

# Functional Calculus of a Transferable Scalar in a Turbulent Flow

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The problem of dispersion of a transferable scalar in a turbulent fluid is considered. The Hopf functional equation for the characteristic functional of the velocity vector and transferable scalar is derived and discussed. The special case of heat conduction with random initial condition is studied in detail. It is shown that the Hopf equation accepts a Gaussian characteristic functional solution and several examples are discussed.

## 1. Introduction

The instability of the Navier-Stokes equation at large Reynolds number together with nonlinear interaction of waves leads to the complex turbulent fluid motions. It is well known that such a complicated field can only be described statistically<sup>1</sup>. The works on the statistical theory of turbulence are almost exclusively restricted to the study of the moments of the random velocity field. It is clear, of course, that the random turbulent field is fully specified in the statistical sense if its probability or characteristic functional is given.

The only attempt to find the general characteristic functional of an incompressible turbulent field is the remarkable paper of Hopf<sup>2</sup> where the functional equation governing the characteristic functional is derived. In the present work the derivation of Hopf is extended to the case of coupled problems of the dispersion of a transferable scalar in the turbulent flow. The characteristic functional is defined and the Hopf governing functional equation is derived. The correspondence to the simple fluid case is established. The trial functional method of the solution is discussed and it is observed that in general the equation does not accept a Gaussian solution. The hierarchy of equations governing the various moments are derived and the characteristic nonlinearity of the turbulent closure problem is identified.

The special case of the heat conduction is then considered. It is shown that the functional equation accepts a Gaussian solution and the corresponding partial differential equation for the second order correlation is derived which is observed to be identical to the one derived by Ahmadi<sup>3</sup>. The characteristic functionals for several previously studied examples<sup>3</sup> are then obtained and discussed.

## 2. Basic Equation

The equations governing the motion of an incompressible viscous fluid and dispersion of a transferable scalar are

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u}, \quad (2)$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = D \nabla^2 T. \quad (3)$$

In these equations  $\mathbf{u}$  is the velocity vector,  $p$  is pressure,  $T$  is the intensity of transferable scalar (for instance, temperature),  $\rho$  is the mass density,  $\nu$  is the coefficient of kinematic viscosity, and  $D$  is the diffusivity of the transferable scalar (heat).

When the flow becomes turbulent, Eq. (1) – (3) are valid and govern the instantaneous values of  $\mathbf{u}$  and  $T$ . It is possible to find the equations for various moments of  $(\mathbf{u}, T)$ . It is well known that because of the nonlinear convective terms in Eq. (2), (3) the equation for the moments of order  $n$  involve the moments of order  $n+1$  which is the difficulty of the closure problem of turbulence. Hopf<sup>2</sup> has shown that it is possible to obtain an equation for the characteristic functional of the turbulent field. This equation is equivalent to the hierarchy of the moment equations.

Following<sup>2</sup> we introduce the characteristic functional of the random field  $u_\alpha, T$

$$Q(k_\alpha, \theta, t) = \langle \exp \{ [ (k_\alpha, u_\alpha) + (\theta, T) ] \} \rangle \quad (4)$$

where  $\langle \rangle$  stand for the expected value (ensemble average) and the inner product is defined by

$$(\theta, T) = \int \theta(\mathbf{x}) T(\mathbf{x}) d\mathbf{x} \quad (5)$$



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and summation convention on repeated index  $\alpha$  from one to three is assumed. The characteristic functional (4) must be positive definite and is subjected to the following condition:

$$Q|_{k=\theta=0} = 1. \quad (6)$$

Various moments of the random field are related to the functional derivatives of  $Q$ . For instance

$$\frac{\delta Q}{\delta k_a(\mathbf{x})} = i \langle u_a(\mathbf{x}) \exp\{i[(k_\beta, u_\beta) + (\theta, T)]\} \rangle \quad (7)$$

where  $\delta Q/\delta k_a$  stands for the functional derivative. (Note that in the notation of Hopf<sup>2</sup> this reads  $\partial Q/\partial k_a dx$ ). More generally

$$\begin{aligned} & \frac{\delta^n Q}{\delta k_a(\mathbf{x}_1) \delta k_\beta(\mathbf{x}_2) \dots \delta \theta(\mathbf{x}_n)} \\ &= i^n \langle u_a(\mathbf{x}_1) u_\beta(\mathbf{x}_2) \dots T(\mathbf{x}_n) \\ & \cdot \exp\{i[(k_\beta, u_\beta) + (\theta, T)]\} \rangle. \end{aligned} \quad (8)$$

Evaluating (7) and (8) at  $\mathbf{k} = \theta = 0$  we find

$$\left. \frac{\delta Q}{\delta k_a(\mathbf{x})} \right|_{\mathbf{k}=\theta=0} = i \langle u_a(\mathbf{x}) \rangle \quad (9)$$

and

$$\left. \frac{\delta^n Q}{\delta k_a(\mathbf{x}_1) \dots \delta \theta(\mathbf{x}_n)} \right|_{\mathbf{k}=\theta=0} = i^n \langle u_a(\mathbf{x}_1) \dots \theta(\mathbf{x}_n) \rangle \quad (10)$$

which are the expected values of  $u_a(\mathbf{x})$  and the  $n$ -th moment of  $u_a(\mathbf{x}_1) \dots \theta(\mathbf{x}_n)$ , respectively. The incompressibility condition (1) becomes<sup>2</sup>

$$\frac{\partial}{\partial x_a} \left( \frac{\delta Q}{\delta k_a} \right) \equiv 0. \quad (11)$$

We now proceed to find the functional differential equation for  $Q$ .

### 3. Functional Differential Equation

Taking the partial time derivative of (4) we find

$$\begin{aligned} \frac{\partial Q}{\partial t} = & \int_{\mathbf{x}} \left( i k_a \frac{\partial u_a}{\partial t} + i \theta \frac{\partial T}{\partial t} \right) \\ & \exp\{i[(k_\beta, u_\beta) + (\theta, T)]\} d\mathbf{x}. \end{aligned} \quad (12)$$

Employing Eqs. (2) and (3) in (12) gives

$$\begin{aligned} \frac{\partial Q}{\partial t} = & i \int_{\mathbf{x}} \left[ k_a \left( -\frac{\partial}{\partial x_\beta} (u_a u_\beta) - \frac{1}{\varrho} \frac{\partial p}{\partial x_a} + \nu \frac{\partial^2 u_a}{\partial x_\beta \partial x_\beta} \right) \right. \\ & \left. + \theta \left( -\frac{\partial}{\partial x_a} (u_a T) + D \frac{\partial^2 T}{\partial x_\beta \partial x_\beta} \right) \right] \\ & \exp\{i[(k_a, u_a) + (\theta, T)]\} d\mathbf{x}. \end{aligned} \quad (13)$$

Interchanging the order of differentiation and expectation and making use of (8) we find

$$\begin{aligned} \frac{\partial Q}{\partial t} = & \int_{\mathbf{x}} \left\{ k_a \left[ i \frac{\partial}{\partial x_\beta} \frac{\delta^2 Q}{\delta k_a \delta k_\beta} + \nu \frac{\partial^2}{\partial x_\beta \partial x_\beta} \frac{\delta Q}{\delta k_a} - \frac{\partial \pi}{\partial x_a} \right] \right. \\ & \left. + \theta \left[ i \frac{\partial}{\partial x_a} \frac{\delta^2 Q}{\delta k_a \delta \theta} + D \frac{\partial^2}{\partial x_a \partial x_a} \frac{\delta Q}{\delta \theta} \right] \right\} d\mathbf{x} \end{aligned} \quad (14)$$

where

$$\pi(k_a, \theta, t) = i \langle (p/\varrho) \exp\{i[(k_a, u_a) + (\theta, T)]\} \rangle \quad (15)$$

is to be determined as part of the solution. Equations (14) and (11) are the basic functional differential equations for the characteristic functional  $Q$  and  $\pi$ . It is easily observed that when  $\theta \equiv 0$  Eq. (14) reduces to the Hopf equation of non heat conducting fluid.

Assume that a Taylor expansion exists for  $Q$ , i.e.,

$$Q = Q_{00} + Q_{10} + Q_{01} + \dots + Q_{mn} + \dots \quad (16)$$

with

$$Q_{00} = 1 \quad (17)$$

and

$$\begin{aligned} Q_{mn} = & \int_{\mathbf{x}_1} \dots \int_{\mathbf{x}_{m+n}} k_Q(\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{x}_{m+1} \dots \mathbf{x}_{m+n}) \\ & k_a(\mathbf{x}_1) \dots k_\omega(\mathbf{x}_m) \theta(\mathbf{x}_{m+1}) \dots \theta(\mathbf{x}_{m+n}) d\mathbf{x}_1 \dots d\mathbf{x}_{m+n} \end{aligned} \quad (18)$$

where

$$\begin{aligned} k_Q(\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{x}_{m+1} \dots \mathbf{x}_{m+n}) = & \frac{1}{(m+n)!} \\ & \cdot \frac{\delta^{m+n} Q}{\delta k_a(\mathbf{x}_1) \dots \delta k_\omega(\mathbf{x}_m) \delta \theta(\mathbf{x}_{m+1}) \dots \delta \theta(\mathbf{x}_{m+n})} \Big|_{\mathbf{k}=\theta=0} \end{aligned} \quad (19)$$

It is obvious that

$$\begin{aligned} k_Q = & \frac{i^{m+n}}{(m+n)!} \\ & \cdot \langle u_a(\mathbf{x}_1) \dots u_\omega(\mathbf{x}_m) \theta(\mathbf{x}_{m+1}) \dots \theta(\mathbf{x}_{m+n}) \rangle. \end{aligned} \quad (20)$$

A similar expansion for  $\pi$  gives

$$\pi = \sum_m \sum_n \pi_{mn} \quad (21)$$

with

$$\pi_{00} = \frac{1}{\varrho} \langle p \rangle \quad (22)$$

and

$$\begin{aligned} \pi_{mn} = & \int_{\mathbf{x}_1} \dots \int_{\mathbf{x}_{m+n}} k_\pi(\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{x}_{m+1}, \dots, \mathbf{x}_{m+n}) \\ & \cdot k_a(\mathbf{x}_1) \dots k_\omega(\mathbf{x}_m) \\ & \cdot \theta(\mathbf{x}_{m+1}) \dots \theta(\mathbf{x}_{m+n}) d\mathbf{x}_1 \dots d\mathbf{x}_{m+n} \end{aligned} \quad (23)$$

where

$$k_\pi(\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{x}_{m+1} \dots \mathbf{x}_{m+n}) = \frac{1}{(m+n)!} \frac{\delta^{m+n} \pi}{\delta k_\alpha(\mathbf{x}_1) \dots \delta k_\omega(\mathbf{x}_m) \delta \theta(\mathbf{x}_{m+1}) \dots \delta \theta(\mathbf{x}_{m+n})} \Big|_{\mathbf{k}=\theta=0} \quad (24)$$

It can be easily seen that

$$k_\pi = \frac{i^{m+n}}{(m+n)!} \quad (25)$$

$$\cdot < \langle (\mathbf{x}) u_\alpha(\mathbf{x}_1) \dots u_\omega(\mathbf{x}_m) \theta(\mathbf{x}_{m+1}) \dots \theta(\mathbf{x}_{m+n}) \rangle .$$

Substituting the expansion (16) and (17) into Eq. (14) and equating the coefficients of the same power of  $\mathbf{k}$ ,  $\theta$  we find the equations for the correlation functions.

$$\begin{aligned} \frac{\partial Q_{mn}}{\partial t} = & \int_{\mathbf{x}} \left\{ k_\alpha \left[ i \frac{\partial}{\partial x_\beta} \frac{\delta^2 Q_{m+1n}}{\delta k_\alpha \delta k_\beta} \right. \right. \\ & + \nu \frac{\partial^2}{\partial x_\beta \partial x_\beta} \frac{\delta Q_{mn}}{\delta k_\alpha} \frac{\partial \pi_{m-1n}}{\partial x_\alpha} \Big] \\ & + \theta \left[ i \frac{\partial}{\partial x_\alpha} \frac{\delta^2 Q_{m+1n}}{\delta k_\alpha \delta \theta} \right. \\ & \left. \left. + D \frac{\partial^2}{\partial x_\beta \partial x_\beta} \frac{\delta Q_{mn}}{\delta \theta} \right] \right\} d\mathbf{x} . \quad (26) \end{aligned}$$

The equation of continuity (11) for the correlations becomes

$$\frac{\partial}{\partial x_\alpha} \left( \frac{\delta Q_{mn}}{\delta k_\alpha} \right) = 0 . \quad (27)$$

The occurrence of  $Q_{m+1n}$  in the equation for  $Q_{mn}$  is the characteristic difficulty of turbulence closure problems.

The mathematical theory of functional analysis is still in its infancy and hence a general method for solving such a complicated equation is not available. One may hope to find a solution by trial and error ad hoc method. For instance a Gaussian characteristic functional

$$Q_G = \exp \left\{ i \int_{\mathbf{x}} (k_\alpha \langle u_\alpha \rangle + \theta \langle T \rangle) d\mathbf{x} - \frac{1}{2} \int_{\mathbf{x}_1 \mathbf{x}_2} \theta_i(\mathbf{x}_1) \theta_j(\mathbf{x}_2) b_{ij}(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \right\} \quad (28)$$

where

$$\theta_i = [k_\alpha, \theta], \quad i = 1, \dots, 4$$

and

$$b_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \langle (T_i - \langle T_i \rangle) (T_j - \langle T_j \rangle) \rangle \quad (29)$$

where  $T_i = [u_i, T]$ ,  $i = 1, \dots, 4$ , might be a reasonable trial function. Unfortunately, as discussed by

Hopf<sup>2</sup> for the form of (28) appropriate for a fluid which does not conduct heat, this does not satisfy Equation (14). Evaluating Eq. (14) for  $k=0$  we find

$$\begin{aligned} \frac{\partial Q}{\partial t} \Big|_{k=0} = & \int_{\mathbf{x}} \left\{ \theta \left[ i \frac{\partial}{\partial x_\alpha} \frac{\delta Q}{\delta k_\alpha \delta \theta} \right]_{k=0} \right. \\ & \left. + D \frac{\partial^2}{\partial x_\alpha \partial x_\alpha} \frac{\partial Q}{\partial \theta} \Big|_{k=0} \right\} d\mathbf{x} . \quad (30) \end{aligned}$$

It may be easily shown that Eq. (30) accepts a Gaussian solution (28) if the velocity field is identically zero or uncorrelated with temperature field. This trivial solution is discussed in the next section.

It is possible to find the equation for the functional  $Q$  in the wave number space but we do not pursue this matter here.

#### 4. Heat Conduction with Random Initial Conditions

The equation governing the heat conduction is

$$\partial T / \partial t = D \nabla^2 T \quad (31)$$

with boundary condition

$$T = T_s \text{ on } S \quad (32)$$

and initial condition

$$T|_{t=0} = T_0(\mathbf{x}) . \quad (33)$$

Assuming that  $T_0(\mathbf{x})$  is a random function of space, the temperature becomes also a random function. This problem has been recently studied by Ahmadi<sup>3</sup> where the equations for the second order correlation are derived and several examples are solved. In the present work we would like to find the characteristic functional or probability density functional of the temperature field.

Let us define the characteristic functional of the temperature field by

$$Q_T = \langle e^{i(\theta, T)} \rangle . \quad (34)$$

With an argument similar to that in Sect. 3 we find

$$\frac{\partial Q_T}{\partial t} = \int_{\mathbf{x}} \theta D \frac{\partial^2}{\partial x_\alpha \partial x_\alpha} \frac{\delta Q}{\delta \theta} d\mathbf{x} . \quad (35)$$

This equation is identical to Eq. (30) with  $\delta Q / \delta k$  taken to be zero.

Assuming that the mean temperature is zero, let us use a Gaussian trial functional of the form

$$Q_G = \exp \left\{ -\frac{1}{2} \int_{\mathbf{x}_1 \mathbf{x}_2} \theta(x_1) R_T(\mathbf{x}_1, \mathbf{x}_2, x) \theta(\mathbf{x}_2) \cdot d\mathbf{x}_1 d\mathbf{x}_2 \right\} \quad (36)$$

where

$$R_T(\mathbf{x}_1, \mathbf{x}_2, t) = \langle T(\mathbf{x}_1, t) T(\mathbf{x}_2, t) \rangle. \quad (37)$$

Substituting (36) into (35) we find  $Q_G$  is a solution if

$$\begin{aligned} & \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \theta(\mathbf{x}_1) \theta(\mathbf{x}_2) (\partial R_T / \partial t) d\mathbf{x}_1 d\mathbf{x}_2 \\ &= \int_{\mathbf{x}} \theta(\mathbf{x}) D \frac{\partial^2}{\partial x_a \partial x_a} \left[ \int_{\mathbf{x}_1} \theta(\mathbf{x}_1) R_T(\mathbf{x}_1, \mathbf{x}) d\mathbf{x}_1 \right. \\ & \quad \left. + \int_{\mathbf{x}_2} R_T(\mathbf{x}, \mathbf{x}_2) \theta(\mathbf{x}_2) d\mathbf{x}_2 \right] d\mathbf{x}. \end{aligned} \quad (38)$$

Setting  $\mathbf{x}$  equal to  $\mathbf{x}_2$  and  $\mathbf{x}_1$  in the first and second double integrals on the right hand side of (38) respectively, we find

$$\begin{aligned} \frac{\partial}{\partial t} R_T(\mathbf{x}_1, \mathbf{x}_2, t) &= D [\nabla_1^2 R_T(\mathbf{x}_1, \mathbf{x}_2, t) \\ & \quad + \nabla_2^2 R_T(\mathbf{x}_1, \mathbf{x}_2, t)] \end{aligned} \quad (39)$$

where  $\nabla_1^2$  and  $\nabla_2^2$  are the Laplacian at  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , respectively.

Equation (39) is identical with Eq. (4) of Reference<sup>3</sup>. Therefore we conclude that the temperature field accept a Gaussian solution with its characteristic functional given by Eq. (36) if it is Gaussian at the initial time.

Several examples were solved in<sup>3</sup> where the time development of the correlation functions are obtained. We can now easily derive the corresponding characteristic functionals.

For one dimensional heat conduction in a slab of length  $l$  with temperature being zero on both boundaries and purely random initial condition, i.e.

$$R_{T0}(x_1, x_2) = S_0 \delta(x_1 - x_2), \quad (40)$$

the correlation function is given by Eq. (16) of<sup>3</sup> and thus the corresponding characteristic functional is

$$\begin{aligned} Q[\theta(x), t] &= \exp \left\{ -\frac{S_0}{l} \int_0^l dx_1 \int_0^l dx_2 \theta(x_1) \theta(x_2) \right. \\ & \quad \left. \sum_{n=1}^{\infty} \sin \frac{n\pi x_1}{l} \sin \frac{n\pi x_2}{l} \exp[-2Dn^2\pi^2 t/l^2] \right\}. \end{aligned} \quad (41)$$

In the case of a semi-infinite medium with zero boundary condition and purely random initial condition (40) the correlation function is given by Eq. (21) of<sup>3</sup>. Therefore the characteristic functional is given by

$$\begin{aligned} Q[\theta(x), t] &= \exp \left\{ -\frac{S_0}{2\sqrt{8\pi Dt}} \int_0^\infty dx_1 \int_0^\infty dx_2 \theta(x_1) \theta(x_2) \right. \\ & \quad \left. [\exp\{- (x_1 - x_2)^2 / 8Dt\} - \exp\{x_1 + x_2\}^2 / 8Dt\}] \right\} \end{aligned} \quad (42)$$

(Note that the omission of the minus sign in the argument of the last exponential is a typographical error in<sup>3</sup>.)

For the three dimensional solid with purely random initial condition,

$$R_{T0}(\mathbf{x}_1, \mathbf{x}_2) = S_0 \delta(\mathbf{x}_1 - \mathbf{x}_2). \quad (43)$$

The correlation function is given by Eq. (9) of<sup>3</sup> and the characteristic functional becomes

$$\begin{aligned} Q[\theta(x), t] &= \exp \left\{ -\frac{DS_0 H(t)}{2(2D\pi t)^{3/2}} \int_{\mathbf{x}_1} d\mathbf{x}_1 \int_{\mathbf{x}_2} d\mathbf{x}_2 \right. \\ & \quad \left. \theta(\mathbf{x}_1) \theta(\mathbf{x}_2) \exp \left[ -\frac{(\mathbf{x}_1 - \mathbf{x}_2)^2}{8Dt} \right] \right\}. \end{aligned} \quad (44)$$

Expressions (41), (42), and (44) are examples of the characteristic functionals of the heat conduction problems with random initial conditions. With these known characteristic functionals the random temperature is completely specified in the statistical sense. That is, all the cross correlations of any order can be obtained by functional differentiation of the corresponding  $Q$ .

## 5. Further Remarks

In the present paper the Hopf functional equation for the joint characteristic functional of the turbulent velocity vector and transferable scalar fields is derived. The method of solution of such partial functional equations is not known and even the existence of a solution is not clear. At the present time only the ad hoc method of trial functions is possible. We have observed that the Gaussian characteristic functional does not satisfy the functional Eqs. (26) and (27). Therefore, it is concluded that the process of turbulent diffusion is non-Gaussian. Several other trial characteristic functionals also have been considered without any success. The simple Gaussian solution for the heat conduction equation with random initial condition is a trivial case where the trial function method gives the exact solution. A method of an approximate solution of the functional Eqs. (26) and (27) which is based

on nearly Gaussianity is under study which seems to be quite promising, but we leave it for a future communication.

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