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Reassessment of the classical closures for scalar turbulence

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In deducing the consequences of the Direct Interaction Approximation, Kraichnan was sometimes led to consider the properties of special classes of nonlinear interactions in degenerate triads in which one wavevector is very small. Such interactions can be described by simplified models closely related to elementary closures for homogeneous isotropic turbulence such as the Heisenberg and Leith models. These connections can be exploited to derive considerably improved versions of the Heisenberg and Leith models that are only slightly more complicated analytically. This paper applies this approach to derive some new simplified closure models for passive scalar advection and investigates the consistency of these models with fundamental properties of scalar turbulence. Whereas some properties, such as the existence of the Kolmogorov–Obukhov range and the existence of thermal equilibrium ensembles, follow the velocity case closely, phenomena special to the scalar case arise when the diffusive and viscous effects become important at different scales of motion. These include the Batchelor and Batchelor–Howells–Townsend ranges pertaining, respectively, to high and low molecular Schmidt number. We also consider the spectrum in the diffusive range that follows the Batchelor range. We conclude that improved elementary models can be made consistent with many nontrivial properties of scalar turbulence, but that such models have unavoidable limitations.

Keywords: isotropic turbulence; homogeneous turbulence; passive scalar turbulence; solvable or simplified models; turbulent mixing

1. Introduction

The quadratic nonlinearity of the Navier–Stokes equation is expressed in the Fourier representation by the condition that modes with wavevectors $\mathbf{p}$ and $\mathbf{q}$ interact to excite mode $\mathbf{k}$, subject to the 'triad condition' $\mathbf{k} = \mathbf{p} + \mathbf{q}$. The first attempts to model energy transfer in homogeneous isotropic turbulence by Kovasznay, Heisenberg, Obukhov, and many others [1], which might be called the *classical turbulence closures*, ignored this 'triadic' structure, so that the Navier–Stokes nonlinearity had no explicit role in their formulation. Batchelor [2] criticized these models on precisely these grounds. Whatever its defects are, the quasinormality theory [1] did incorporate the Navier–Stokes nonlinearity explicitly, through geometric factors linked to triad interactions, as did Kraichnan's direct interaction approximation (DIA) [3] and its various modifications.

The oversimplifications inherent in the classical closures result in numerous difficulties, including questionable or even extremely unrealistic predictions of the dissipation range [1], and other defects like forward-only energy transfer and inability to fill unexcited modes by nonlinear interactions alone [4,5]. Although these problems are addressed by

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analytical closures of the DIA family, these theories have some practical drawbacks. Whereas classical closures appeal to easily grasped physical pictures (or perhaps, cartoons), like stepwise cascade and eddy viscosity, the derivation of analytical closures, including the quasinormality theory, may seem abstract and unintuitive. Moreover, whereas their analytical simplicity makes computational implementation of the classical closures quite straightforward, computational implementation of DIA-based closures is actually quite difficult. Considerations like these make the classical closures rather attractive.

Thus, some practical compromise between simplicity and theoretical rigor could be a desirable feature of a class of models intermediate between DIA and the classical closures. One such model is the model for inhomogeneous turbulence by Besnard et al. [6]. Canuto and Dubovikov [7] have developed and applied such models to a variety of problems including shear and rotating turbulence. In [4] and [5], it is shown that models closely related to the Leith and Heisenberg models result from taking suitable limits of DIA-based closures. These models are only slightly more complex than the original closures, and thus retain their appealing analytical simplicity, but overcome many of their theoretical limitations.

The present paper applies these methods to the problem of passive scalar advection by a random velocity field. Both the classical closures and the improved models suggested by analytical closures of the DIA family are easily extended to the scalar case. Although the linearity of passive scalar dynamics simplifies the problem significantly, new possibilities arise when the diffusivity and viscosity are of different orders of magnitude, or equivalently, when the Schmidt number is very large or very small. Then diffusive and viscous effects become important at different scales of motion; the difference leads to the *Batchelor* [8] (or viscous-convective) and *Batchelor–Howells–Townsend* [9] (or inertial-diffusive) ranges, which occur at high and low molecular Schmidt number, respectively. Another problem unique to scalar turbulence is the behavior of the scalar spectrum in the diffusive range following the Batchelor range. We consider the consistency of closures for scalar turbulence with these ranges. A new version of the scalar Leith model [10] can be consistent with the Batchelor range and the correct Batchelor diffusive range, but not with the Batchelor–Howells–Townsend range. Conversely, scalar Heisenberg models are necessarily inconsistent with the Batchelor range, but a modified Heisenberg model can predict a Batchelor–Howells-Townsend range. In all cases, consistency is demonstrated for our new models, not for the original ‘classical’ formulations; this fact supports the reformulation of classical closures. On the other hand, whereas Kraichnan has demonstrated the consistency of the Lagrangian History DIA with all of these scaling regimes [11], the failure of any one simplified model to be consistent with all of them demonstrates that such models have unavoidable limitations.

2. Classical closures for scalar turbulence

The spectrum $C(k)$ of the variance of a passive scalar θ advected by a statistically homogeneous and isotropic random velocity field u_i satisfies

$$\dot{C}(k) = P_\theta(k) - \frac{\partial \mathcal{F}_\theta}{\partial k} - 2\mathcal{D}k^2 C(k), \tag{1}$$

where $P_\theta(k)$ is the spectrum of a source of scalar fluctuations, $\mathcal{D}$ is the scalar diffusivity, and the scalar flux is

$$\mathcal{F}_\theta(k) = \Im \int_{|\mathbf{k}|\le k} d\mathbf{k} \int d\mathbf{p}d\mathbf{q}\; \delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) k_p \langle u_p(\mathbf{p})\theta(\mathbf{q})\theta(-\mathbf{k})\rangle. \tag{2}$$

The time argument is understood but not written explicitly.

The linearity of the advection equation in θ implies that any closure for $\mathcal{F}_\theta$ must be linear in the scalar spectrum. This condition makes it trivial to extend the original Heisenberg, Leith, and Kovasznay models [1,12] to the scalar case:

$$\mathcal{F}_\theta(k) = \mathsf{C}\int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dp\ \sqrt{\frac{E(p)}{p^3}} \quad \text{(Heisenberg)} \tag{3}$$

$$\mathcal{F}_\theta(k) = \mathsf{C}\sqrt{k^3 E(k)} k^4 \frac{\partial}{\partial k}\left[\frac{C(k)}{k^2}\right] \quad \text{(Leith)} \tag{4}$$

$$\mathcal{F}_\theta(k) = \mathsf{C}\sqrt{k^3 E(k)} k C(k) \quad \text{(Kovasznay)}, \tag{5}$$

where $E(k)$ is the energy spectrum of the velocity field and C denotes a constant, but not necessarily the same constant each time it appears. The arguments justifying these models follow the arguments justifying the velocity models very closely: the Heisenberg model equates the scalar flux to 'production' of scalar variance at scale k by an 'eddy diffusivity' (the second integral) multiplying the square of the scalar gradient (the first integral); the Kovasznay model states that the scalar flux is the product of a frequency at scale k, namely $\sqrt{k^3 E(k)}$, and a measure of the scalar variance at scale k, namely $kC(k)$. The Leith model simply adds a diffusive contribution to the Kovasznay model. The Leith model (1967) is much newer than the Kovasznay and Heisenberg models (1948), but its formulation in terms of the wavenumber k alone, without explicit reference to 'triad' geometry, justifies grouping it with what we have called 'classical' models. Leith's velocity model [12] suggests a more general form of Equation (4); however, we follow [10] and [13] in formulating a special case consistent with the existence of equilibrium ensembles. This point will be discussed more fully later.

Although these equations state the *scalar* Heisenberg, Leith, and Kovasznay models, we omit 'scalar' in what follows. These models have been formulated for any velocity spectrum $E(k)$; no assumptions have been made about the analytical form of this spectrum or about how it has been obtained.

Although the Kovasznay model is not suggested by analytical theory, it is included because it is the simplest conceivable model, and because it occurs in any argument based entirely on dimensional analysis with an implicit locality assumption [14]. Formally, the Kovasznay model is a limit of the Heisenberg model, since if we cut-off the interactions in the Heisenberg model so that

$$\mathcal{F}_\theta(k) = \mathsf{C}(\lambda)\int_{k/\lambda}^k d\kappa\ \kappa^2 C(\kappa) \int_k^{\lambda k} dp\ \sqrt{\frac{E(p)}{p^3}} \tag{6}$$

and adjust $\mathsf{C}(\lambda)$ so that the limit $\lambda \to 1$ is nonzero, the result will be the Kovasznay model. We remark that the effect of finite $\lambda < \infty$ in Equation (6) is obviously to reduce the effect of distant interactions; in fact, Orszag [15] had suggested that modifying the Heisenberg model to reduce the effect of extremely distant interactions produces a more realistic model; however, we will not pursue this point. The completely local interactions described by the Kovasznay model correspond to the intuitive idea of a stepwise cascade.

We briefly summarize previous work connecting classical closures to analytical closure based on DIA; more details appear in the Appendix. In [4], it was shown following [16] that considering only degenerate wavevector triads corresponding to distant interactions such that $0 \approx k \ll p, q$ (here, $k = |\mathbf{k}|$, $p = |\mathbf{p}|$, and $q = |\mathbf{q}|$, and the triad condition $\mathbf{k} = \mathbf{p} + \mathbf{q}$ is assumed) in DIA, and making some other simplifications of the triad relaxation time leads to a model with the structure of the classical Heisenberg model.[1] For the scalar, the analogous result is

$$\mathcal{F}_\theta(k) = \mathsf{C} \int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dp\ \Theta_T(\kappa, p) E(p), \tag{7}$$

where Θ_T is a relaxation time corresponding to a pair of modes, rather than a triad as in DIA-based models. Although the derivation begins with DIA, in which no arbitrary constants appear, the interactions isolated to arrive at Equation (7) do not conserve scalar variance among themselves. Imposing conservation requires introducing an arbitrary constant, which could be chosen to match a known form of the Kolmogorov–Obukhov scalar spectrum [1].

Adding a class of local interactions such that $0 \approx q \ll k \approx p$ leads to a generalized Heisenberg model [4]; the scalar analog is

$$\begin{aligned}\mathcal{F}_\theta(k) = \mathsf{C} \Bigg\{ &- \int_0^k d\kappa\ \kappa^4 \int_k^\infty dp\ \Theta_T(\kappa, p) \frac{C(p)E(p)}{p^2} \\ &+ \int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dp\ \Theta_T(\kappa, p) E(p) \Bigg\}.\end{aligned} \tag{8}$$

The second term on the right side coincides with the Heisenberg model; the first term gives a scalar analog of the 'backscatter' term in the velocity model. Because of this term, the scalar flux can take either sign, whereas in Equation (7), the flux is necessarily positive. A somewhat different treatment of local interactions leads to a generalized Leith model [5]. The scalar analog is

$$\mathcal{F}_\theta(k) = -\mathsf{C} \left[\int_0^k d\kappa\ \kappa^2 E(\kappa) \Theta_T(\kappa, k) \right] k^4 \frac{\partial}{\partial k} \left[\frac{C(k)}{k^2} \right]. \tag{9}$$

In the interest of simplicity, following our previous work [4] on the velocity field models, the timescales in Equations (7)–(9) are further abridged by replacing the pair relaxation time by a single-mode relaxation time determined by the larger wavenumber. Although the models with a pair relaxation time might be interesting, reduction to a single-mode relaxation time does not appear to compromise any important theoretical property. The result is a set of models closer to the classical models than Equations (7)–(9), but more general than the original models Equations (3)–(5). We propose then the modified Heisenberg model,

$$\mathcal{F}_\theta(k) = \mathsf{C} \int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dp\ \Theta_T(p) E(p) \quad \text{(modified Heisenberg)}, \tag{10}$$

the modified Leith model

$$\mathcal{F}_\theta(k) = -\mathsf{C} \left[\int_0^k d\kappa\ \kappa^2 E(\kappa) \right] \Theta_T(k) k^4 \frac{\partial}{\partial k} \left[\frac{C(k)}{k^2} \right] \quad \text{(modified Leith)} \tag{11}$$

and, by simply evaluating the integrands in Equation (10) at the same wavenumber k and multiplying by k^2 to make the units consistent, the modified Kovasznay model,

$$\mathcal{F}_\theta(k) = \mathsf{C}k^3 E(k)\Theta_T(k)kC(k) \quad \text{(modified Kovasznay).} \tag{12}$$

We can add the scalar version of the 'generalized Heisenberg model' [4]

$$\mathcal{F}_\theta(k) = \mathsf{C}\left\{\int_0^k d\kappa\ \kappa^2 C(\kappa)\int_k^\infty dp\ \Theta_T(p)E(p) - \int_0^k dq\ q^4\int_k^\infty dp\ \Theta_T(p)\frac{C(p)E(p)}{p^2}\right\}. \tag{13}$$

The limit discussed in connection with Equation (6) that leads from the Heisenberg model to the Kovasznay model can be applied to Equations (10) and (12) as well. The same limiting process applied to Equation (13) yields the Leith model, but we acknowledge that this analysis is purely formal.

Following [4], we suggest the following models for Θ_T:

$$\dot{\Theta}_T(k) = 1 - \eta_T(k)\Theta_T(k) - \mathcal{D}k^2\Theta_T(k) \tag{14}$$

$$\dot{\Theta}_T(k) = 1 - \eta_T(k)\Theta_T(k) \tag{15}$$

$$0 = 1 - \eta_T(k)\Theta_T(k) - \mathcal{D}k^2\Theta_T(k) \tag{16}$$

$$0 = 1 - \eta_T(k)\Theta_T(k). \tag{17}$$

The first equation imitates the structure of Kraichnan's test-field model [17,18]; the subsequent equations are steady-state and/or nondiffusive simplifications. A consequence of the dependence on k alone is suppression of the viscosity dependence of the scalar timescale in the theory of [18]. The frequency $\eta_T(k)$ can be modeled by the algebraic expression,

$$\eta_T(k) = \mathsf{C}\Theta_T(k)k^3 E(k) \tag{18}$$

or by the integral expression, again obtained by imitating Kraichnan's theories,

$$\eta_T(k) = \mathsf{C}\Theta_T(k)\int_0^k d\kappa\ \kappa^2 E(\kappa). \tag{19}$$

The formulation of Equations (10)–(12) in terms of a timescale Θ_T is useful because in some cases, 'external agencies' like rotation and shear can be modeled by suitably generalizing Θ_T; for the velocity case, compare, for example [14,19].

The velocity field models suggested in [4] differ analytically from Equations (14)–(19) only in the appearance of the scalar diffusivity instead of the viscosity. However, although Equations (70) and (71) in [4], rewritten in the present notation, formulate the model

$$\eta(k) = c_\eta\Theta(k)\int_0^k d\kappa\ \kappa^2 E(\kappa),$$

where η and Θ now pertain to the velocity field, the proportionality constant c_η need not equal the corresponding constant C in Equation (19). On the contrary, the ratio c_η/C is a 'turbulent Schmidt number.'

In a more complete theory like DIA, such constants are computed in terms of scalar and velocity field *response functions* [3], which are not the same, and which reflect the relative differences of scalar transfer compared to momentum transfer. A more precise link between the semi-phenomenological models proposed here and the much more sophisticated timescale modeling in comprehensive closure theories is beyond the scope of this paper.

The simplest timescale model combines the nondiffusive static model Equation (17) with the algebraic frequency model Equation (18). The result is

$$\Theta_T(k) = \mathsf{C}\frac{1}{\sqrt{k^3 E(k)}}. \tag{20}$$

Substituting Equation (20) in Equations (10) and (12) reproduces the classical Heisenberg and Kovasznay models Equations (3) and (5), respectively.

A simple way to move beyond the classical models is to combine Equation (17) with the integral model Equation (19), so that

$$\Theta_T(k) = \mathsf{C}\frac{1}{\sqrt{\int_0^k d\kappa\ \kappa^2 E(\kappa)}}. \tag{21}$$

Substituting Equation (21) in Equation (11) gives the modified Leith model,

$$\mathcal{F}_\theta(k) = \mathsf{C}\sqrt{\int_0^k d\kappa\ \kappa^2 E(\kappa)}k^4 \frac{\partial}{\partial k}\left[\frac{C(k)}{k^2}\right] \quad \text{(LWN)}, \tag{22}$$

advocated in [13]. Following the terminology of that reference, we can call it the scalar LWN (local wave-number) model.

Another possibility not envisioned in the classical models is diffusive damping of the timescale. Combining Equations (16) and (18), the timescale is found by solving

$$k^3 E(k)\Theta_T(k)^2 + \mathcal{D}k^2\Theta_T(k) = 1. \tag{23}$$

The positive solution has the limits

$$\Theta_T \sim \begin{cases} \left(k^3 E(k)\right)^{-1/2} & \text{if } k^3 E(k) \gg \mathcal{D}k^2 \\ \left(\mathcal{D}k^2\right)^{-1} & \text{if } k^3 E(k) \ll \mathcal{D}k^2. \end{cases} \tag{24}$$

The diffusive limit is important for the Batchelor–Howells–Townsend spectrum discussed later.

The introduction of a timescale evolution equation as in Equations (14) and (15) departs further from the classical models: if steady-state models like Equations (20) and (21) are combined with the corresponding steady-state timescale models for the velocity field [4], the result is proportionality of the scalar and velocity timescales; the proportionality constant will be the 'turbulent Schmidt number' noted earlier. However, if the scalar and velocity timescales satisfy evolution equations, then there is no simple universal relation between them. We believe that this observation may be applicable to 'advanced' single-point models that allow a variable ratio of the turbulent diffusivity and eddy viscosity; however, such developments must be left to future research.

Eliminating the diffusion term in Equation (22) results in a modified Kovasznay model,

$$\mathcal{F}_\theta(k) = \mathsf{C}\sqrt{\int_0^k d\kappa\ \kappa^2 E(\kappa)}kC(k) \quad \text{(Ellison)}, \tag{25}$$

which might be called the scalar *Ellison* model [1]. This model is more consistent with the elementary character of the Kovasznay model than the result of substituting Equation (21) in Equation (12).

Our experience with the velocity models suggests that the models of Equations (22) and (25) should be very much superior to the models of Equations (4) and (5), and this expectation will be confirmed: just as for the velocity field, some dependence on distant interactions appears indispensable for any realistic model of scalar turbulence. We note, however, that introducing the integral timescale of Equation (21) in Equation (10) leads to numerical instabilities; compare [4] for the velocity field.

3. Constraints on models of scalar turbulence

Like closures for the velocity field, closures for scalar turbulence must satisfy some basic general constraints. Two of them: the existence of a constant flux scalar Kolmogorov–Obukhov (or inertial-convective) range and the scalar equipartition ensemble are formulated by analogy to the velocity case as follows.

(1) *Existence of a Kolmogorov–Obukhov range:* If the velocity field is in a Kolmogorov steady state with dissipation rate ϵ, the constant scalar flux condition $\mathcal{F}_\theta = \chi =$ constant should permit the solution,

$$C(k) = \mathsf{C}\chi\epsilon^{-1/3}k^{-5/3}, \tag{26}$$

where χ is the scalar dissipation rate

$$\chi = \int_0^\infty dk\ 2\mathcal{D}k^2C(k). \tag{27}$$

(2) *Equipartition solution:* The *nondiffusive truncated system* for the passive scalar, defined by $\mathcal{D} = 0$ and the spectral truncation $k \leq k_{\max}$, should permit the solution $\mathcal{F}_\theta = 0$ with an equipartition spectrum,

$$C(k) \sim k^2. \tag{28}$$

This solution should exist for advection by an arbitrary solenoidal velocity field [11]. Although the possibility of equipartition may seem somewhat esoteric, it has important qualitative consequences for models: if it is satisfied, then both 'forward' (large to small scale) and 'backward' (small to large scale) transfer of scalar excitation must be possible. This issue will be discussed in more detail later.

If the molecular diffusivity and viscosity are not of comparable magnitude, then diffusive and viscous effects in the scalar and velocity spectra can exist at different scales of motion. Consequently, scalar spectra with no direct analog in the velocity case are possible: scalar fluctuations can persist even when the velocity fluctuations are damped by viscosity; conversely, the scalar fluctuations can be damped by diffusivity even when significant velocity fluctuations exist. When the velocity field exhibits a Kolmogorov inertial range, these possibilities define the *Batchelor* [8] and *Batchelor–Howells–Townsend* [9] ranges, respectively. Denoting the inverse Kolmogorov scale by $k_d \propto (\epsilon/\nu^3)^{1/4}$, where ν is the viscosity, these additional basic constraints are formulated as follows.

(3) *Possibility of a Batchelor range:* If the velocity field is in a Kolmogorov steady state, and scalar fluctuations persist when $k \gg k_d$, then the constant scalar flux condition is satisfied by the Batchelor spectrum,

$$C(k) = \mathsf{C}\sqrt{\frac{\nu}{\epsilon}}\chi k^{-1}. \tag{29}$$

This spectrum is expected to exist in the range $k_d \ll k \ll k_B$, where k_B is the wavenumber at which the viscous frequency κk_B^2 equals the Kolmogorov frequency $\sqrt{\epsilon/\nu}$; as $k_B \sim (\epsilon/\mathcal{D}^2\nu)^{1/4} = Sc^{1/2}k_d$, where $Sc = \nu/\mathcal{D}$ is the Schmidt number, the Batchelor range can exist when the Schmidt number is very large.

(4) *Possibility of a Batchelor–Howells–Townsend range:* If the velocity field is in a Kolmogorov steady state, and scalar fluctuations are damped by molecular diffusivity when $k \ll k_d$, then the scalar fluctuations can exhibit a power-law diffusive range of the form,

$$C(k) = \mathsf{C}\chi\frac{\epsilon^{2/3}}{\mathcal{D}^3}k^{-17/3}. \tag{30}$$

This spectrum is expected to exist for $k \gg k_{\text{BHT}}$, where k_{BHT} is a wavenumber at which the Kolmogorov viscosity $\epsilon^{1/3}k^{-4/3}$ equals the scalar diffusivity $\mathcal{D}$. As $k_{\text{BHT}} = (\epsilon/\mathcal{D}^3)^{1/4} = Sc^{3/4}k_d$, this range can exist if the Schmidt number Sc is very small.

It may also be useful to recall the arguments for the spectra Equations (29) and (30). The derivation of Equation (29) assumes that when the Batchelor range exists, the scalar field is randomly strained by the velocity field. Since necessarily $C(k) \propto \chi$ and the total strain is proportional to $\sqrt{\epsilon/\nu}$, the Kolmogorov frequency of the velocity field, dimensional analysis gives Equation (29). The spectrum Equation (30) applies when power-law velocity fluctuations act against scalar diffusivity. The dominant balance in such a range is [9]

$$\mathbf{u} \cdot \nabla\theta = \mathcal{D}\nabla^2\theta. \tag{31}$$

Squaring and assuming that $\mathbf{u}$ and θ are independent gives the spectral balance,

$$E(k)\frac{\chi}{\mathcal{D}} = \mathcal{D}^2k^4C(k). \tag{32}$$

Equation (30) follows by substituting a Kolmogorov spectrum for $E(k)$. Despite its power-law form, this spectral law does not express a constant flux condition. We should add that the actual existence of the Batchelor–Howells–Townsend range remains a topic of occasional discussion [20,21], but we consider it as at least theoretically plausible because it is supported by a simple, elementary argument.

We next consider the consistency of closures with each of these ranges in turn.

3.1. *Kolmogorov–Obukhov range*

Because the Kolmogorov–Obukhov range is a nondiffusive steady state, all of the timescale models reduce to either Equations (20) or (21), and for Kolmogorov scaling, both equations give

$$\Theta_T(k) \propto \left(\epsilon^{1/3}k^{2/3}\right)^{-1}. \tag{33}$$

The constant flux states with $\mathcal{F}_\theta = \chi$ are therefore found for each model as follows.

3.1.1. *Kovasznay and Leith models*

For the Kovasznay model,

$$\chi = \mathsf{C}\epsilon^{1/3}k^{5/3}C(k) \tag{34}$$

so that $C(k)$ has the required form Equation (26). For the Leith model,

$$\mathsf{C}\chi\epsilon^{-1/3}k^{-14/3} = \frac{d}{dk}\left[\frac{C(k)}{k^2}\right]. \tag{35}$$

has a solution $C(k) \sim k^{-5/3}$.

3.1.2. *Heisenberg and generalized Heisenberg models*

In both of these models,

$$\int_k^\infty dp\ \Theta_T(p)E(p) \propto \epsilon^{1/3}k^{-4/3}, \tag{36}$$

therefore the constant scalar flux condition for the Heisenberg model is

$$\chi\epsilon^{-1/3}k^{4/3} = \mathsf{C}\int_0^k d\kappa\ \kappa^2 C(\kappa). \tag{37}$$

Differentiating with respect to k gives the required solution. For the generalized Heisenberg model, the constant scalar flux condition is

$$\chi = \mathsf{C}\left\{\epsilon^{1/3}k^{-4/3}\int_0^k d\kappa\ \kappa^2 C(\kappa) - \frac{1}{5}k^5\int_k^\infty dp\ \epsilon^{1/3}p^{-13/3}C(p)\right\}. \tag{38}$$

Direct substitution shows the existence of the required solution. In all cases, the constant C could be chosen by requiring agreement with an observed value of the constant in Equation (26), the so-called 'Batchelor constant.'

3.2. *Equipartition solution*

3.2.1. *Classical Kovasznay and Heisenberg models*

For the Kovasznay model the zero flux condition $\mathcal{F}_\theta = 0$ forces $C(k) = 0$; the equipartition solution does not exist no matter how the timescale is determined. The same is obviously also true for the Heisenberg model. Returning to an earlier remark about equipartition and the direction of transfer, note that for both the Kovasznay and Heisenberg models, $\mathcal{F}_\theta$ is necessarily positive; thus, transfer of scalar excitation must be from large to small scales.

3.2.2. *Leith models*

All variants of the Leith model developed here contain the term $\partial(C/k^2)/\partial k$ and are therefore automatically consistent with vanishing scalar flux when $C \propto k^2$. Again referring to the connection between the direction of transfer and the equipartition property, all versions of the Leith model permit the scalar flux to take either sign.

3.2.3. *Generalized Heisenberg models*

Rewriting Equation (13) as

$$\mathcal{F}_\theta = \mathsf{C} \int_0^k d\kappa\, \kappa^4 \int_k^\infty dp\; \Theta_T(p) E(p) \left[\frac{C(\kappa)}{\kappa^2} - \frac{C(p)}{p^2} \right] \tag{39}$$

shows that the equipartition solution exists regardless of the timescale model, and that the flux vanishes for this solution. Note that the second integral must be cut-off at some large wavenumber in order that it can be absolutely convergent, but such a cut-off is consistent with the definition of the equilibrium ensemble. In this model as well, the scalar flux can have either sign.

3.3. ***Batchelor spectrum***

3.3.1. *Classical Kovasznay, Leith, and Heisenberg models*

Recall that the Batchelor spectrum has a constant scalar flux when the velocity spectrum is in its dissipation range. It is obvious that none of the classical models Equations (3)–(5) can support a constant scalar flux when $E(k)$ is exponentially small unless $C(k)$ becomes exponentially large. The Batchelor spectrum is impossible for all of these models.

3.3.2. *Modified Kovasznay and Leith models*

Consider the scalar flux models of Equations (22) and (25). In the Batchelor regime with $k \gg k_d$,

$$\int_0^k d\kappa\, \kappa^2 E(\kappa) \to \frac{\epsilon}{\nu}. \tag{40}$$

This nonzero limit is the crucial advantage of the integral expression Equation (19) over the algebraic model of Equation (18). For the Ellison model, imposing the constant scalar flux condition with Equation (25) gives

$$\chi = \sqrt{\frac{\epsilon}{\nu}} k C(k) \tag{41}$$

and Equation (29) follows immediately.

For the LWN model, Equation (22), the constant scalar flux condition

$$\chi = -\mathsf{C}\sqrt{\frac{\epsilon}{\nu}}k^4 \frac{d}{dk}\frac{C(k)}{k^2} \tag{42}$$

is obviously satisfied by the Batchelor spectrum Equation (29).

Equation (42) coincides with the result of Kraichnan's analysis [11] of the Batchelor range in the rapid change limit of the velocity field; compare also [18], where the Batchelor range is related to a diffusive limit of the test-field model.

3.3.3. *Scalar Heisenberg and generalized Heisenberg models*

It is evident in advance that the Heisenberg models cannot be consistent with the Batchelor spectrum because these models express the eddy diffusivity at any wavenumber k in terms of modes with wavenumbers *larger* than k, whereas the Batchelor spectrum requires the random straining of the scalar by modes with wavenumbers *smaller* than k. The physical mechanism responsible for the Batchelor spectrum is therefore inconsistent with the formulation of the scalar Heisenberg models. Under the conditions that generate the Batchelor spectrum, the constant scalar flux condition,

$$\chi = \mathsf{C}\int_0^k d\kappa\ \kappa^2 C(\kappa)\int_k^\infty dp\ \Theta_T(p)E(p) \tag{43}$$

cannot be satisfied by a power-law $C(k)$, because the second integral is exponentially small in the dissipation range $k \gg k_d$, regardless of how Θ_T is chosen. The backscatter term in the generalized Heisenberg model does not change this conclusion.

3.4. *The Batchelor diffusive range*

Batchelor [8] had originally proposed that the k^{-1} range is terminated by a scalar diffusive range proportional to e^{-ak^2}: this dependence followed from an assumption of effectively static straining by the velocity field of the scalar spectrum which is then averaged over an ensemble of strain fields. In a reconsideration of Batchelor's arguments, Kraichnan [11] suggested that this diffusive range will scale instead as e^{-ak}, the exponential decay found for the velocity field. This conclusion was the outcome of an assumption that the strain varied rapidly in time; the limit in which the velocity field is white noise in time has become known as the *Kraichnan model*.

The only scalar models consistent with the Batchelor range are the Ellison and LWN models Equations (25) and (22). Let us consider the diffusive range for each. For the Ellison model, the diffusive range of the Batchelor spectrum is found by solving

$$\frac{d}{dk}\sqrt{\frac{\epsilon}{\nu}}kC(k) + \mathcal{D}k^2C(k) = 0 \tag{44}$$

which has the solution

$$C(k) \propto k^{-1}e^{-\mathcal{D}\sqrt{\nu/\epsilon}k^2} \tag{45}$$

with the squared exponential diffusive range predicted originally by Batchelor. For the LWN model, we have instead

$$\frac{d}{dk}k^4\frac{d}{dk}\left(\frac{C}{k^2}\right)+\mathcal{D}k^2C(k)=0, \tag{46}$$

which simplifies to

$$\frac{4}{k}\frac{d}{dk}\left(\frac{C}{k^2}\right)+\frac{d^2}{dk^2}\left(\frac{C}{k^2}\right)=-\mathcal{D}\sqrt{\frac{\nu}{\epsilon}}\left(\frac{C}{k^2}\right) \tag{47}$$

with the asymptotic decaying solution

$$C(k)\propto k^2e^{-(\mathcal{D}^2\nu/\epsilon)^{1/4}k} \tag{48}$$

in agreement with the prediction of Kraichnan's refinement of Batchelor's argument. The prefactor k^2 in Equation (48) is related to a property of the Leith model noted earlier: consistency with an equipartition solution $C(k)\propto k^2$ in the limit of zero diffusivity. Note that Equation (45) does not lead to equipartition in the non-diffusive limit, but instead to an indefinitely long Batchelor scaling regime.

To understand the difference between these predictions, note that whereas Equation (47) coincides with Equation (3.12) of [11] for scalar advection in the 'rapid change' limit, Equation (44) is related to Equation (3.9) of the same reference, where the large-scale strain rate γ is $\sqrt{\epsilon/\nu}$ (note that Kraichnan's Ψ is the scalar mode density such that $k^2\Psi(k)\propto C(k)$.) According to Kraichnan, Equation (44) is appropriate if the straining is effectively static in each realization. Some further discussion is given in Appendix.

3.5. *Batchelor–Howells–Townsend spectrum*

To find this range, we solve the equation,

$$\frac{d}{dk}\mathcal{F}_\theta(k)=-2\mathcal{D}k^2C(k), \tag{49}$$

where the velocity is assumed to have a Kolmogorov scaling range.

3.5.1. *Kovasznay, Ellison, and Leith models*

The Kovasznay and Ellison models have the common form,

$$\frac{d}{dk}\left[\eta_T(k)kC(k)\right]=2\mathcal{D}k^2C(k) \tag{50}$$

with $\eta_T(k)\propto\sqrt{k^3E(k)}$ and $\eta_T(k)\propto\sqrt{\int_0^k d\kappa\;\kappa^2E(\kappa)}$, respectively. The solution of Equation (49) then has the form

$$\eta_T(k)kC(k)=\exp\left(-\int dk\;\frac{2\mathcal{D}k}{\eta_T(k)}\right). \tag{51}$$

No choice of η_T consistent with the present models yields the correct power law. Consider, for example, the limit of Equation (23) in which the scalar timescale is purely diffusive, $\Theta_T = 1/(\mathcal{D}k^2)$, so that $\eta_T \sim (\epsilon^{2/3}/\mathcal{D})k^{-2/3}$. Then $C(k) \sim k^{-5/3}\exp(-ak^{8/3})$, where $a \propto \mathcal{D}^2/\epsilon^{2/3}$.

The analysis for the Leith models is similar and leads to the same conclusion that the Batchelor–Howells–Townsend spectrum does not exist. For example, Leith [12] shows that the flux model Equation (4) leads to a solution in terms of exponentially decaying Bessel functions; this is qualitatively consistent with the results for the Kovasznay model. If the scalar timescale is purely diffusive, Equation (49) becomes

$$\frac{d}{dk}\left[\frac{\epsilon^{2/3}}{\mathcal{D}}k^{10/3}\frac{d}{dk}\frac{C(k)}{k^2}\right] \propto \mathcal{D}k^2 C(k) \tag{52}$$

and it can be verified directly that this equation has no power-law solution.

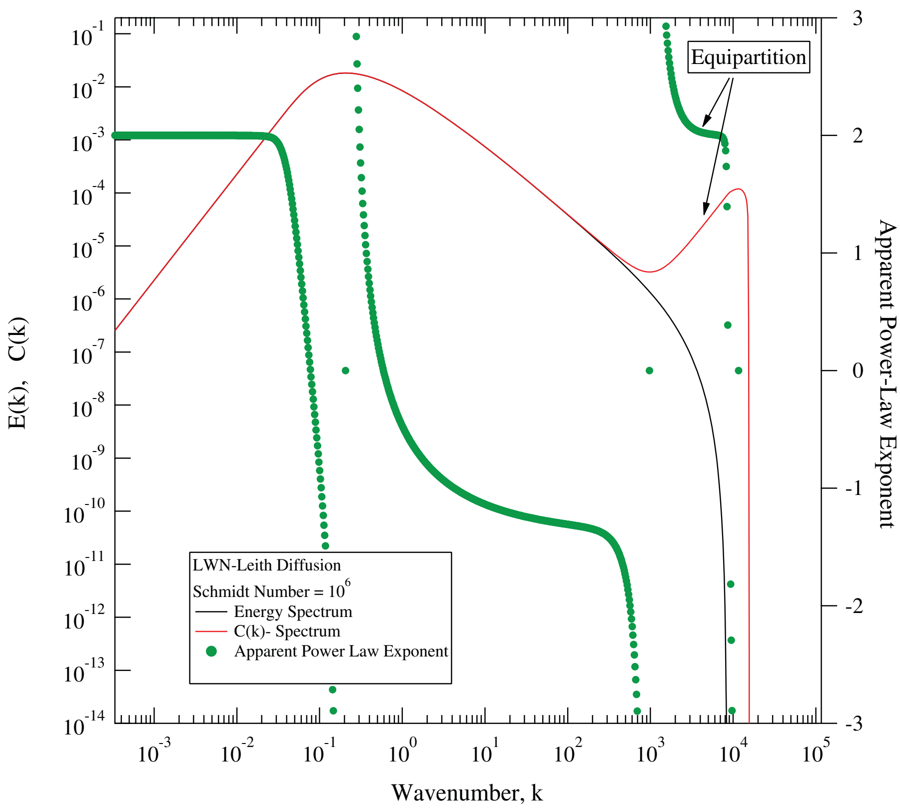

Figure 1. Scalar spectra for the Leith diffusion model at high Sc showing an equipartition at high wavenumbers. Note that the energy and scalar spectra terminate at high wavenumber.

3.5.2. *Heisenberg and generalized Heisenberg models*

Equation (49) takes the form

$$\frac{d}{dk}\int_0^k d\kappa\ \kappa^2 C(\kappa)\int_k^\infty dp\ E(p)\Theta_T(p) = 2\mathcal{D}k^2 C(k). \tag{53}$$

For scales in this spectral regime, scalar fluctuations are strongly damped, so that

$$\int_0^k d\kappa\ \kappa^2 C(\kappa) \approx \frac{\chi}{\mathcal{D}}. \tag{54}$$

Assuming, as we did for the scalar Kovasznay and Leith models, that Θ_T is dominated by molecular diffusivity according to the lower limit in Equation (24), we obtain

$$\frac{d}{dk}\frac{\chi}{\mathcal{D}}\frac{\epsilon^{2/3}k^{-2/3}}{\mathcal{D}k^2} = 2\mathcal{D}k^2 C(k) \tag{55}$$

and Equation (30) follows. This derivation requires the possibility of a viscous timescale; thus, the classical Heisenberg model is not consistent with this scalar spectrum. Because it

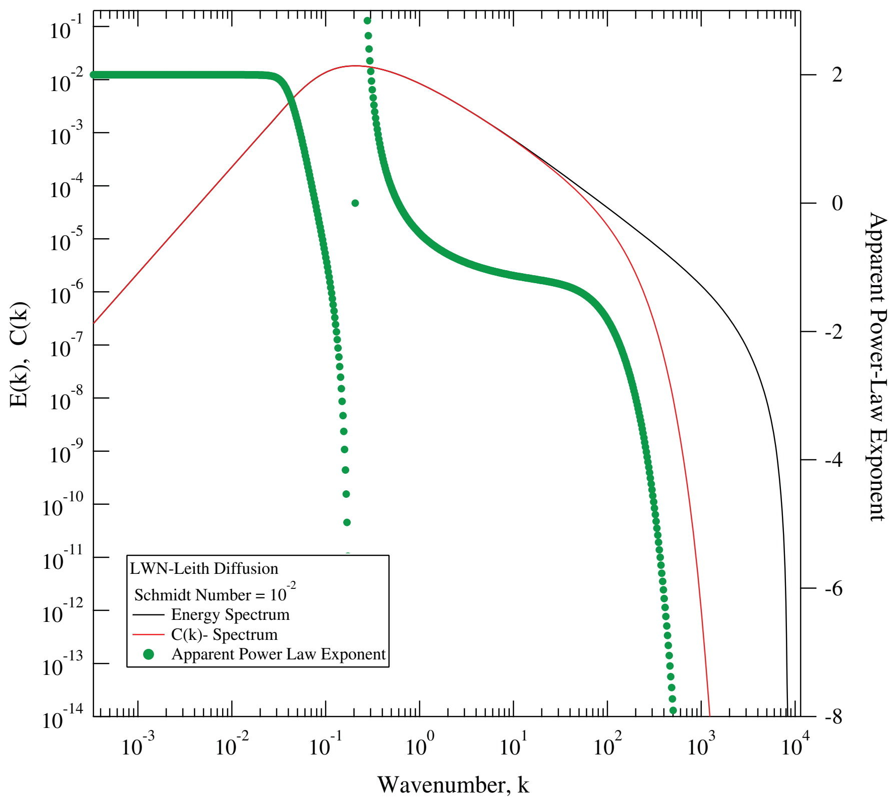

Figure 2. Scalar spectra for the Leith diffusion model at low Sc . Note that the energy and scalar spectra terminate at high wavenumber.

assumes that scalar damping is due to the velocity inertial range, it gives instead

$$C(k) = \mathsf{C}\frac{\chi}{\mathcal{D}^2}\epsilon^{1/3}k^{-13/3}. \tag{56}$$

To prove the existence of the Batchelor–Howells–Townsend spectrum for the generalized Heisenberg model, it is necessary to establish that the backscatter term cannot upset the relevant balance. Substituting the Batchelor–Howells–Townsend spectrum in the backscatter term gives

$$\frac{d}{dk}\int_0^k d\kappa\, \kappa^4 \int_k^\infty dp\, \Theta_p(p)\frac{E(p)C(p)}{p^2} \sim k^{-5}, \tag{57}$$

which is much smaller than $k^2C(k) \sim k^{2-17/3} = k^{-11/3}$ for large k. We conclude that the backscatter term decays more rapidly that the eddy damping term, and therefore does not change the balance in Equation (55) to leading order.

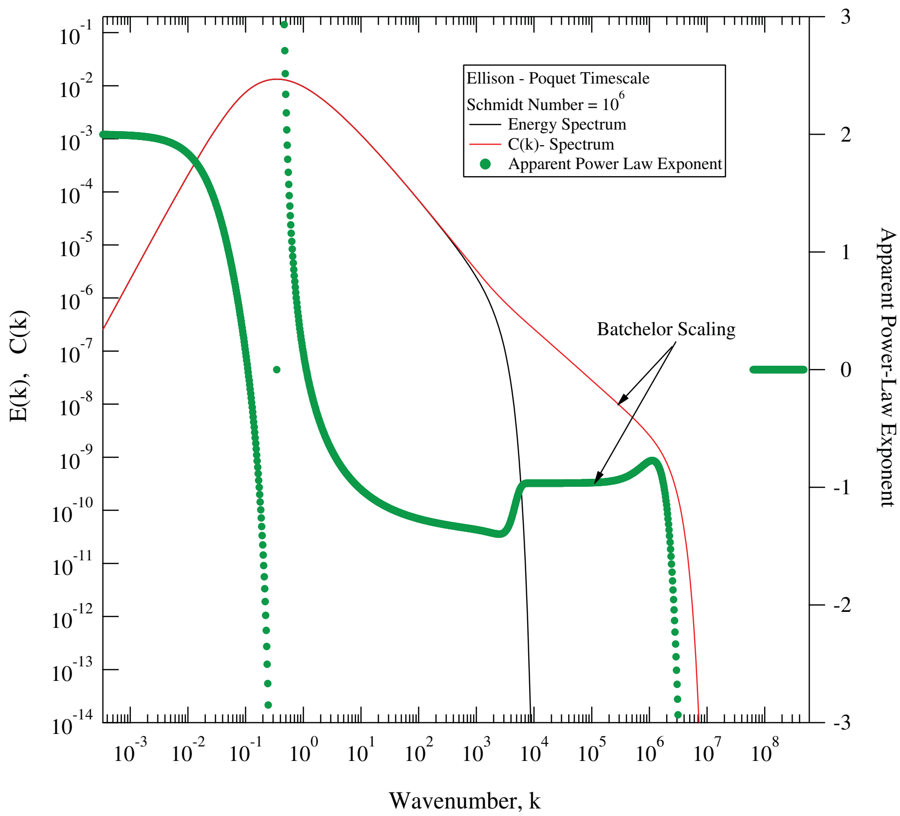

Figure 3. Scalar spectra for the Ellison model at high Sc showing equipartition at small scales.

In deriving the Batchelor–Howells–Townsend spectrum, we have assumed that the integral,

$$\int_0^\infty d\kappa\ \kappa^2 C(\kappa), \tag{58}$$

converges at infinity in order to assert Equation (54) for arbitrarily large k; clearly, the scaling $C(\kappa) \sim \kappa^{-17/3}$ is consistent with this assumption.

4. Model calculations

Calculations have been performed to demonstrate the predictions of these closures at high and low Schmidt numbers. The equations were solved using finite difference methods with second-order accuracy in time and space. To improve the computational efficiency, the equations are rewritten so that the wavenumber space, k, is logarithmic, *i.e.* we have equal increments of $z = \log(k/k_{\text{scale}})$ with $k_{\text{scale}} = 1$. In addition, we have found it useful to compute the evolution of $kE\,(k,t)$ and $kC\,(k,t)$, rather than $E\,(k,t)$ and $C\,(k,t)$. The calculations used a grid spacing of $\delta z = 0.02$ and a total of 1400 grid points. The time steps are adaptive and are selected by stability criteria. The well-resolved scaling regions exhibited in the numerical results confirm that the numerical methods with these choices of wavenumber resolution and time step are adequate. We stress that satisfactory numerical

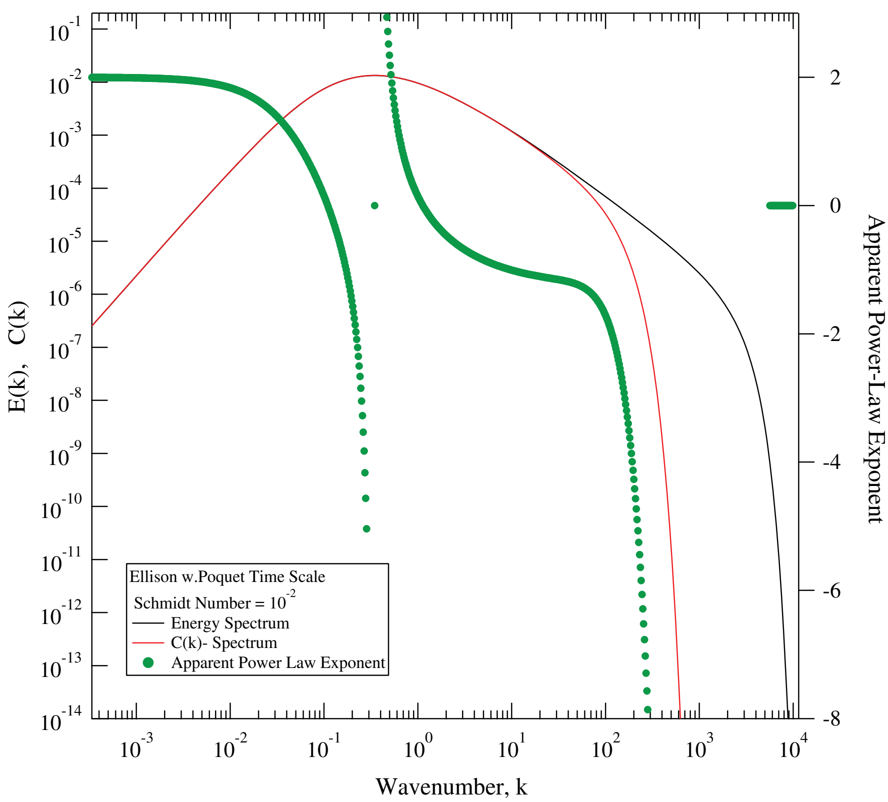

Figure 4. Scalar spectra for the Ellison model at low Sc showing BHT spectrum at small scales.

resolution, even in a calculation that resolves very small scales, is much more easily obtained and verified in statistical calculations like these, than in direct numerical simulations. Each calculation required approximately 4×10^5 time steps.

The problem simulated is simultaneous decay of the energy and scalar spectra; for this problem, it is appropriate to evaluate the velocity spectrum evolution using the velocity closure corresponding to the scalar closure [5]. The initial energy and scalar spectra have the common form,

$$K_0 \frac{\left(\frac{k}{k_0}\right)^2 \exp\left(-\left(\frac{k}{k_0}\right)^2\right)}{\int_0^\infty dq \left(\frac{q}{k_0}\right)^2 \exp\left(-\left(\frac{q}{k_0}\right)^2\right)}, \tag{59}$$

where the constant K_0 determines either the total energy or total scalar variance as appropriate, and k_0 determines the wavenumber at which the velocity or scalar spectrum reaches a maximum; we have set $K_0 = 1$ and $k_0 = 1$ for both spectra. Two cases were run for each model, a low Schmidt number case with $Sc = 10^{-2}$ and a high Schmidt number case with $Sc = 10^{+6}$.

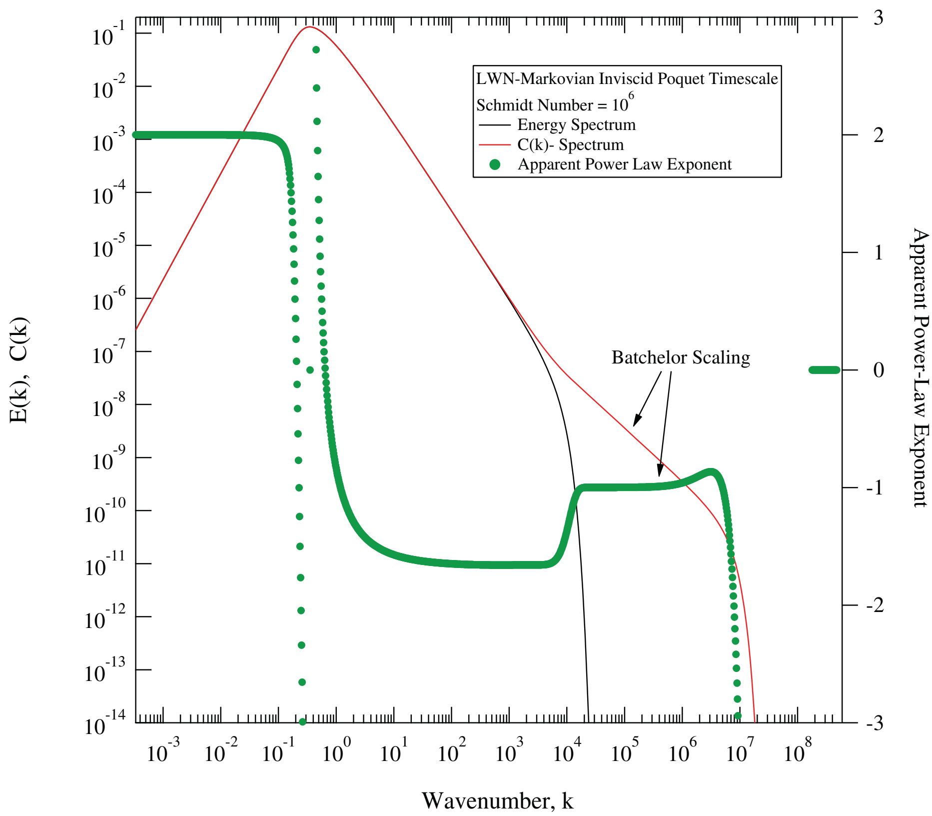

Figure 5. Scalar spectra for the LWN modification of the 'classic' Leith diffusion model using the integral timescale, for high Sc showing Batchelor regime.

It was noted in the Introduction that one attractive feature of these closures is the relative ease with which the model equations can be solved on modern computers. To give some idea of the computational resources required, all calculations were performed on a Macintosh MacBook Pro with a 2.6 Ghz Intel Core i7 processor. The code is written in C and compiled with the Gnu C Compiler (gcc) and is not heavily optimized. Each calculation required at most 4 minutes. Our previous experience suggests that the computation time required to simulate the same problems using a more fundamental Markovianized closure can be estimated as roughly the square of the time required by the present closures; this estimate is consistent with the requirement to compute two-dimensional rather than one-dimensional integrations in wavenumber space in order to resolve triad interactions.

The figures show the energy and scalar spectra at a nondimensional time of $tk_0\sqrt{K_0} = 25$, when the energy and scalar spectral evolution are both self-similar. Self-similarity is verified by collapse of both spectra using suitable scaling variables. The self-similar regime in both the velocity and scalar is by now very standard, therefore we do not show the verification of self-similarity explicitly. To exhibit possible scaling regions, we evaluate a local exponent,

$$\gamma_j = \frac{\log \dfrac{E_{j+1} - E_j}{E_j - E_{j-1}}}{\log(\Delta z)} \tag{60}$$

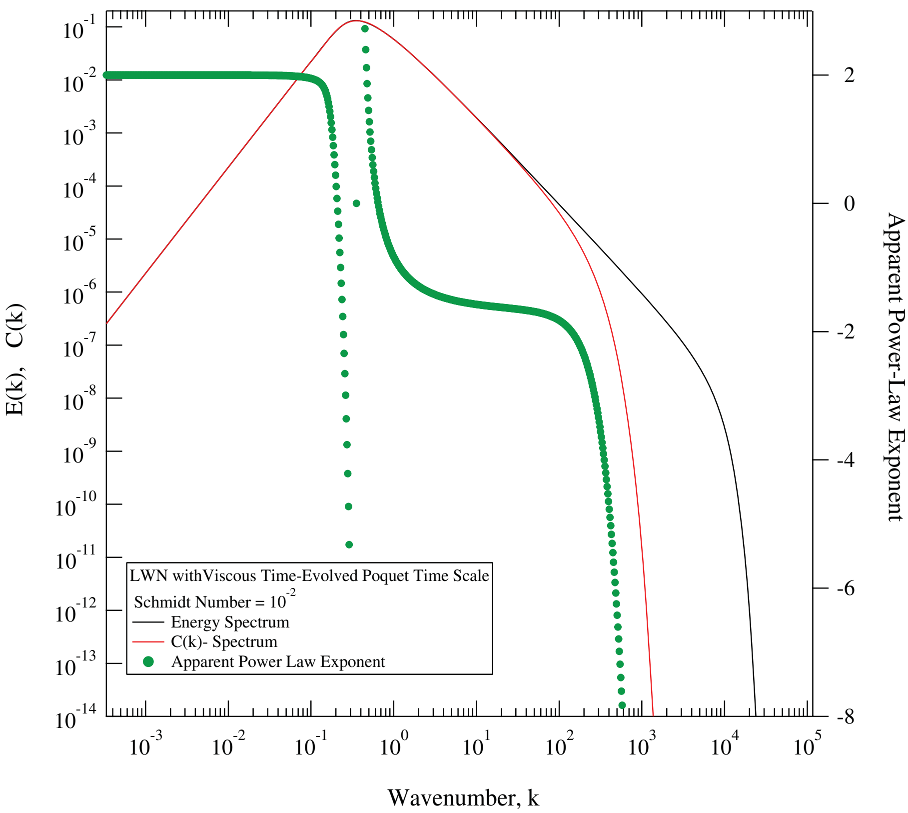

Figure 6. Scalar spectra for the LWN modification of the ‘classic’ Leith diffusion model using the integral timescale, for low Sc showing equipartition at small scales.

over the entire spectrum. In spectral regions in which $E(k) \sim k^{\gamma}$, $\gamma_j = \gamma$; we believe that this method of exhibiting power-law scaling is preferable to visual comparison with straight lines in a log-log plot. Note, however, that γ_j is not meaningful in spectral regions without power-law scaling, in particular, near the peak of the spectrum.

Figures 1 and 2 show predictions of the 'classical' Leith model Equation (4), for high and low Schmidt numbers, respectively. In both the high (Figure 1) and low (Figure 2) Schmidt number cases, the energy and scalar spectra terminate at some high wavenumber beyond which both vanish identically [6,12]. The cause lies in a peculiarity the classical Leith velocity spectrum model shares with the Kovasznay model: since both are purely local, the bizarre but dimensionally possible spectrum $E(k) \sim E_0 - \nu^2 k$ is consistent with both models and moreover defines the 'dissipation range:' the velocity spectrum decays linearly, reaches zero at some finite wavenumber, and is zero thereafter. This obviously undesirable property transfers to the Leith scalar model, because it causes the diffusivity to vanish at sufficiently large k. In the high Schmidt number case, the scalar spectrum first reaches equipartition before it terminates. The equipartition spectrum is shown by the effective power-law exponents of Equation (60). The low-Schmidt number computation does not exhibit any Batchelor–Howells–Townsend regime.

Figures 3 and 4 show the results for the scalar Ellison model for high and low Schmidt number, respectively. The Ellison model produces Batchelor scaling at high wavenumbers

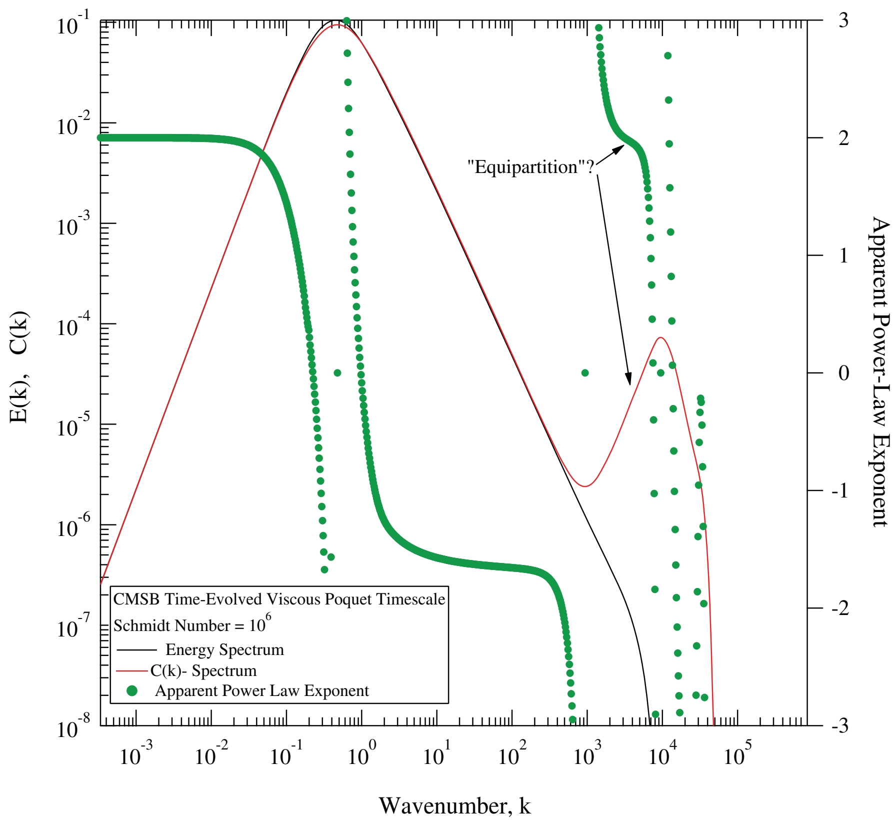

Figure 7. Scalar spectra for generalized Heisenberg model at high Sc showing equipartition at small scales.

in the high Schmidt number case. However, the Batchelor–Howells–Townsend spectrum does not occur in the low Schmidt number regime, despite the well-resolved inertial range in the velocity field.

Figures 5 and 6 show the results for the calculation with the LWN model for the high and low Schmidt number cases, respectively. Like the Ellison model, the LWN model does produce the Batchelor scaling regime for the high-Schmidt number case, but not the Batchelor–Howells–Townsend for the low-Schmidt number case.

Theoretically, the Ellison and LWN models make different predictions for the diffusive range following the Batchelor range; unfortunately however, even in these quite well resolved closure calculations, it has not been possible to find unambiguous confirmation of the spectra Equations (45) and (48). Kraichnan [11] commented that it did not seem possible to find an analytical form of the spectrum consistent with both the Batchelor spectrum and the Batchelor diffusive range of Equation (48). Another feature of these calculations is the prediction of a ‘bottleneck’ before the Batchelor diffusive range in both the Ellison and LWN models, but we will not speculate on any significance it might have. Perhaps both of these topics warrant further investigation.

Figures 7 and 8 show the results for the generalized Heisenberg model for high and low Schmidt numbers. The generalized Heisenberg model is the only model tested that produced the Batchelor–Howells–Townsend scaling for the low-Schmidt number case, but

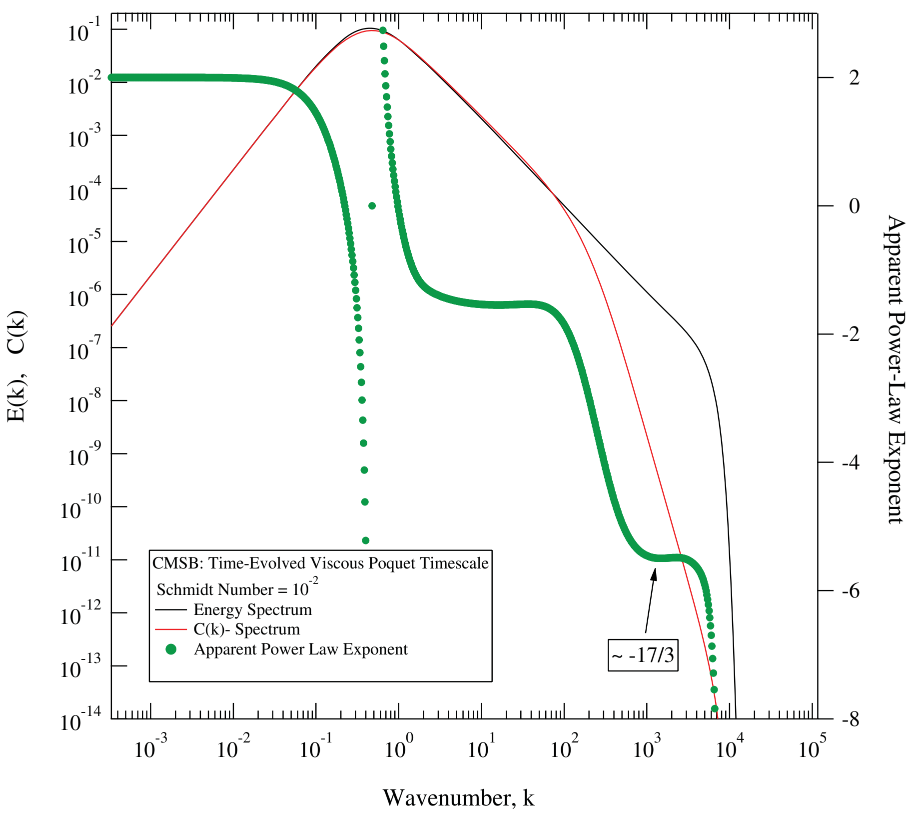

Figure 8. Scalar spectra for generalized Heisenberg model at low Sc showing BHT spectrum at small scales.

it failed to produce the Batchelor scaling at high Schmidt number, and instead produced an equipartition of the scalar spectrum.

5. Conclusions

In this paper, we have explored some models of scalar turbulence that are intermediate in complexity between analytical closures that explicitly resolve triad interactions, and 'classical' closures in which the exact velocity-scalar coupling has no explicit role. We have examined the consistency of these models with some nontrivial properties of scalar turbulence. We summarize the results in the table.

Consistency of models with properties of scalar turbulence.

Model	Kolmo–Obukh	Equipart	Batchelor	BHT
Kovasznay Equation (5)	Yes	No	No	No
Leith Equation (4)	Yes	Yes	No	No
Heisenberg Equation (3)	Yes	No	No	No
Ellison Equation (25)	Yes	No	Yes	No
LWN Equation (22)	Yes	Yes	Yes	No
New Heisenberg	Yes	No	No	Yes
Gen. Heisenberg Equation (8)	Yes	Yes	No	Yes

where BHT denotes the Batchelor–Howells–Townsend spectrum. By 'new Heisenberg' we mean the model Equation (10) with a timescale that admits a diffusive limit, such as Equation (23).

Evidently, the classical Kovasznay and Heisenberg models are the least satisfactory, while the LWN and generalized Heisenberg models come closest to satisfying all constraints. But none of these models satisfies all four. We noted earlier that this fact underscores the limitations of simplified models, since Kraichnan [11] shows the consistency of Lagrangian closure with all of these special cases. On the other hand, this limitation is perhaps not extremely serious, since a problem in which the Schmidt number takes both very high and very low values is unlikely. We note that the consistency of simple spectral models with the properties of scalar advection at high and low Schmidt numbers may suggest the possibility of applications to single-point models.

One overall conclusion can certainly be drawn: distant interactions must be possible in any turbulence theory that is at all realistic. The table conclusively demonstrates that merely changing the timescale from algebraic to integral produces major improvements in models.

Acknowledgements

We very gratefully acknowledge Prof. Yukio Kaneda's invaluable discussions of the role of local and nonlocal interactions in the Batchelor diffusive range. We are also grateful for the careful reading and helpful comments of Drs. Thomasz Drozda and Stephen L. Woodruff of NASA Langley Research Center.

Note

1. This derivation confirms Batchelor's assessment [2] of the Heisenberg model: '...the underlying physical idea seems to be suited more to the exchange of energy between distant wavenumbers than to the more important case of exchange between wavenumbers of the same order of magnitude.'

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Appendix. Analytical theories of scalar turbulence

The purpose of this appendix is to simplify the closures of the DIA family by replacing integrations over mode triads by integrations over a single wavenumber. It will entail repeating some earlier arguments [4,5] for velocity field closures in the simpler context of scalar turbulence. We stress at the outset that *these results are not approximations* of DIA or any other analytical closure; they are simplifications that highlight some of the properties of interactions in scalar turbulence, at least as they are captured by closure theories.

We give a condensed account of the analytical theory and refer to standard references like [18] for details. Define the scalar spectral density in homogeneous scalar turbulence,

$$Z(\mathbf{k}) = \langle \theta(\mathbf{k})\theta(-\mathbf{k})\rangle. \tag{A1}$$

As before, the time variable is understood but not written explicitly. The evolution equation for $Z(\mathbf{k})$ is

$$\dot{Z}(\mathbf{k}) = F_\theta(\mathbf{k}) - S_\theta(\mathbf{k}) - 2\mathcal{D}k^2 Z(\mathbf{k}), \tag{A2}$$

where $F_\theta(\mathbf{k})$ is a source of scalar fluctuations, and the scalar transfer term is

$$S_\theta(\mathbf{k}) = \int d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q})\Im\{q_m\langle u_m(\mathbf{p})\theta(\mathbf{q})\theta(-\mathbf{k})\rangle\} \tag{A3}$$

Consequently, the spectrum of scalar fluctuations

$$C(k) = \tfrac{1}{2}\oint dS(\mathbf{k})Z(\mathbf{k}) \tag{A4}$$

satisfies

$$\dot{C}(k) = P_\theta(k) - T_\theta(k) - 2\mathcal{D}k^2 C(k), \tag{A5}$$

where in Equations (A4) and (A5), $\oint dS(\mathbf{k})$ denotes integration over a sphere of radius k, and

$$P_\theta(k) = \tfrac{1}{2}\oint dS(\mathbf{k})F_\theta(\mathbf{k}) \quad T_\theta(k) = \tfrac{1}{2}\oint dS(\mathbf{k})S_\theta(\mathbf{k}). \tag{A6}$$

Conservation of scalar variance by the velocity-scalar interaction implies

$$\int d\mathbf{k}\ S_\theta(\mathbf{k}) = 0; \tag{A7}$$

consequently, the transfer term T_θ is the gradient of a flux,

$$T_\theta(\mathbf{k}) = \frac{\partial\mathcal{F}_\theta}{\partial k}, \tag{A8}$$

which gives the spectral evolution equation in the form of Equation (1). If the scalar field is statistically isotropic, then

$$T_\theta(k) = 4\pi k^2 S_\theta(k). \tag{A9}$$

Markovianized analytical closures for isotropic scalar turbulence have the common structure,

$$S_\theta(k) = \int d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) \times q_m q_n \Theta_T(k,p,q) P_{mn}(\mathbf{p}) U(p)[Z(k) - Z(q)], \tag{A10}$$

where $U(p)$ is the mode density of the velocity field and $P_{mn}(\mathbf{p}) = \delta_{mn} - p^{-2}p_m p_n$ is the transverse projection operator. This equation *without time dependence* would describe a steady state under a two-time theory like the DIA; by applying it to a statistically nonstationary problem, we are making approximations consistent with Markovianization. These issues are carefully discussed by Carnevale and Martin [22].

In a scalar analog of the test-field model [18], the relaxation time Θ_T would evolve by

$$\dot{\Theta}_T(k,p,q) = 1 - [\eta_T(k) + \eta(p) + \eta_T(q)]\Theta_T(k,p,q) - [\mathcal{D}k^2 + \nu p^2 + \mathcal{D}q^2]\Theta_T(k,p,q), \tag{A11}$$

where η_T is a scalar frequency defined by

$$\eta_T(k) = \mathsf{C} k_m k_n \int d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q})\Theta_T(k,p,q)P_{mn}(\mathbf{p})U(p) \tag{A12}$$

and $\eta(p)$ is an analogous quantity for the velocity field. The dependence of Θ_T on both a scalar and a velocity frequency complicates any attempt to replace triad interactions by pair interactions. At the risk of oversimplification, we propose to ignore the dependence on the velocity frequency scale entirely, and assume that Θ_T depends only on the scalar frequency.

Following [4], we distinguish two contributions to scalar transfer as defined by Equation (A10): an 'input' or 'replenishing' term,

$$S_\theta^+(k,p,q) = -\int d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) q_m q_n \Theta_T(k,p,q) P_{mn}(\mathbf{p})U(p)Z(q) \tag{A13}$$

and a 'damping' or 'eddy diffusivity' term,

$$S_\theta^-(k,p,q) = \int d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) q_m q_n \Theta_T(k,p,q) P_{mn}(\mathbf{p})U(p)Z(k) \tag{A14}$$

so that $S_\theta = S_\theta^+ + S_\theta^-$. (The terminology 'input' and 'damping' is consistent with the signs in Equations (A13) and (A14) because S_θ appears in Equation (A2) with a negative sign.) Continuing to follow [4], we will evaluate these terms in the two limits of *distant interactions* $k \ll p, q \to \infty$ and *local interactions* $q \ll k \approx p$. In both limits, the triangle formed by the wavevectors $\mathbf{k}$, $\mathbf{p}$, $\mathbf{q}$ with $\mathbf{k} = \mathbf{p} + \mathbf{q}$ degenerates into collinear line segments and permits the replacement of integrals over wavevector triads by integrals over a single wavenumber.

The procedure is as follows:

1. Evaluate the integrands in Equations (A13) and (A14) in the distant and local interaction limits.

2. Replace all mode interactions in which $q \geq k$ by their distant interaction limit, and all interactions in which $q \leq k$ by their local interaction limit.
3. Replace the triad interaction time by a pair interaction time.

Steps (1) and (2) were introduced by Kraichnan [16] for distant interactions to connect analytical theories to renormalization group formalisms. These steps undeniably entail some arbitrary choices: in step (2), we could replace k by λk with $\lambda > 1$; recall the comment by Orszag cited earlier [15]. Also, in step (3), there is no 'rational' way to replace the triad time by a pair interaction time; we simply do it. However to repeat, we are seeking simplifications, not approximations.

Consider the distant interaction limit of the integrand of S_θ^-. In this limit, $p \approx q$, thus

$$q_m q_n \Theta_T(k, p, q) P_{mn}(\mathbf{p}) U(p) Z(k) \approx k_m k_n \Theta_T(k, p, p) P_{mn}(\mathbf{q}) U(q) Z(k), \tag{A15}$$

where we have substituted $\mathbf{q} = \mathbf{k} - \mathbf{p}$. Using the elementary result for integration over a sphere of radius p,

$$\oint dS(\mathbf{p})\ P_{mn}(\mathbf{p}) = \tfrac{8}{3}\pi p^2 \delta_{mn} \tag{A16}$$

and following step (2) in replacing the integration over triads by an integral over all $q \geq k$, the outcome is

$$S_\theta^- \to \mathsf{C} k^2 Z(k) \int_k^\infty dq\ \Theta_T(k, q, q) E(q), \tag{A17}$$

where the symbol $\to$ simply denotes the result of the indicated operations. We used $U(q) d\mathbf{q} \propto E(q) dq$, valid for isotropy, to replace mode density $U(q)$ by the energy spectrum $E(q)$. Step (3), brute force introduction of a pair relaxation time, leads to

$$S_\theta^- \to \mathsf{C}_d^- k^2 Z(k) \int_k^\infty dq\ \Theta_T(k, q) E(q)\ \text{(distant interactions)}. \tag{A18}$$

Analytical evaluation of C_d^- and subsequent analogous constants is straightforward, however, as in [4], they will be treated as disposable parameters.

The distant interaction limit of S_θ^+ is similar and leads after the same three steps to

$$S_\theta^+ \to -\mathsf{C}_d^+ k^2 \int_k^\infty dq\ \Theta_T(k, q) \frac{E(q) Z(q)}{q^2}\ \ \text{(distant interactions)}. \tag{A19}$$

Next consider the local interactions in which $p \approx k$. Clearly,

$$q_m q_n \Theta_T(k, p, q) P_{mn}(\mathbf{p}) U(p) Z(k) \approx q_m q_n \Theta_T(k, k, q) P_{mn}(\mathbf{k}) U(k) Z(k) \tag{A20}$$

in this limit. Again following the same steps,

$$S_\theta^- \to \mathsf{C}_\ell^- Z(k) U(k) \int_0^k dq\ \Theta_T(k, q) q^4\ \ \text{(local interactions)}. \tag{A21}$$

Since in the local interaction limit,

$$q_m q_n \Theta_T(k, p, q) P_{mn}(\mathbf{p}) U(p) Z(q) \approx q_m q_n \Theta_T(k, k, q) P_{mn}(\mathbf{k}) U(k) Z(q), \tag{A22}$$

we find

$$S_\theta^+ \to \mathsf{C}_\ell^+ U(k) \int_0^k dq\ \Theta_T(k, q) q^2 C(q) \quad \text{(local interactions)} \tag{A23}$$

(as in Equation (A17), we use $Z(q)d\mathbf{q} \propto E(q)dq$.) In this case, we have used the notation to emphasize that the constants in each of Equations (A18)–(A23) are different.

By multiplying the terms proportional to $Z(k)$, Equations (A18) and (A23), by k^2 and adding, and choosing $\mathsf{C}_d^- = \mathsf{C}_\ell^+ = \mathsf{C}$, we obtain the closure

$$T_\theta(k) = \mathsf{C}\left\{k^2 C(k) \int_k^\infty dq\ \Theta_T(k, q) E(q) - E(k) \int_0^k dq\ \Theta_T(k, q) q^2 C(q)\right\} \tag{A24}$$

so that, consistent with conservation properties, T_θ is a gradient:

$$T_\theta(k) = \frac{\partial}{\partial k} \mathsf{C} \int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dq\ \Theta_T(k, q) E(q), \tag{A25}$$

which gives the scalar Heisenberg model with a pair relaxation time stated earlier as Equation (7).

Adding the two additional contributions Equations (A19) and (A21) and again requiring $\mathsf{C}_d^+ = \mathsf{C}_\ell^- = \mathsf{C}$, we obtain the scalar generalized Heisenberg model of Equation (8),

$$\begin{aligned} S_\theta = \frac{\partial}{\partial k} \mathsf{C} \bigg\{ &\int_0^k d\kappa\ \kappa^4 \int_k^\infty dp\ \Theta_T(\kappa, p) \frac{C(p)E(p)}{p^2} \\ &- \int_0^k d\kappa\ \kappa^2 C(\kappa) \int_k^\infty dp\ \Theta_T(\kappa, p) E(p) \bigg\}. \end{aligned} \tag{A26}$$

The condition $\mathsf{C}_d^+ = \mathsf{C}_\ell^-$ makes the scalar transfer a gradient, and equating both to the constant C of the Heisenberg model ensures the possibility of equipartition ensembles.

Up to this point, we have not considered the local interactions in which $p \to 0, q \to k$. This limit is rather deeper and more subtle: it is linked to the *locality* property of scalar transfer, namely the finiteness of the scalar flux even when the velocity field exhibits Kolmogorov scaling at all wavenumbers $0 < k < \infty$. Clearly, if we simply set $p = 0$ in Equation (A10), it appears that $U(p)$ would cause the transfer to diverge. However in this limit, $Z(q) - Z(k)$ also approaches zero; thus, the limit must be evaluated more carefully.

Write the scalar flux as

$$\begin{aligned} \mathcal{F}_\theta(k) = \int_{|\mathbf{k}| \geq k} d\mathbf{k} \int_{|\mathbf{p}| \leq k} d\mathbf{p} d\mathbf{q}\ \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) q_m q_n \Theta_T(k, p, q) P_{mn}(\mathbf{p}) U(p) \\ \times [Z(k) - Z(q)]. \end{aligned} \tag{A27}$$

Expanding the integrand in a Taylor series about k to second order in $\mathbf{p}$,

$$
\begin{aligned}
& q_m q_n \Theta_T(k, p, q) P_{mn}(\mathbf{p}) U(p)[Z(\mathbf{k}) - Z(\mathbf{k} - \mathbf{p})] \\
& \approx (k_m - p_m)(k_n - p_n) \left(\Theta_T(k, p, k) - p_c \frac{\partial \Theta_T(k, p, m)}{\partial m_c} \Big]_{\mathbf{m}=\mathbf{k}} \right) \\
& \quad \times P_{mn}(\mathbf{p}) U(p) \left(p_a \frac{\partial Z}{\partial k_a} - \tfrac{1}{2} p_a p_b \frac{\partial^2 Z}{\partial k_a \partial k_b} \right) \\
& = -k_m k_n P_{mn}(\mathbf{p}) U(p) p_a p_c \frac{\partial Z}{\partial k_a} \frac{\partial \Theta_T(k, p, m)}{\partial m_c} \Big]_{\mathbf{m}=\mathbf{k}} \\
& \quad - \tfrac{1}{2} k_m k_n \Theta_T(k, p, k) P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial^2 Z}{\partial k_a \partial k_b} + \cdots
\end{aligned}
\tag{A28}
$$

where we have used $p_n P_{mn}(\mathbf{p}) = p_m P_{mn}(\mathbf{p}) = 0$ and $\cdots$ denotes terms that vanish on integration over $\mathbf{p}$.

At this point, we consider only the last term in Equation (A28); following the previous steps, we will use this term to represent *all* interactions in which $p \leq k$ and replace $\Theta_T(k, p, k)$ by a pair interaction time $\Theta_T(k, p)$. Then

$$
\mathcal{F}_\theta(k) \to -\tfrac{1}{2} \int_{|\mathbf{k}| \geq k} d\mathbf{k} \int_{|\mathbf{p}| \leq k} d\mathbf{p}\, k_m k_n \Theta_T(k, p) P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial^2 Z}{\partial k_a \partial k_b} \tag{A29}
$$

where, as in Equation (A17), $\to$ simply denotes the result of carrying out the stated steps. Elementary analysis leads to

$$
\begin{aligned}
& \int_{|\mathbf{k}| \geq k} d\mathbf{k} \int_{|\mathbf{p}| \leq k} d\mathbf{p}\, k_m k_n \Theta_T(k, p) P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial^2 Z}{\partial k_a \partial k_b} \\
& = \int_{|\mathbf{p}| \leq k} d\mathbf{p} \int_{|\mathbf{k}| \geq k} d\mathbf{k}\, \frac{\partial}{\partial k_a} \left[k_m k_n \Theta_T(k, p) P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial Z}{\partial k_b} \right] \\
& \quad - \int_{|\mathbf{p}| \leq k} d\mathbf{p} \int_{|\mathbf{k}| \geq k} d\mathbf{k}\, \frac{\partial}{\partial k_a} \left[k_m k_n \Theta_T(k, p) \right] P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial Z}{\partial k_b} \\
& = \int_{|\mathbf{p}| \leq k} d\mathbf{p} \oint dS(\mathbf{k})\, k_m k_n \Theta_T(k, p) P_{mn}(\mathbf{p}) U(p) k_a k_b k^{-2} p_a p_b \frac{\partial Z}{\partial k} \\
& \quad - \int_{|\mathbf{p}| \leq k} d\mathbf{p} \int_{|\mathbf{k}| \geq k} d\mathbf{k}\, k_m k_n \left(\frac{\partial}{\partial k_a} \Theta_T(k, p) \right) P_{mn}(\mathbf{p}) U(p) p_a p_b \frac{\partial Z}{\partial k_b}
\end{aligned}
\tag{A30}
$$

where we note that in going from line 3 to line 5, the contribution from $(\partial/\partial k_a)(k_m k_n) = \delta_{am} k_n + \delta_{an} k_m$ vanishes.

Considering only the first integral after the last equality,

$$
\begin{aligned}
& \int_{|\mathbf{p}| \leq k} d\mathbf{p} \oint dS(\mathbf{k})\, k_m k_n \Theta_T(k, p) P_{mn}(\mathbf{p}) U(p) k_a k_b k^{-2} p_a p_b \frac{\partial Z}{\partial k} \\
& \quad = \mathsf{C} \int_0^k dp\, k^4 p^4 \Theta_T(k, p) U(p) \frac{\partial Z}{\partial k}
\end{aligned}
\tag{A31}
$$

consequently, we have the expression for the flux

$$\mathcal{F}_\theta(k) = -\mathsf{C} \int_0^k d\kappa\ \kappa^2 \Theta_T(k,\kappa) E(\kappa) k^4 \frac{\partial Z}{\partial k}. \tag{A32}$$

This is the scalar LWN model with a pair relaxation time, formulated earlier as Equation (9). However, we have arrived at this result somewhat less cleanly than the Heisenberg model, because we have discarded some terms generated by the original closure. Nevertheless, the analysis establishes that analytical closure incorporates an effect of diffusive transfer described by a model closely related to the Leith model. However, we stress that the result is not the original model proposed by Leith but rather a modification in which the effect of distant interactions is explicitly retained through the integration in Equation (A32).

One important feature is that the model depends on the strain $\int_0^k dp\ p^2 E(p)$ rather than on the mean square velocity fluctuation $\int_0^k dp\ E(p)$. This dependence on strain is responsible for the locality of the Kolmogorov–Obukhov range, since the integral over p is convergent even if $E(p) \propto p^{-5/3}$.

However, we see that in closure, dependence on strain is tightly linked to the diffusive character of the corresponding interactions: interaction of the scalar field at wavenumber k with velocity modes with asymptotically small wavenumbers in a range $0 \leq p \leq \Delta p$, say, spreads the scalar excitation over wavenumbers κ in the range $k - \Delta p \leq \kappa \leq k + \Delta p$; this effect is of course diffusive. In the Ellison model, the dependence on strain is present, but the diffusive effect is lost.

This conclusion can perhaps help clarify the discussion of Batchelor's and Kraichnan's picture of the Batchelor diffusive range in Section 3.4: in Kraichnan's picture, the strain field is at large but finite wavenumbers, and local interactions cause the scalar excitation to be diffused as discussed above. This diffusion in wavenumber is consistent with the LWN variant of Leith's model. However, in Batchelor's picture, the large-scale strain field is at effectively zero wavenumber; it therefore acts like a mean field (here, 'mean field' is understood in the sense of Reynolds averaging), distorting the scalar field and possibly the wavevector $\mathbf{k}$, but at most transferring the excitation from k to a different (single) wavenumber. Consequently, there is no diffusive effect. The perhaps surprising outcome is that the k^{-1} constant flux scaling is unchanged, and only the diffusive range is altered [11].