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Rederivation and further assessment of the LET theory of isotropic turbulence, as applied to passive scalar convection

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A simpler and more rigorous derivation is presented for the LET (Local Energy Transfer) theory, which generalizes the theory to the non-stationary case and which corrects some minor errors in the original formulation (McComb 1978), Previously, *ad hoc* generalizations of the LET theory (McComb & Shanmugasundaram 1984) gave good numerical results for the free decay of isotropic turbulence. The quantitative aspects of these previous computations are not significantly affected by the present corrections, although there are some important qualitative improvements.

The revised LET theory is also extended to the problem of passive scalar convection, and numerical results have been obtained for freely decaying isotropic turbulence, with Taylor–Reynolds numbers in the range $5 \leqslant R_\lambda \leqslant 1060$, and for Prandtl numbers of 0.1, 0.5 and 1.0. At sufficiently high values of the Reynolds number, both velocity and scalar spectra are found to exhibit Kolmogorov-type power laws, with the Kolmogorov spectral constant taking the value $\alpha = 2.5$ and the Corrsin–Oboukhov constant taking a value of $\beta = 1.1$.

1. Introduction

The Local Energy Transfer (LET) theory belongs to the general class of renormalized perturbation theories, and is a two-point, two-time closure of the Navier–Stokes hierarchy in the Eulerian coordinate frame. Originally, the development of this theory was motivated by the need to eliminate the infrared divergence, which occurs when one assumes that the Kolmogorov energy spectrum applies at all wavenumbers in the limiting case of infinite Reynolds number. (This corresponds to a gedanken experiment, in which the fluid viscosity is allowed to shrink to zero, while the rate at which the arbitrary stirring forces do work on the system is maintained constant.) The basic *ansatz* of the LET theory is that the renormalized (or turbulent) response may be obtained from a consideration of the local energy balance in k-space. The theory has been developed in a series of papers, which first considered the single-time stationary case (McComb 1974, 1976) and then the two-time stationary case (McComb 1978, hereinafter referred to as I). Subsequently, it was shown that an heuristic modification of the LET theory to the two-time, non-stationary case could be used successfully to calculate the free decay

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of isotropic turbulence from arbitrary initial conditions (McComb & Shanmugasundaram 1984; McComb & Shanmugasundaram & Hutchinson 1989, hereinafter referred to as II and III, respectively). In the latter case (reference III), our numerical results led us to question the importance of connective scaling in two-time correlations. We also put forward in III arguments which questioned the relevance of random Galilean invariance as a criterion for turbulence theories of this kind.

In the present paper our first objective is to give a direct derivation of the LET theory for the general non-stationary case. This new treatment is not only simpler, but can claim to be more rigorous, insofar as certain inconsistencies in I have been eliminated. For instance, the derivation given in I appears to rely on the propagator exhibiting time-reversal symmetry; an unrealistic property for a chaotic system, let alone a dissipative one. This is not a requirement in the new derivation given here. We also take the opportunity to correct an error in the limits on the integration over intermediate times, as given in I.

Our second objective is to begin the task of assessing the potential of the LET theory for application to problems of practical significance. As is well known, recent developments in computers and in numerical methods have not been matched by any comparable progress with the central problem of turbulence modelling. Ideally, renormalized perturbation theories would provide a possible way forward in this area, but evidently they must recognize the engineer's need for predictive methods which can be applied to flows with a mean rate of shear and which can also handle heat and mass transfer. However, the difficulties involved in taking inhomogeneity and anisotropy into account are formidable, so as a first step in taking the LET theory along the road to practical applications, we consider here the prediction of passive scalar convection for the homogeneous, isotropic case. We also note in passing that this has proved in the past to be a severe test for other two-point, two-time closures.

Lastly, and especially for those readers whose immediate concern is with applications, we should emphasize that the LET theory makes no claim to being a rational approximation to the Navier–Stokes equations. Like all other closures of this type, it relies on a second-order truncation of a renormalized perturbation series of unknown convergency properties. At this stage, therefore, our strategy is both pragmatic and conventional. We aim to test the LET theory on a hierarchy of increasingly more complex problems, and this paper should be seen as part of that process.

2. Basic equations

In this section we briefly summarize those aspects of the Fourier analysis of the Navier–Stokes equation which will be needed in this paper. We begin by considering an incompressible fluid in a cubical box of side L. This is our basis for decomposing the velocity field into its discrete Fourier components. At a later stage we take the limit as L tends to infinity (which is required for rigorous isotropy) and summations are replaced by integrals.

If we let the velocity field be $u_\alpha(\boldsymbol{x},t)$, then the Fourier components $u_\alpha(\boldsymbol{k},t)$ are defined by

$$u_\alpha(\boldsymbol{x},t) = \sum_{\boldsymbol{k}} u_\alpha(\boldsymbol{k},t)\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{2.1}$$

For an incompressible fluid, the Navier–Stokes equation then becomes

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]u_\alpha(\boldsymbol{k},t) = \sum_{j} M_{\alpha\beta\gamma}(\boldsymbol{k})\, u_\beta(\boldsymbol{j},t)\, u_\gamma(\boldsymbol{k}-\boldsymbol{j},t)), \tag{2.2}$$

while the continuity equation takes the form

$$k_\alpha u_\alpha(\boldsymbol{k},t) = 0. \tag{2.3}$$

The inertial-transfer operator $M_{\alpha\beta\gamma}(\boldsymbol{k})$ is defined by

$$M_{\alpha\beta\gamma}(\boldsymbol{k}) = (2\mathrm{i})^{-1}[k_\beta D_{\alpha\gamma}(\boldsymbol{k})+k_\gamma D_{\alpha\beta}(\boldsymbol{k})], \tag{2.4}$$

where the projection operator $D_{\alpha\beta}(\boldsymbol{k})$ is given by

$$D_{\alpha\beta}(\boldsymbol{k}) = \delta_{\alpha\beta}-k_\alpha k_\beta|\boldsymbol{k}|^{-2}. \tag{2.5}$$

As always in this kind of work, we consider velocity fields with zero mean, and so the main statistical quantity of interest is the pair-correlation of velocities, which is introduced through the relationship

$$(L/2\pi)^3\langle u_\alpha(\boldsymbol{k},t)\, u_\beta(-\boldsymbol{k},t')\rangle = Q_{\alpha\beta}(\boldsymbol{k};t,t'). \tag{2.6}$$

For isotropic turbulence, we simplify matters by introducing the correlation function $Q(k;t,t')$, which is defined by the relationship

$$Q_{\alpha\beta}(\boldsymbol{k};t,t') = D_{\alpha\beta}(\boldsymbol{k})\, Q(k;t,t'), \tag{2.7}$$

and can be expressed in terms of the energy spectrum $E(k,t)$ as follows:

$$E(k,t) = 4\pi k^2 Q(k;t,t). \tag{2.8}$$

The basic hypothesis of the LET theory has been (see I) that the turbulent response can be represented by an exact propagator, which connects the velocity field, associated with mode $\boldsymbol{k}$, to itself at a later time. (It may be worth noting that the graphical methods used by Wyld 1961 to construct partial sums of the primitive perturbation series imply the existence of a propagator, at the level of a line-renormalized expansion in the moments of the exact velocity field: we shall say a little more about this, in the next section.) In I, we defined the velocity-field propagator $H_{\alpha\sigma}(\boldsymbol{k};t,s)$ by the relationship

$$u_\alpha(\boldsymbol{k},t) = H_{\alpha\sigma}(\boldsymbol{k};t,t')\, u_\sigma(\boldsymbol{k},t'), \tag{2.9}$$

where

$$\left.\begin{aligned} H_{\alpha\sigma}(\boldsymbol{k};t,s)\, H_{\sigma\beta}(\boldsymbol{k};s,t') &= H_{\alpha\beta}(\boldsymbol{k};t,t');\\ H_{\alpha\beta}(\boldsymbol{k};t,t) &= 1. \end{aligned}\right\} \tag{2.10}$$

Again, for the case of isotropic turbulence, we can express this in terms of a scalar function, thus

$$H_{\alpha\beta}(\boldsymbol{k};t,t') = D_{\alpha\beta}(\boldsymbol{k})\, H(k;t,t'), \tag{2.11}$$

where $H(k;t,t')$ is referred to as the propagator function. In the present paper, we shall replace (2.9) by a statistical form, based on correlation functions. This will make the statistical character of the propagator more apparent.

3. A modified derivation of the LET equations

In this section, we shall give a short account of the way in which the LET equations may be derived using renormalized perturbation theory. In physical terms, we may think of a fluid which is arbitrarily set into motion, with a velocity field which varies randomly with position and time, and which has Gaussian statistics. This is our zero-order field, and we shall denote it by $u_\alpha^{(0)}(\boldsymbol{k},t)$. We now imagine that the nonlinear term is switched on, whereupon the exact, non-Gaussian, velocity field is generated by the mode-couplings induced by the convolution sums in $\boldsymbol{k}$-space. That is, in mathematical terms, the exact velocity field can be rigorously expressed in terms of an infinite series in the zero-order Gaussian velocity field. Naturally, the coefficients in this series are obtained by iterating the Navier–Stokes equation. (It is perhaps worth noting that this formulation of the turbulence problem is often discussed in terms of arbitrary random forces. However, such stirring forces, although an essential feature of certain theories, are not intrinsic to a general formulation of this type, and we shall not require them here.)

It is an obvious corollary of the above statements, that the exact correlation function can be obtained as an infinite series in the moments of the zero-order field. It also follows, from the Gaussian nature of the zero-order field, that this infinite series can be further expressed solely in terms of the products and convolutions of the pair correlation of the zero-order field. However, although the resulting series corresponds to a rigorous solution of the Navier–Stokes equations, it should be understood that it will in general be wildly divergent. This is because the iteration is in terms of the inverse of the viscous operator on the left-hand side of (2.2). Hence, the expansion is effectively in powers of the Reynolds number, and diverges in all cases of interest.

The possibility of obtaining a renormalized expansion, which might have better properties than the primitive series, was first recognized by Kraichnan (1959), in the form of the Direct-Interaction Approximation or DIA; and was given a more general, diagrammatic analysis by Wyld (1961). The basic idea is quite simple. One replaces the zero-order correlation and response functions at all points in the expansion by their exact forms. This procedure corresponds to summing certain classes of terms in the primitive series to all orders (Wyld 1961). Also, more recently, Kraichnan (1977) has reinterpreted this formalism in terms of the technique of reversion of power series.

The problem now becomes one of defining the renormalized (turbulent) response, such that one may truncate the series at low order (usually second order) and hence obtain closed equations for the exact correlation and response functions. In DIA, the closure is obtained by concentrating on the relationship between the velocity field and the stirring forces. In the LET theory (in I), we introduced the propagator through equation (2.9) and obtained its governing equation from a consideration of the local energy balance in $\boldsymbol{k}$-space. We shall adopt a slight variation on this approach in the following sections.

3.1. *Perturbation expansion of the Navier–Stokes equations*

Formally, we introduce the perturbation series for the velocity as an expansion in terms of a book-keeping parameter λ, thus

$$u_\alpha(\boldsymbol{k},t) = u_\alpha^{(0)}(\boldsymbol{k},t)+\lambda u_\alpha^{(1)}(\boldsymbol{k},t)+O(\lambda^2), \tag{3.1}$$

where λ is put equal to one at the end of the calculation.

We also introduce the zero-order propagator as the Green's function of the linear operator on the left-hand side of (2.2), or through

$$[\partial/\partial t+\nu k^2]\,H_{\alpha\beta}^{(0)}(\boldsymbol{k};t,t') = D_{\alpha\beta}(\boldsymbol{k})\,\delta(t-t'), \tag{3.2}$$

and hence,

$$H_{\alpha\beta}^{(0)}(\boldsymbol{k};t,t') = \begin{cases} D_{\alpha\beta}(\boldsymbol{k})\exp\{-\nu k^2(t-t')\}, & t>t', \\ 0, & t<t'. \end{cases} \tag{3.3}$$

The perturbation solution may be obtained in the usual way, by substituting the expansion for $u_\alpha(\boldsymbol{k},t)$ into the right-hand side of (2.2), and associating the book-keeping parameter λ with the inertial-transfer operator $M_{\alpha\beta\gamma}(\boldsymbol{k})$, thus

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]u_\alpha(\boldsymbol{k},t)=\lambda M_{\alpha\beta\gamma}(\boldsymbol{k})\sum_{\boldsymbol{j}}[u_\beta^{(0)}(\boldsymbol{j},t)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},t)+\lambda u_\beta^{(0)}(\boldsymbol{j},t)\,u_\gamma^{(1)}(\boldsymbol{k}-\boldsymbol{j},t)$$
$$+\lambda u_\beta^{(1)}(\boldsymbol{j},t)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},t)+\ldots]. \quad (3.4)$$

The individual coefficients $u^{(1)}$, $u^{(2)}, \ldots$, are readily obtained by expanding the left-hand side of (2.2) and equating coefficients of each power of λ. This can be done to all orders, but we shall only require the first order here; and this is

$$u_\alpha^{(1)}(\boldsymbol{k},t)=\int_0^t \mathrm{d}s\,H_{\alpha\sigma}^{(0)}(\boldsymbol{k};t,s)M_{\alpha\beta\gamma}(\boldsymbol{k})\sum_{\boldsymbol{j}}u_\beta^{(0)}(\boldsymbol{j},s)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},s). \quad (3.5)$$

3.2. *Basic ansatz of the LET theory*

Since the velocity-field propagator exists, in principle, as an expansion in the moments of the Gaussian zero-order velocity field, two of its properties follow immediately. First, it is statistically sharp, so we have

$$\langle H_{\alpha\beta}(\boldsymbol{k};t,t')\rangle=H_{\alpha\beta}(\boldsymbol{k};t,t'). \quad (3.6)$$

Secondly, its expansion in powers of the book-keeping parameter λ contains only even-order terms, thus

$$H_{\alpha\beta}(\boldsymbol{k};t,t')=H_{\alpha\beta}^{(0)}(\boldsymbol{k};t,t')+\lambda^2H_{\alpha\beta}^{(2)}(\boldsymbol{k};t,t')+O(\lambda^4). \quad (3.7)$$

The statistical form of the LET theory's basic hypothesis is introduced in the following way. Let us invert the operator on the left-hand side of (2.2), multiply both sides by $u_\epsilon(-\boldsymbol{k},t')$, and average, to obtain the exact result for the correlation tensor

$$Q_{\alpha\epsilon}(\boldsymbol{k};t,t')=\int_0^t \mathrm{d}s\,H_{\alpha\sigma}^{(0)}(\boldsymbol{k};t,s)\left(\frac{L}{2\pi}\right)^3\sum_{\boldsymbol{j}}M_{\alpha\beta\gamma}(\boldsymbol{k})\langle u_\beta(\boldsymbol{j},t)\,u_\gamma(\boldsymbol{k}-\boldsymbol{j},t)\,u_\epsilon(-\boldsymbol{k},t')\rangle. \quad (3.8)$$

We may also derive a relationship for the correlation tensor by carrying out the same sequence of operations on equation (2.9), but this time we also need the property (3.6), and this gives us

$$Q_{\alpha\epsilon}(\boldsymbol{k};t,t')=H_{\alpha\sigma}(\boldsymbol{k};t,t')\,Q_{\sigma\epsilon}(\boldsymbol{k};t,t'). \quad (3.9)$$

This now replaces (2.9) as the defining equation for H, and our basic *ansatz* for closure of the Navier–Stokes equation becomes a postulate of the equivalence of (3.8) and (3.9).

3.3. *The generalized covariance equation*

As a preliminary to obtaining closed equations for the correlator and propagator functions, we first derive the generalized covariance equation. To do this, we invoke (2.9) in order to write the Navier–Stokes equation in the form

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]u_\alpha(\boldsymbol{k},t)=\lambda M_{\alpha\beta\gamma}(\boldsymbol{k})\sum_{\boldsymbol{j}}u_\beta(\boldsymbol{j},t)\,u_\gamma(\boldsymbol{k}-\boldsymbol{j},t). \quad (3.10)$$

We then multiply both sides by $u_\epsilon(-\boldsymbol{k},t')$ and average, thus

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]\langle u_\alpha(\boldsymbol{k},t)\,u_\epsilon(-\boldsymbol{k},t')\rangle=\lambda\sum_{\boldsymbol{j}}M_{\alpha\beta\gamma}(\boldsymbol{k})\langle u_\beta(\boldsymbol{j},t)\,u_\gamma(\boldsymbol{k}-\boldsymbol{j},t)\,u_\epsilon(-\boldsymbol{k},t')\rangle. \quad (3.11)$$

The triple moment on the right-hand side can be expanded out, using (3.1),

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]\langle u_\alpha(\boldsymbol{k},t)\,u_\epsilon(-\boldsymbol{k},t')\rangle = \lambda\sum_{\boldsymbol{j}} M_{\alpha\beta\gamma}(\boldsymbol{k})\,[\langle u_\beta^{(0)}(\boldsymbol{j},t)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},t)\,u_\epsilon^{(0)}(-\boldsymbol{k},t')\rangle$$
$$+\lambda\langle u_\beta^{(0)}(\boldsymbol{j},t)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},t)\,u_\epsilon^{(1)}(-\boldsymbol{k},t')\rangle+2\lambda\langle u_\beta^{(1)}(\boldsymbol{j},t)\,u_\gamma^{(0)}(\boldsymbol{k}-\boldsymbol{j},t)\,u_\epsilon^{(0)}(-\boldsymbol{k},t')\rangle+O(\lambda^2)], \tag{3.12}$$

and, substituting from (3.5) for $u^{(1)}$, we obtain the generalized covariance equation, at second order in $u^{(0)}$, with higher orders readily being obtained by iteration.

Now we follow much the same procedure as was used to derive the DIA (Kraichnan 1959). We do this as follows:

(i) Evaluate the moments of the zero-order velocity field (in principle, to all orders) in terms of $Q^{(0)}$, using the Gaussian statistics of the zero-order field.

(ii) Make the replacements $Q^{(0)}\to Q$ and $H^{(0)}\to H$, put the book-keeping parameter $\lambda = 1$, and truncate the expansion, which is the right-hand side of the generalized covariance equation, at second order.

(iii) Lastly, we make the usual simplification for isotropic turbulence, by substituting the tensor forms given by (2.7) and (2.11), and summing over $\alpha = \epsilon$.

The result is easily found to be the exact generalized covariance equation at second order, thus

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]Q(k;t,t') = \int d^3j L(\boldsymbol{k},\boldsymbol{j})\left[\int_0^{t'} dt''\,H(k;t',t'')\,Q(j;t,t'')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\right.$$
$$\left.-\int_0^{t} dt''\,H(j;t,t'')\,Q(k;t'',t')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')+O(\lambda^4)\right], \tag{3.13}$$

where it can be shown that the coefficient $L(\boldsymbol{k},\boldsymbol{j})$ takes the form

$$L(\boldsymbol{k},\boldsymbol{j}) = \frac{[\mu(k^2+j^2)-kj(1+2\mu^2)]\,(1-\mu^2)\,kj}{k^2+j^2-2kj\mu}, \tag{3.14}$$

and μ is the cosine of the angle between the vectors $\boldsymbol{k}$ and $\boldsymbol{j}$.

3.4. *The LET equations for the correlation and propagator functions for isotropic turbulence*

We summarize here the equations which make up the LET theory for the particular case of isotropic turbulence. First, we invoke (2.7) and (2.11), so that we may write (3.9), which defines the propagator, in the form

$$Q(k;t,t') = H(k\!:t,t')\,Q)k;t',t'), \quad t>t'. \tag{3.15}$$

Then, for completeness, we repeat here (3.13), with the term $O(\lambda^4)$ dropped, as our equation for the two-time correlation function, thus

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]Q(k;t,t') = \int d^3j L(\boldsymbol{k},\boldsymbol{j})\left[\int_0^{t'} dt''\,H(k;t',t'')\,Q(j;t,t'')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\right.$$
$$\left.-\int_0^{t} dt''\,H(j;t,t'')\,Q(k;t'',t')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\right]; \tag{3.16}$$

along with the energy equation in the form

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]Q(k;t,t) =$$

$$2\int d^3jL(\boldsymbol{k},\boldsymbol{j})\int_0^t dt''\, Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\,[H(k;t,t'')\,Q(j;t,t'')-H(j;t,t'')\,(Q(k;t,t')], \quad (3.17)$$

which is just the special case of the correlation equation, evaluated on the time diagonal, when $t = t'$.

It should be noted that (3.15)–(3.17) form a closed set for the three functions $Q(k;t,t')$, $Q(k;t,t')$ and $Q(k;t,t')$. This set is the basis of our numerical calculations of freely decaying turbulence, which we shall present later on in this paper. However, it should also be noted that previously an essential feature of the LET theory has been an evolution equation for the propagator (also referred to as the response equation). Although we do not need such an equation for the purpose of numerical calculation, it is nevertheless of some interest in elucidating the difference between the corrected form of the LET theory presented here and the form reported previously.

Accordingly, we close this section by remarking that substitution from (3.15) into the left-hand side of (3.16) leads to

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]H(k;t,t')\,Q(k;t',t')= \int d^3jL(\boldsymbol{k},\boldsymbol{j})\left[\int_0^{t'} dt''\, H(k;t',t'')\,Q(j;t,t'')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\right.$$

$$\left. - \int_0^t dt''\, Q(k;t'',t')\,H(j;t,t'')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\right]; \quad (3.18)$$

and this is the LET response equation.

3.5. *Comparison of LET with DIA*

Comparison with DIA (Kraichnan 1959) has been made previously (I, II and III), and our object here is only to modify those previous comparisons insofar as the current version of the LET response equation is different from earlier forms. To begin with, we mention for completeness that (3.16) and (3.17) are, notational differences aside, identical to their DIA equivalents. The differences between the two formulations lie solely in their respective response equations.

We may demonstrate this by dividing up the integral over $0 < t'' < t$ on the right-hand side of (3.18) into two ranges $0 < t'' < t'$ and $t' < t'' < t$; using (3.15) to write

$$Q(k;t',t'') = Q(k;t'',t') = H(k;t'',t')\,Q(k;t',t'), \quad t' < t'' < t,$$

and rearranging (3.18) to obtain

$$\left[\frac{\partial}{\partial t}+\nu k^2\right]H(k;t,t')+\int d^3jL(\boldsymbol{k},\boldsymbol{j})\int_{t'}^t dt''\, H(k;t'',t')\,H(j;t,t'')\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')$$

$$= \frac{1}{Q(k;t',t')}\int d^3jL(\boldsymbol{k},\boldsymbol{j})\left[\int_0^{t'} dt''\, Q(|\boldsymbol{k}-\boldsymbol{j}|;t,t'')\,\{H(k;t',t'')\,Q(j;t,t'')\right.$$

$$\left. -Q(k;t',t'')\,H(j;t,t'')\}\right]. \quad (3.19)$$

The comparable form in DIA is the equation for the response function $G(k;t,t')$, which is analogous to $H(k;t,t')$ here. Comparison of (3.19) with the corresponding

DIA form (Kraichnan 1959), shows that the two left-hand sides are the same, but that (3.19) has additional nonlinear terms on the right-hand side.

As is well known, the DIA response equation is divergent when the limit of infinite Reynolds number is taken: its wavenumber convolution integral diverges at $\boldsymbol{k} = \boldsymbol{j}$, when the Kolmogorov distribution is taken to apply at all wavenumbers. It is quite easily shown that the additional term on the right-hand side of the LET response equation (3.19) will cancel this divergence, as we take the limit $\boldsymbol{k}$ tends to $\boldsymbol{j}$.

4. Numerical analysis

Equations (3.15)–(3.17) for the velocity-field correlations and propagators were applied to four test problems. These are summarized in table 1, where all the relevant initial parameters are given. Evolved values of the same parameters, corresponding to the end of each calculation, will be found in table 2. It should be noted that test problems 1–3 are based on spectral shapes which may be found in figure 1 of II, and cover low to intermediate values of the Taylor–Reynolds number. The calculations at high Reynolds numbers were based on an initial spectrum suggested by Herring (see III), which is given here as test problem 4.

In order to carry out the calculations, both wavenumbers and times were discretized and equations integrated forward in time from arbitrarily chosen initial spectra. Full details of the numerical procedures will be found in Section 4 of II, and will not be repeated here. However, for convenience we shall summarize the definitions of the various integral parameters in this section.

4.1. *Definitions of the integral parameters*

The general form of the trial spectrum is given by

$$E(\kappa, 0) = c_1 \kappa^{c_2} \exp(-c_3 k^{c_4}), \tag{4.1}$$

where the values of the constants for each spectrum are given in table 1. The r.m.s. velocity of any velocity component, $u(t)$, and the rate of dissipation per unit mass are

$$E(t) = \int_0^\infty E(k,t)\,\mathrm{d}k = \tfrac{3}{2}[u(t)]^2 \tag{4.2}$$

and

$$\epsilon(t) = 2\nu \int_0^\infty k^2 E(k,t)\,\mathrm{d}k. \tag{4.3}$$

The transfer spectrum is given by

$$T(k,t) = 8\pi k^2 P(k;t,t), \tag{4.4}$$

where $P((k;t,t)$ is given by the right-hand side (3.17), with $t' = t$. The total rate at which energy is transferred from all the modes $p < k$ to all the modes $p > k$ is given by the transport power $\Pi(k,t)$, which is related to the transfer spectrum, thus

$$\Pi(k,t) = \int_0^\infty \mathrm{d}p\, T(p,t). \tag{4.5}$$

The modal time-correlation is defined by

$$R(k;t,t') = \frac{Q(k;t,t')}{[Q(k;t,t)\,Q(k;t',t')]^{\frac{1}{2}}} \tag{4.6}$$

Test problem no.	Basic spectral shape	Values of c in the initial spectrum shape $E(k,0) = c_1 k^{c_2} \exp(-c_3 k^{c_4})$: c_1	c_2	c_3	c_4	k_{bot}	k_{top}	ν	$E(0)$	$\epsilon(0)$	$u(0)$	$R_L(0)$	$R_\lambda(0)$
1	I	0.00524169	4	0.0883881	2	1.834	29.3	0.01189	1.485	1.009	0.995	43.0	35.0
2	II	0.0662912	1	0.210224	1	1.0905	41.50	0.05	1.466	19.88	0.989	7.98	3.80
3	IV	0.4	1	0.5	1	0.281	35.9	0.008	1.59	0.616	1.029	133	58.5
4	Herring's test problem	$E(k,0) = 2\pi k^2(0.02+k)^{-\frac{11}{3}}$				0.01	103.2	0.005	56.1	22.7	6.116	39108	429.8

TABLE 1. Velocity calculations: initial conditions

Test problem no.	Old form: Final time	E	ϵ	$u(0)$	R_L	R_λ	$S_{u\theta}$	Current form: Final time	E	ϵ	$u(0)$	R_L	R_λ	$S_{u\theta}$
1	0.841	0.533	0.710	0.596	25.29	14.98	0.493	0.830	0.579	0.716	0.621	26.70	16.21	0.459
2	0.395	0.310	0.594	0.455	7.37	4.65	0.461	0.395	0.312	0.592	0.456	7.38	4.69	0.397
3	1.00	0.953	0.508	0.797	119.96	38.61	0.423	0.994	0.987	0.491	0.811	121.08	40.67	0.415
4	0.600	52.957	3.673	5.942	39627	1009	0.369	0.600	53.063	3.471	5.948	39609	1040	0.351

TABLE 2. Velocity calculations: evolved integral parameters

such that
$$R(k;t,t) = 1. \tag{4.7}$$

The integral lengthscale $L(t)$ and the Taylor microscale $\lambda(t)$ are defined by

$$L(t) = \left[\frac{3\pi}{4}\int_0^\infty k^{-1}E(k,t)\,\mathrm{d}k\right]\Big/E(t), \tag{4.8a}$$

$$\lambda(t) = \left[5E(t)\Big/\int_0^\infty k^2E(k,t)\,\mathrm{d}k\right]^{\frac{1}{2}}, \tag{4.8b}$$

with the associated Reynolds numbers

$$R_L(t) = L(t)\,u(t)/\nu, \tag{4.9}$$

and
$$R_\lambda(t) = \lambda(t)\,u(t)/\nu. \tag{4.10}$$

The skewness of the longitudinal velocity derivative is given by

$$S(t) = -\frac{\langle(\partial u_1(\boldsymbol{x},t)/\partial x_1)^3\rangle}{\langle(\partial u_1(\boldsymbol{x},t)/\partial x_1)^2\rangle^{\frac{3}{2}}} = \frac{2}{35}\left[\frac{\lambda(t)}{u(t)}\right]\int_0^\infty k^2T(k,t)\,\mathrm{d}k, \tag{4.11}$$

while the one-dimensional energy spectrum, $\phi_1(t)$, is given by

$$\phi_1(t) = \frac{1}{2}\int_k^\infty (1-k^2/p^2)\,p^{-1}E(p,t)\,\mathrm{d}p, \tag{4.12}$$

and the Kolmogorov dissipation wavenumber is defined by

$$k_d = (\epsilon/\nu^3)^{\frac{1}{4}}. \tag{4.13}$$

5. Passive scalar convection

One of the most important practical aspects of fluid turbulence is its mixing ability, particularly in the transport of heat and mass. Here we shall make a preliminary assessment of the performance of the LET closure on this aspect of turbulence, by considering the idealized problem of passive scalar convection. As in the case of the velocity field, we shall consider the free decay of isotropic turbulence.

We shall represent the general scalar property by $\theta(\boldsymbol{x},t)$, which can stand for any contaminant or tracer. But, for definiteness, we shall take it to be temperature, so that the relevant dimensionless parameter (in addition to the Reynolds number) is the Prandtl number Pr, which is given by

$$Pr = \nu/\kappa,$$

where κ is the thermal diffusivity and is given by the thermal conductivity divided by the density of the fluid.

5.1. *Basic equations*

The governing equation for the scalar field $\theta(\boldsymbol{x},t)$ takes the well-known form

$$\partial\theta(\boldsymbol{x},t)/\partial t + (u_\beta(\boldsymbol{x},t)\,\partial/\partial x_\beta)\,\theta(\boldsymbol{x},t) = \kappa\nabla^2\theta(\boldsymbol{x},t), \tag{5.1}$$

where κ is the thermal diffusivity. A source term can also be added, but as we shall only be considering the free decay from arbitrary initial distributions of temperature, we shall not pursue that aspect here. The same approach may be adopted as earlier, in the case of the velocity field, by the introduction of the Fourier components of the temperature field, thus

$$\theta(\boldsymbol{k},t) = \sum_{\boldsymbol{k}} \theta(\boldsymbol{x},t)\,\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{5.2}$$

Then, direct substitution into (5.1) immediately yields the governing equation for $\theta(\boldsymbol{k},t)$ in the form

$$\left(\frac{\partial}{\partial t}+\kappa k^2\right)\theta(\boldsymbol{k},t) = -ik_\beta \sum_{\boldsymbol{j}} u_\beta(\boldsymbol{k}-\boldsymbol{j},t)\,\theta(\boldsymbol{j},t). \tag{5.3}$$

This equation is, of course, the scalar equivalent of the Navier–Stokes equation, in the form of (2.2); and we can generalize other such relationships to the scalar case, in the process of introducing a statistical treatment. Taking the scalar field to have zero mean, then the lowest non-trivial statistical moment is the two-point correlation, and (2.6) for the isotropic, homogeneous velocity field generalizes to the corresponding relationship for the scalar field, thus

$$(L/2\pi)^3\langle\theta(\boldsymbol{k},t)\,\theta(\boldsymbol{k}',t)\rangle = \Theta(k;t,t')\,\delta^3(\boldsymbol{k}+\boldsymbol{k}'). \tag{5.4}$$

Then, the analogue of the energy spectrum – the distribution of mean-square temperature fluctuations with wavenumber – follows at once as

$$E_\theta(k,t) = 4\pi k^2\Theta(k;t,t); \tag{5.5}$$

along with the dissipation rate of mean-square temperature fluctuations

$$\epsilon_\theta(t) = \int_0^\infty 2\kappa k^2 E_\theta(k,t)\,\mathrm{d}k, \tag{5.6}$$

and the balance equation

$$\partial E_\theta(k,t)/\partial t + 2\kappa k^2 E_\theta(k,t) = T_\theta(k,t), \tag{5.7}$$

where the transfer spectrum $T_\theta(k,t)$, is defined by analogy with (4.4) for the velocity field.

We conclude this section by listing some definitions which will be helpful in analysing our results for scalar spectra. First, we note that the dissipation-range velocity scale,

$$v_d(t) = (\epsilon(t)\,\nu)^{\frac{1}{4}}, \tag{5.8}$$

can be supplemented by an analogous scale for the dissipation range of wavenumbers of temperature fluctuations, namely

$$\theta_d(t) = [\nu\epsilon_\theta^2(t)/\epsilon(t)]^{\frac{1}{4}}. \tag{5.9}$$

Also, the additional parameters introduced with the scalar problem require the introduction of additional wavenumber scales in order to permit the characterization of the possible combinations of velocity and scalar fields. For our purposes here, it will be sufficient to introduce the Batchelor wavenumber

$$k_{\mathrm{B}}(t) = (\epsilon(t)/\nu\kappa^2)^{\frac{1}{4}} \tag{5.10}$$

and the Oboukhov–Corrsin wavenumber

$$k_{\mathrm{OC}}(t) = (\epsilon(t)/\kappa^3)^{\frac{1}{4}}. \tag{5.11}$$

These can be used in conjunction with the Kolmogorov dissipation-range wavenumber, which we defined earlier in (4.14).

5.2. *The LET equations for passive scalar convection*

Although (5.3) for the scalar field is linear, when we attempt a statistical treatment we still face a closure problem. This is because it is the fluctuations in the velocity field which induce the fluctuations in the scalar field. Accordingly we treat this problem by an extension of the existing LET theory for the velocity field. This may be accomplished by generalizing the basic hypothesis of LET, as stated in (3.15), to introduce a propagator $H^{\theta\theta}(k;t,t')$ which connects the scalar field to itself at later time. That is, by analogy with (3.15), we write

$$\Theta(k;t,t') = H^{\theta\theta}(k;t,t')\,\Theta(k;t',t'), \tag{5.12}$$

for the scalar case.

We could also introduce cross-relations of the velocity and scalar fields, with corresponding cross-propagators *scalar → velocity* and *velocity → scalar*, but the first is ruled out by our restriction to passive convection, and the second by the symmetry requirements of istropic turbulence.

The application of the renormalized perturbation theory, which follows the introduction of (5.12) as basic *ansatz*, involves some lengthy algebra which has been given by Filipiak (1991), and will not be repeated here. The end result is a closed equation for the two-time scalar field autocorrelation, which (at second order in renormalized perturbation theory) is given by

$$\left(\frac{\partial}{\partial t}+\kappa k^2\right)\Theta(k;t,t') = \int \mathrm{d}^3j\,\frac{k^2j^2(1-\mu^2)}{k^2+j^2-2jk\mu}\left[-\int_{t_0}^{t'}\mathrm{d}s\,H^{\theta\theta}(j;t,s)\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,s)\,\Theta(k;s,t') \right.$$
$$\left. +\int_{t_0}^{t'}\mathrm{d}s\,H^{\theta\theta}(k;t',s)\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,s)\,\Theta(j;t,s)\right], \tag{5.13}$$

with a corresponding result for the single-time case; thus

$$\left(\frac{\partial}{\partial t}+2\kappa k^2\right)\Theta(k;t,t) = 2\int \mathrm{d}^3j\,\frac{k^2j^2(1-\mu^2)}{k^2+j^2-2jk\mu}$$
$$\times\int_{t_0}^{t}\mathrm{d}s\,[H^{\theta\theta}(j;t,s)\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,s)\,\Theta(k;s,t)+H^{\theta\theta}(k;t,s)\,Q(|\boldsymbol{k}-\boldsymbol{j}|;t,s)\,\Theta(j;t,s)] \tag{5.14}$$

It should be noted that the above three equations for the scalar field are analogous to (3.15)–(3.17) for the velocity field; in that they form a complete set for the functions $H^{\theta\theta}(k;t,t')$, $\Theta(k;t,t')$ and $\Theta(k;t,t)$; and that they can be integrated forward in time from arbitrary initial scalar spectra, provided that the velocity field is either already known at all points and times, or is simultaneously calculated from (3.15)–(3.17). Some of the results obtained in this way will be given in §6.3.

6. Results

In this section, we present and discuss results obtained from the numerical integrations of (3.15)–(3.17) for the velocity field, and from the integration of (5.12)–(5.14) for the scalar field. we begin by comparing the corrected form of LET, as presented here, with the results obtained previously.

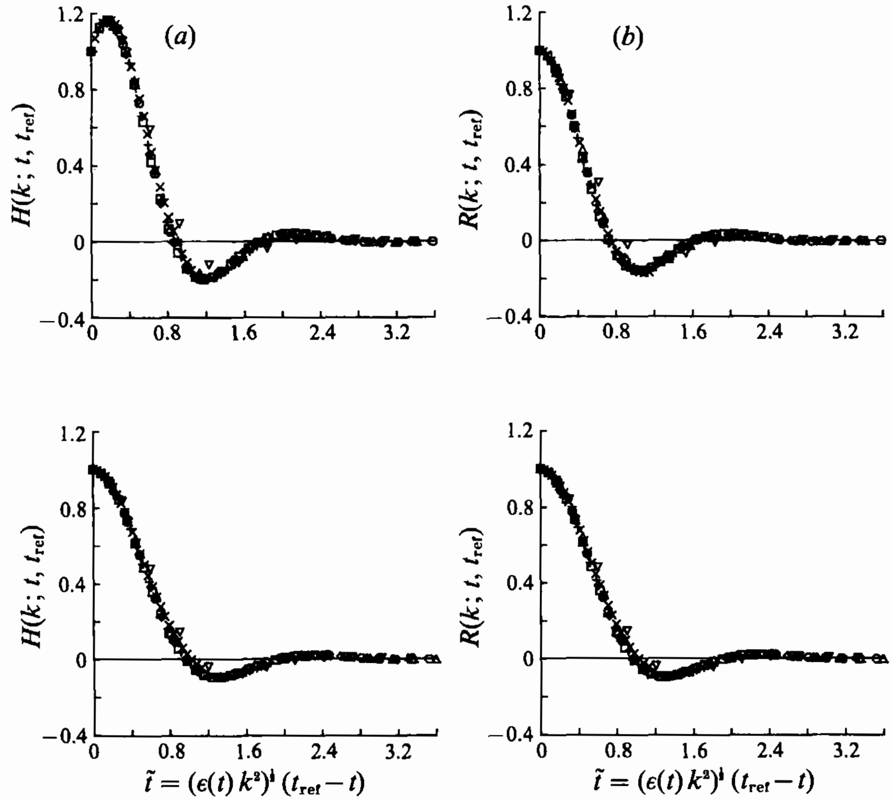

FIGURE 1. Scaling behaviour of (*a*) velocity propagator function and (*b*) velocity correlation function for test problem 4: results from old (top plot, $R_\lambda = 1009$) and new (bottom plot, $R_\lambda = 1040$) forms of LET theory for various wavenumbers: ×, 2.28; +, 4.56; □, 7.24; ◇, 11.49; ○, 18.24; △, 28.96; ▽, 45.97. $t_{ref} = 0.6$.

6.1. *Comparison with earlier results for LET*

The difference between the present and corrected forms of LET lies in the equation for the propagator function for the velocity field. If we compare (3.18) of the present work with (2.4) of III, it may be seen that the corrected propagator equation contains an extra term. As we shall now see, the effect of this extra term is to produce some improvements in the qualitative behaviour of LET.

In figures 1(*a*) and 1(*b*), we show the response and correlation functions respectively, as computed for test problem 4 at high Reynolds numbers. Beginning with figure 1(*a*) for H, we see that there is quite a marked qualitative difference between the corrected form of LET and the previous results (III). In particular, the unphysical overshoot at short times has been eliminated. In quantitative terms, we also note that the undershoot at longer times, a feature which LET shares with DIA, is reduced in the corrected form of LET. Similar qualitative changes may also be observed in the corresponding results for the correlation function, as given in figure 1(*b*); and for both functions we might also note a marginal improvement in the collapse of data at different wavenumbers under the effect of Kolmogorov scaling.

As a convenient way of summarizing the overall quantitative effect of the change in LET, we present calculations of the evolution of the skewness of the longitudinal velocity derivative (or skewness factor, for short) for test problem 1 in figure 2. The

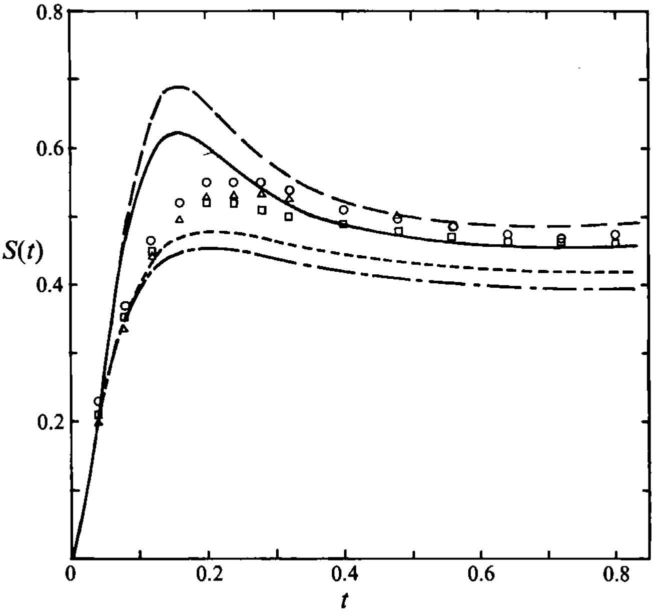

FIGURE 2. Comparison of the evolution of one-dimensional skewness factor for test problem 1: ————, LET (new); ———, LET (old); -----, DIA; —·—·—, SCF. ○, △, □, DNS results (Orszag & Patterson 1972).

use of the skewness factor as a sensitive indicator of the relative performance of different theories is well established, and in figure 2 we show results for the old and new forms of LET compared with the results of the well-known numerical simulation by Orszag & Patterson (1972), along with our own calculations of DIA and the self-consistent field theory (SCF: Herring 1965, 1966) for test problem 1. It should be noted that the corrected LET agrees with the results from the numerical simulation within the 'experimental error' of the latter. This seems to be a satisfactory result.

We should also note that, qualitatively, our results for these two theories are in agreement with the similar calculations of Herring & Kraichnan (1972); but, before we deal with the quantitative comparison, this would seem to be a suitable point to comment on important differences in the two approaches to numerical calculation. These reside mainly in the initial formulation. Herring & Kraichnan employ an initial analytical reduction to mathematical forms based on the scalar magnitudes of vectors $\boldsymbol{k}, \boldsymbol{j}$ and $\boldsymbol{l}$ (say), which must then always be constrained to form the sides of a triangle. In our case, the preliminary reduction leads to mathematical forms which depend on the scalar magnitudes k and j, along with the cosine of the angle between the two vectors. Of course, the two approaches are mathematically fully equivalent. But there are non-trivial differences in the way the various approximations of the numerical representation may affect the two formulations. It is our impression that here are significant advantages in using our formulation (see II; also, Lee 1965), but we shall not pursue that here. The essential point is that we should not expect absolute identity of results between the two kinds of approach.

With all these points in mind, it is nevertheless of interest to compare results for DIA and SCF. From Herring & Kraichnan (1971) we find that the evolved skewness for SCF is about 96% of that for DIA; whereas our present calculations give the evolved skewness for SCF as about 94% of that for DIA. This is typical of what we find in general, that our numerical results are within about 2% of those due to Herring & Kraichnan, which is quite reassuring. According to LET, the evolved skewness takes the value $S = 0.351$, while DIA gives $S = 0.344$ and SCF gives $S = 0.318$.

6.2. *Development of an inertial range*

A direct criterion for the existence of the inertial range is that the rate of energy transfer (as defined by the transport power: see 5.5)) is constant (with respect to wavenumber) and equal to the dissipation rate. A second, indirect, criterion would be the existence of a power-law region in the energy spectrum, with exponent of $-\frac{5}{3}$. In fact, it is the latter criterion only which is usually fulfilled in practice. In this paper, we are concerned with freely decaying turbulence, which means that the requirement of stationarity is satisfied in an approximate way, as a local property of some restricted range of wavenumbers. Evidently, what we need is some practical criterion for deciding when this is the case. We begin by writing down the equation for the energy spectrum as

$$\partial E(k,t)/\partial t + 2\nu k^2 E(k,t) = T(k,t). \tag{6.1}$$

This is a familiar form, and is readily deduced from the equations given in the present paper.

In an experimental context, Uberoi (1963) proposed that the condition for an inertial range should be that range of wavenumbers for which the time-derivative and the viscous terms in the above equation are negligible. This would then give us the criteria

$$T(k,t) = 0; \qquad \Pi(k,t) = \epsilon; \tag{6.2}$$

where the transport power $\Pi(k,t)$ is related to the transfer spectrum by (5.5). This is, of course, identical to the rigorous requirement for local stationarity, and Lumley (1964) has argued that, in practice, it may be too restrictive. Drawing an analogy with flow in a porous pipe, where leakage through the walls mainly controls the volumetric flow rate, but affects the mean velocity distribution only slightly, he suggested that a non-uniform spectral transfer rate can be interpreted as a 'leakage' out of mode k. If this leakage is small, then the local spectral form may be unaffected. Accordingly, Lumley proposed the following test for the existence of an inertial range:

$$|kT(k,t)/\Pi| < \Delta, \tag{6.3}$$

where the value of Δ has to be chosen in practice, but in general must be such that $\Delta \ll 1$.

Extensive analyses of experimental data (Bradshaw 1967; Helland, Van Atta & Stegen 1977) have borne out Lumley's view that a necessary condition for Kolmogorov $-\frac{5}{3}$ scaling to hold at a given wavenumber is that the energy transfer through that wavenumber should be approximately equal to the dissipation rate. In particular, Helland *et al.* (1977) measured energy transfer rates at Taylor–Reynolds numbers up to $R_\lambda = 951$, and used analytical spectral correlations to extend their results up to $R_\lambda = 10^6$. However, even at such enormous Reynolds, they were unable to find any appreciable range of wavenumbers over which the transfer spectrum $T(k,t)$ was zero. In all cases, the transfer spectrum exhibited a single sharp zero-crossing although as much as three decades of $-\frac{5}{3}$ behaviour was found in the empirical energy spectrum! On the other hand, when transfer spectra were replotted according to Lumley's criterion, it was possible to reconcile the existence of an inertial range in the transfer spectrum with scaling behaviour in the energy spectrum at the same wavenumbers.

With these points in mind, we investigated the development of a Kolmogorov-type inertial range in the predictions of the LET theory. The results are given in figures 3 and 4. In figures 3(*a*) and 3(*b*), we show the time evolution of the dissipation rate and the maximum value of the transport power (with respect to wavenumber) for

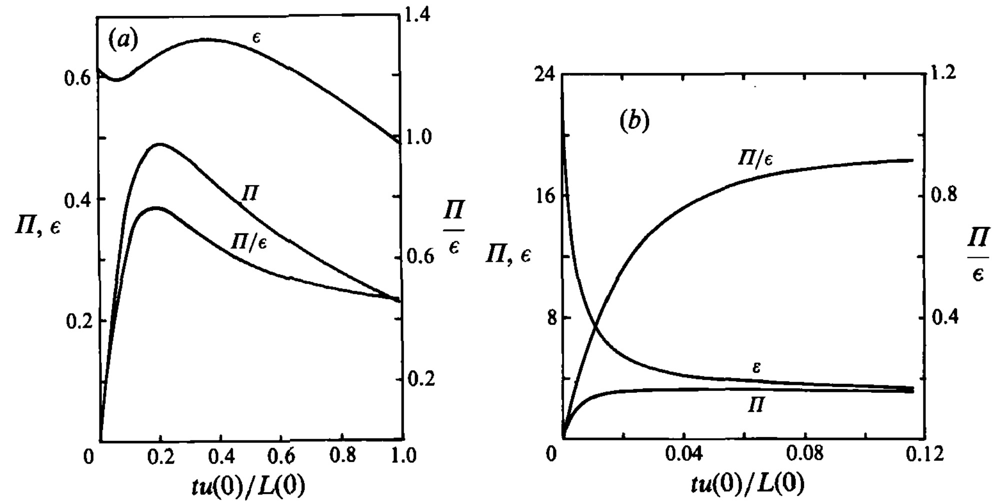

FIGURE 3. Evolution of ϵ and π_{max}. (*a*) LET results for test problem 3: $R_\lambda(t_f) = 41$. (*b*) LET results for test problem 4: $R_\lambda(t_f) = 1040$.

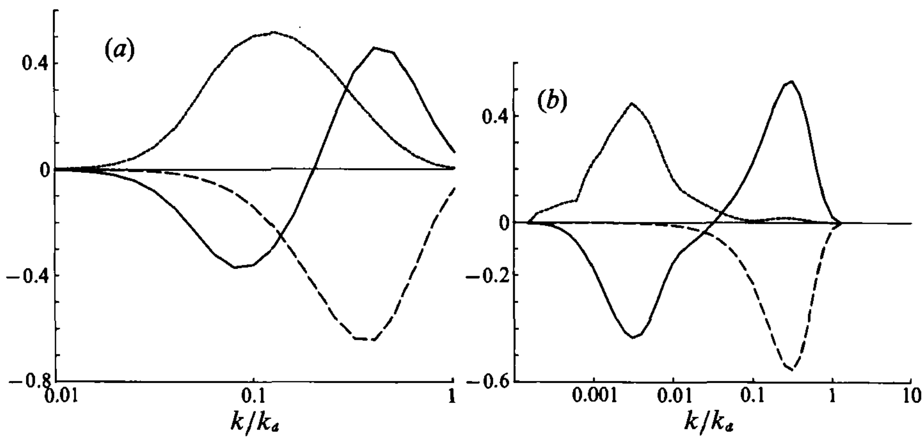

FIGURE 4. Demonstration of energy. (*a*) LET results for test problem 3: $R_\lambda(t_f) = 41$. (*b*) LET results for test problem 4: $R_\lambda(t_f) = 1040$. ———, T; - - - -, $-\partial E/\partial t$; ———, $-2\nu k^2 E$.

test problems 3 ($R_\lambda = 41$) and 4 ($R_\lambda = 1040$), respectively. It is immediately clear that at the lower Reynolds number there is no question of an inertial range existing, with the transport power always much smaller than the dissipation rate. In contrast, at the higher Reynolds number, one notes that the transport power tends asymptotically to the same value as the dissipation rate as time goes on. This contrast is underlined by a consideration of the detailed energy balances in wavenumber, as shown for the same two cases in figures 4(*a*) and 4(*b*). Both sets of results illustrate the action of the nonlinear term rather nicely, but a comparison of the two figures shows that only at the higher Reynolds number could one argue that the input and output regions are becoming clearly delineated. However, even although 1040 is quite a large Reynolds number, it is clear that there is no extended region over which the inertial transfer is zero. At most one could claim that the zero-crossing is a point of inflexion for $T(k,t)$. But, when one replots the result – for all four test problems, now – in figure 5, then it can be seen that the application of the weaker Lumley criterion indicates the development of the inertial range with increasing Reynolds number.

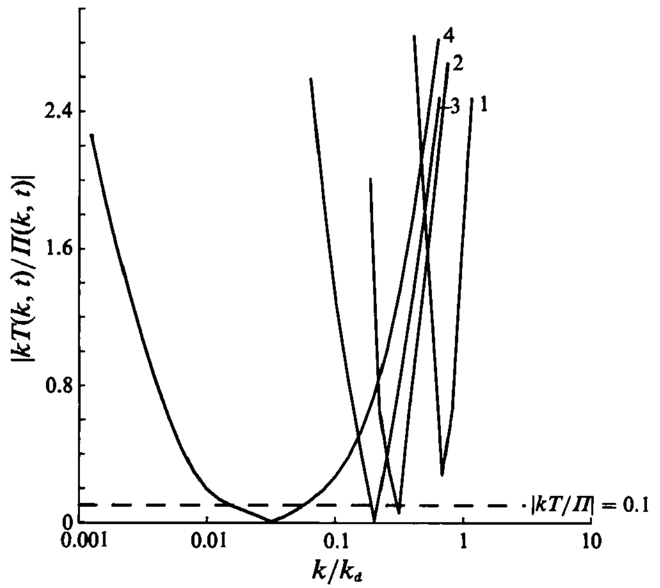

FIGURE 5. Variation of evolved $|kT(k,t)/\pi(k,t)|$ with Reynolds number: LET results. 1, test problem 2 ($R_\lambda = 4.7$); 2, test problem 1 ($R_\lambda = 16.2$); 3, test problem 3 ($R_\lambda = 40.7$); 4, test problem 4 ($R_\lambda = 1040$).

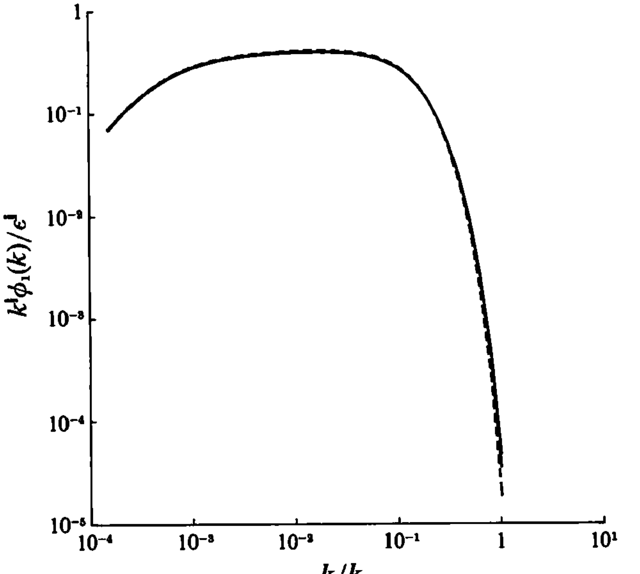

FIGURE 6. Evolved normalized one-dimensional energy spectrum for test problem 4: comparison of results from LET, DIA and SCF. ————, LET; $t = 0.6$, $R_\lambda(t) = 1040$; ————, DIA; $t = 0.6$, $R_\lambda(\tau) = 1039$; – – – –, SCF; $t = 0.6$, $R_\lambda(t) = 1059$.

It should be clear from the above discussion that use of spectra to distinguish between one theory and another is likely to prove rather fraught. In figure 6, we show results for the one-dimensional energy spectrum, obtained by computing test problem 4 with LET, DIA and SCF. On this plot, we note that the three theories are virtually indistinguishable. It should also be noted that, with the normalization used in plotting this figure, a horizontal region in the spectrum corresponds to $-\frac{5}{3}$ scaling. On this basis, all three theories appear to be tangent to the Kolmogorov spectrum for an appreciable range of wavenumbers.

Basic spectral shape	Values of c in the initial spectrum shape $E_\theta(k,0) = c_1 k^{c_2} \exp(-c_3 k^{c_4})$: c_1	c_2	c_3	c_4	k_{bot}	k_{top}	ν	Pr	$E_\theta(0)$	$\epsilon_\theta(0)$	$R_L(0)$	$R_\lambda(0)$
I	0.00524	4	0.0884	2	0.917	29.3	0.0119	0.5	1.00	1.35	44.2	35.4
IV	0.4	1	0.5	1	0.281	35.9	0.008	0.5	1.59	1.23	133	58.5
V	$E_\theta(k,0) = (\frac{4}{3})\pi k^{-\frac{5}{3}}$				0.111	71.8	0.008	0.5	26.8	30.0	5521	245

TABLE 3. Scalar calculations: initial conditions

Initial spectrum	Final time/ eddy turnover time	Pr	E_θ	ϵ_θ	R_L	R_λ	$S_{u\theta}$
I	1.5	0.5	0.162	0.339	29.2	17.0	0.381
IV	0.75	0.5	0.784	0.739	124	43.4	0.346
V	0.38	0.5	22.9	5.09	5424	558	0.357

TABLE 4. Scalar calculations: evolved integral parameters

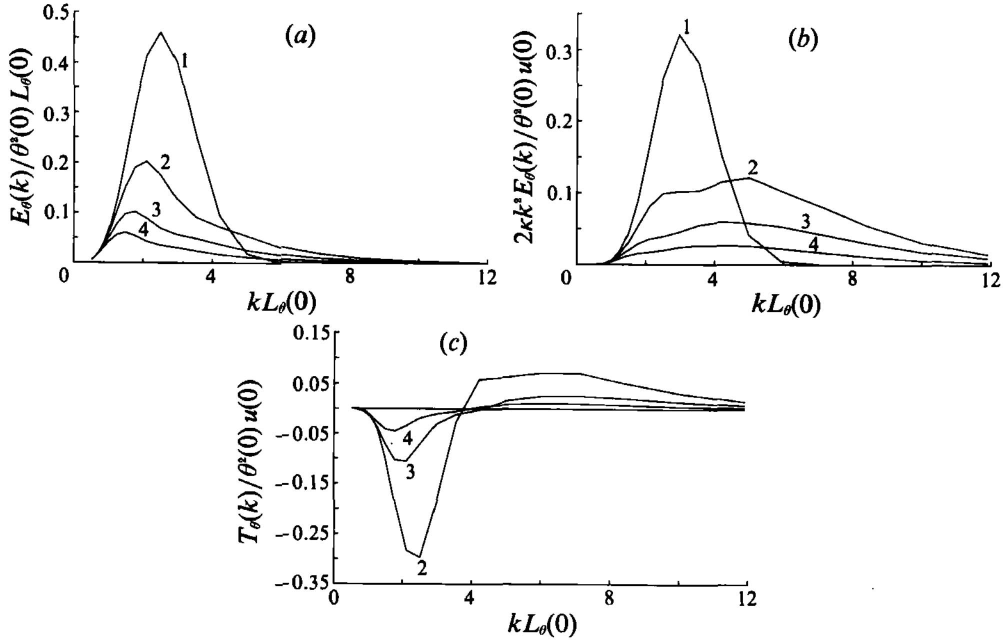

FIGURE 7. The evolution of (*a*) the scalar energy spectrum, (*b*) scalar dissipation spectrum, and (*c*) the scalar transfer spectrum. Basic spectral shape I, $R_\lambda(0) = 35.4$. 1, $tu(0)/L(0) = 0$; 2, $tu(0)/L(0) = 0.5$; 3, $tu(0)/L(0) = 1.0$; 4, $tu(0)/L(0) = 1.5$.

6.3. *Results for passive scalar convection*

Equations (5.12)–(5.14) were integrated forward in time using the same numerical methods as for the velocity field, and the same shapes for initial spectra, as given by (4.1). Values of the constants which determine the shape of the spectrum given by (4.1) can be found in table 3, along with the other initial values. In table 4, we give values of evolved integral parameters. As in the case of the velocity field, we covered a good range of Taylor–Reynolds numbers; and also, in this case, three values of the Prandtl number, namely 0.1, 0.5 and 1.0. details of all these calculations and their results may be found in the thesis by Filipiak (1991).

Here we show in figures 7–9 the evolution in time of decaying scalar spectra E_θ, $2\kappa k^2 E_\theta$ and T_θ, for a Prandtl number of $Pr = 0.5$, and evolved Taylor–Reynolds numbers of 15, 40 and 550, respectively. Various forms of scaling were tried, in order to demonstrate self-similarity in time of these results (Filipiak 1991). It was found that, at medium-to-low Reynolds numbers, scaling based on scalar integral scales gave the best collapse of the scalar energy spectrum but, at the highest Reynolds numbers, the most effective form of scaling was that based on the Kolmogorov variables. However, in the case of the dissipation and transfer spectra, Kolmogorov scaling gave the best collapse of data at all Reynolds numbers.

The high-Reynolds-number case is particularly interesting, as it has been experimentally confirmed (see, for instance, Champagne, Friehe & LaRue 1977) that the scalar spectrum should take the form

$$E_\theta(k) = \beta \epsilon_\theta \epsilon^{-\frac{1}{3}} k^{-\frac{5}{3}}, \tag{6.4}$$

for the inertial–convective range of wavenumbers, provided that we have

$$k < k_{OC} \quad \text{for} \quad Pr < 1. \tag{6.5}$$

This is found to be the case for the LET results, with the range of wavenumbers where the dissipation occurs becoming more distinct from the range where scalar

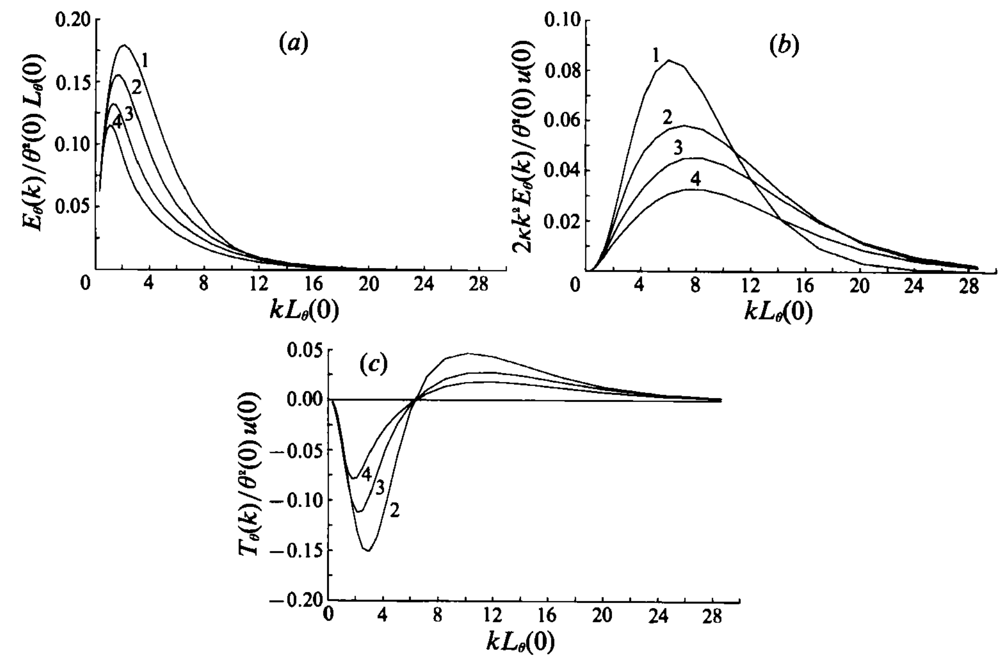

FIGURE 8. The evolution of (*a*) the scalar energy spectrum, (*b*) the scalar dissipation spectrum, and (*c*) the scalar transfer spectrum. Basic spectral shape IV, $R_\lambda(0) = 58.5$. 1, $tu(0)/L(0) = 0$; 2, $tu(0)/L(0) = 0.25$; 3, $tu(0)/L(0) = 0.5$; 4, $tu(0)/L(0) = 0.75$.

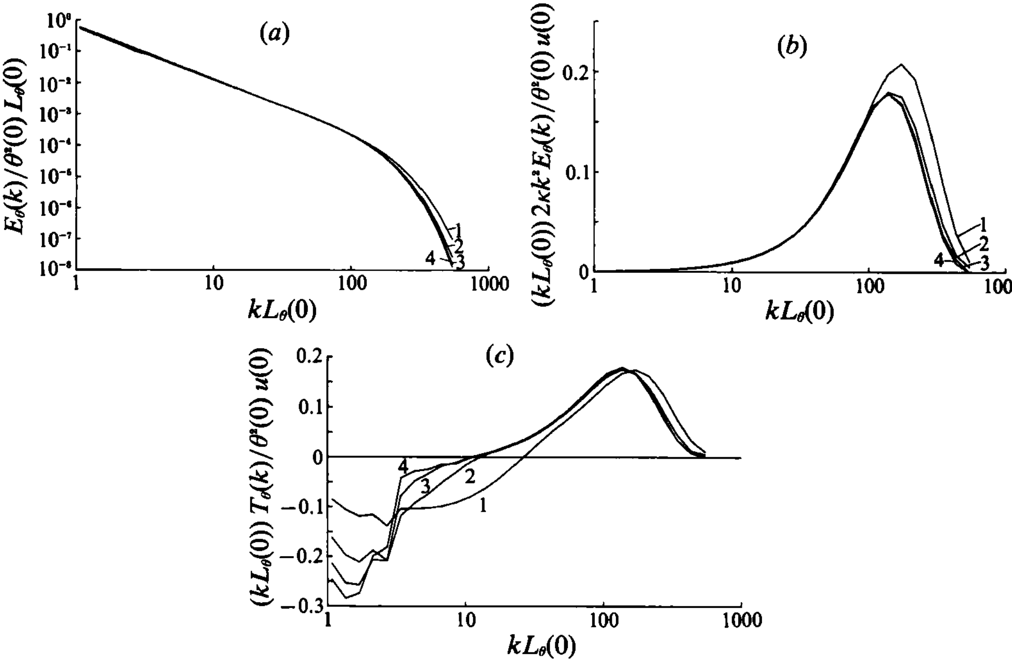

FIGURE 9. The evolution of (*a*) the scalar energy spectrum, (*b*) the scalar dissipation spectrum, and (*c*) the scalar transfer spectrum. Basic spectral shape V, $R_\lambda(0) = 245$. 1, $tu(0)/L(0) = 0.08$; 2, $tu(0)/L(0) = 0.18$; 3, $tu(0)/L(0) = 0.28$; 4, $tu(0)/L(0) = 0.38$.

production occurs, as the Reynolds number increases: see figures 7(*c*), 8(*c*) and 9(*c*). The value of the Oboukhov–Corrsin constant is found to be $\beta = 1.1$ and the value of the Kolmogorov constant is found to be $\alpha = 2.5$ for this computation. These values are rather larger than the accepted experimental values ($0.7 < \beta < 0.8$ and $1.5 < \alpha < 1.7$) but it is interesting to note that the ratio $\beta/\alpha = 0.45$ is close to the accepted experimental value 0.44 (Moeng and Wyngaard 1988).

We finish with brief comments on the scaling behaviour of the two-time correlations and the asymptotic values of the skewness factor, both topics upon which we have placed some emphasis in the past, when dealing with the velocity field (see II, III).

On the first of these topics, we were interested in comparing convective scaling of two-time correlations with inertial-range scaling. In the scalar case we found much the same behaviour as we had with the velocity field. At low-to-medium Reynolds numbers, convective scaling seemed to be more effective at collapsing data, whereas at high Reynolds numbers, inertial-range scaling was distinctly better.

Lastly, the mixed velocity-scalar skewness $S_{u\theta}$ can be defined by analogy with (4.12), for the skewness of one-dimensional derivative of the velocity field. Unfortunately, there are too few measurements of this quantity for one to come to any definite conclusion, except that the results of the LET calculation of $-S_{u\theta}$ give values of the order 0.3–0.5, depending on both Reynolds number and Prandtl number, and that these values are similar to those few results available from experiment (Antonia & Chambers 1980) and direct numerical simulation (Kerr 1985). Detailed results and some further discussion of this point will be found in the thesis by Filipiak (1991).

7. Conclusions

The LET theory would seem to have emerged from this exercise quite well. Its derivation is simpler; some inconsistencies have been eliminated; and a minor error has been corrected. As a result, the agreement with numerical experiment has been marginally improved; unphysical behaviour has been eliminated (in one case) or reduced (in another) and the computational effort required for numerical integration of the theory has been greatly reduced. Moreover, the performance of the theory in predicting scalar transport may be seen as an encouraging first step on the road to practical applications.

We conclude on a rather speculative note, by remarking that (3.15), which may now be seen as the basic *ansatz* of the LET theory, is identical to the fluctuation–dissipation relationship in a form which is not restricted to microscopic systems (Kubo 1966). Of course, an association between turbulence theory and the fluctuation–dissipation theorem (which is rigorously derived for fluctuations about thermal equilibrium), is not new. Herring (1966) noted that the relationship between SCF and DIA was of this form. More recently, Kaneda (1981) found that a variant of Kraichnan's Lagrangian-history theories led to a form of FDT, while Nakano (1988) has made a wave-packet analysis of DIA, and has associated the resulting equations with the FDT. The latter work is particularly interesting from our present point of view, as the result is apparently equivalent to a derivation of the LET response equation by a different method. All in all, the success of the propagator relationship given by (3.15) encourages one to wonder whether or not a viable turbulence theory can be obtained by truncating the renormalized perturbation expansion of the Navier–Stokes equation at second order and invoking a generalized fluctuation–dissipation theorem. This suggests a promising avenue to explore, in order to understand why a theory of this kind gives such good results, and this will be the subject of future work.

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