically.

The fluctuation-relaxation relation survives in any of the Padé approximations, and in any representation, provided that (24) and (25) are treated in parallel. This follows from the fact that forming a Padé approximant commutes with multiplication of the infinite series by a constant. In order to keep the energy conservation property in the internal Padé approximations, the infinite-series integral equations must be cast in a form such that $\int S(k;t,t)d^3k = 0$ is an identity whatever the values of the quantities that are approximated. This can be done by writing S in the form

$$S(k;t,t') = (L/2\pi)^3 \times \mathrm{Im}[k_m \sum_{\vec{p}+\vec{q}=\vec{k}} \langle u_i(\vec{p},t)u_m(\vec{q},t)u_i(-\vec{k},t')\rangle],$$

and expressing the triple moment $\mathrm{Im}\langle u_i(\vec{p},t)u_m \times(\vec{q},t)u_i(-\vec{k},t')\rangle$ in terms of its two defining scalars, which have the form $S_{(1)}(k,p,q;t,t')$ and $S_{(2)}(k,p,q;t,t')$.[6,7] Here L is the side of a large box in which $\vec{u}(\vec{x},t)$ obeys cyclic boundary conditions. Conservation of energy then follows identically from the symmetry properties of $S_{(1)}$ and $S_{(2)}$ under interchange of k, p, and q. These symmetry properties are exhibited in every order of the irreducible expansions for $S_{(1)}$ and $S_{(2)}$, and hence survive in the Padé approximations to these scalars. In order to keep the fluctuation-relaxation relation, parallel manipulations must be carried out on $H(k;t,t')$. A similar reduction to defining scalars serves to keep energy conservation if (24) and (25) are transformed to the wave-number–frequency domain.

Analogous recasting to make the external approximations conservative seems more artificial, and this is a reason for favoring the internal ones.

The irreducible expansion (27) for turbulent dispersion is homologous with that for the random oscillator. If the random velocity field is time independent, G_S and H_S depend on (t,t') only in the combination $t-t'$. The Laplace transform of (27) is then (S subscript dropped)

$$(p+\kappa k^2)G(k,p) = 1 + H(k,p),$$

$$H(k,p) = \sum_{n=1}^{\infty} \lambda^{2n}\theta_{2n}(k,p). \qquad (28)$$

The first two θ_{2n} are

$$\theta_2(k,p) = -\tfrac{1}{2}\int d^3q[\vec{k}\cdot\vec{P}(\vec{q})\cdot\vec{k}]U(q)G(|\vec{k}-\vec{q}|,p)G(k,p),$$

$$\theta_4(k,p) = +\tfrac{1}{4}\int d^3q\int d^3q'[\vec{k}\cdot\vec{P}(\vec{q})\cdot(\vec{k}-\vec{q}')] \times[(\vec{k}-\vec{q})\cdot\vec{P}(q')\cdot\vec{k}] \times G(|\vec{k}-\vec{q}|,p)G(|\vec{k}-\vec{q}-\vec{q}'|,p) \times G(|\vec{k}-\vec{q}'|,p)G(k,p), \qquad (29)$$

where $P_{ij}(\vec{q}) = \delta_{ij} - q_i q_j/q^2$. Each higher θ_{2n} consists of S_{2n} terms, each involving integration over n intermediate wave vector spaces. The S_{2n} are the same numbers as in (7). If $\kappa = 0$, and if $k \gg q$ for any q at which $U(q)$ is appreciable, all the G factors in $\theta_{2n}(k,p)$ may be replaced by $G(k,p)$. The wave number integrations can then be performed, and (28) reduces to

$$H(k,p) = \sum_{n=1}^{\infty} \lambda^{2n}(-v_0^2k^2)^n S_{2n}[G(k,p)]^{2n}, \qquad (30)$$

where v_0 is the root-mean-square turbulent velocity component in any direction $[3v_0^2 = \int U(q)d^3q]$. Thus the high k limit of (28) is identical with (7), in units where $v_0k = 1$.

If $\kappa = 0$, $[k^2G(k,0)]^{-1}$ is the steady-state eddy diffusivity exerted on scalar-field inhomogeneities of wave number k. In particular, the limit $k \to 0$ gives the eddy diffusivity acting on uniform scalar concentration gradients. The author has started an investigation of the random-coupling values and the Padé approximations to $[k^2G(k,0)]^{-1}$ for two shapes of the velocity spectrum: $E(q) \equiv 2\pi q^2U(q) \propto \delta(q-q_0)$ and $E(q) \propto q^4\exp(-2q^2/q_0^2)$. The results have been compared with exact values obtained by a Monte Carlo calculation of particle trajectories in computer realizations of the random velocity field. The largest errors in the random-coupling values are for $E(q) \propto \delta(q-q_0)$, and these range approximately from +25% for $k \gg q_0$ to +8% for $k \ll q_0$. In the (1,1) internal Padé approximation to (28), the errors decrease roughly by a half, without changing sign, except for $k \ll q_0$, where the correction overshoots the exact value. Until higher approximations are calculated, there is too little evidence to elucidate the convergence properties of the Padé sequence. Monte Carlo techniques were used to evaluate the multiple integrals in (29).

7. DISCUSSION

There are major obstacles to an analytical theory of the Padé approximations proposed here. First, the analyticity properties which are needed for convergence of Padé approximants to a function are not known in general. The theory of convergence is well developed for functions representable by a Stieltjes integral, but counterexamples show that this is not a necessary condition for convergence.[4,5] Baker, Jr., has suggested, without proof, that the (r,r) Padé approximants to a power series converge at every point which is not a singularity of the function and which is connected to the origin by a region of the complex plane that is free of singularities.[5] It is likely that the primitive perturbation expansion in powers of λ, for the correlation function of a velocity field that obeys (23), does satisfy this condition. Variation of λ along the real axis is equivalent to scale changes in the velocity field (together with a reflection if λ is negative). Since the initial multivariate-Gaussian statistical ensemble includes all scales with some statistical weight, it is hard to see how a discontinuity or singularity of behavior can occur at a finite, real λ value. Therefore $\lambda = 1$ should be connected to the origin by a singularity-free path. The same conclusion

seems indicated if the turbulence is maintained in a statistically steady state by random driving forces added to the right-hand side of (23). But even if the analyticity properties of the Navier-Stokes equation were fully known, this would not give directly the functional relations among H, S, G, U, and λ which are crucial to the Padé approximants of the irreducible expansions.

Shanks[8] has stressed that the Padé approximants represent well-defined nonlinear operations on an infinite sequence without the need of representing the sequence as partial sums of a power series. Conceivably there are other approaches to a theory of the final $\lambda = 1$ approximations that do not appeal at all to the power series in λ or to analyticity properties in the λ plane. Shanks also presents other nonlinear transforms, distinct from the Padé approximants, which yield convergents to some examples of divergent series. Shank's "iterated e_1 transform" gives remarkably good results on the random oscillator if it is used, instead of the Padé approximants, to form approximate equations for G, like those of Sec. 4.

In the author's opinion, the Padé approximants deserve extensive further study, together with other nonlinear approximations to the irreducible expansions. Despite the absence of underlying mathmatical theory, the performance on the test problem of the random oscillator suggests that these techniques are more powerful than most systematic approximation schemes that have been attempted for turbulence correlations. However, there is a basic and troubling question: Does the perturbation expansion, on which all later manipulations are based, really contain all the information needed to determine the correlation functions unambiguously? If so, is it reasonable that the information can be extracted by considering this complicated functional power series (in unperturbed correlation and response functions) as a simple one-dimensional sequence, the power series in λ?

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