A solitary-wave representation of turbulence in the physical-plus-eddy space

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Abstract. A unique form of turbulent-transport equations is derived based on first principles. The role of nonequilibrium statistical mechanics employed to describe the phenomenology is that it enables to single out the unique form consistent with master equation of Liouville, a prerequisite not met with existing equations for turbulence modeling. The equation is variable-separated to yield a Navier-Stokes equation in 6D(physical-plus-eddy) space with homogeneous boundary conditions. Turbulent transports such as Reynolds’ stress are calculated using a solution of this equation; a solitary-wave function. Satisfactory agreement is observed with existing experiment for mixing shear layer of incompressible flows although no empirical constants to fit with data are involved.

1. Introduction

First principle bases of phenomenologies of fluid dynamics and thermodynamics are due, respectively, to Chapman-Enskog[1],[2] and Prigogine[3], who showed the validity of Navier-Stokes equation and the equality expression of the second law of thermodynamics on common basis of the Boltzmann equation expanded to the first order deviation from equilibrium.

It was, however, an open question whether these equations still hold for turbulent flows where the dependent variables are stochastic and fractal, therefore not differentiable[4]. This problem was solved[5] using the microscopic density[6], namely, unaveraged Boltzmann function, leading to rederivation of the Navier-Stokes equation written in terms of instantaneous quantities without assuming any statistical concepts like local equilibrium, or first order deviation form it. Thus the equations currently employed for the direct numerical simulation(DNS) has acquired the first principle basis.

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Then a question will arise as to whether the alternative methodology of computational fluid dynamics, namely, Reynolds-average formalism can be founded on first principles as well.

In contrast with DNS founded on the microscopic density (the Klimontovich formalism) its Reynolds-average counterpart should be based on its averaged version, namely, the Boltzmann function. Structure of this Boltzmann formalism, so to say, is shown to be identical with what is called the BBGKY hierarchy theory of nonequilibrium statistical mechanics[7].

Each of the two formalisms has advantages as well as disadvantages from computational viewpoints. The most serious disadvantage of the K-formalism lies in the fact that it deals with fractal quantities which are selfsimilarly rugged to a length scale as small as the Kolmogorov scale[8]. It means that if the 3-D Navier-Stokes equation is to be solved by a finite difference method, the grid size be smaller than this length, namely of $O(R^{-3/4})$ ($R$ : Reynolds number). It requires the computer memory size growing with $R^{9/4}$ (the small eddy difficulty). For this reason, the consensus upper limit of applicability of the current DNS falls short of $R \sim 10^4$. To be able to apply the DNS for practical design of transport vehicles ($R \sim 10^7$) we would have to have a computer with memory size greater by the factor of $(10^7/10^4)^{9/4} \sim 10^7$ compared to the currently available ones. This situation is not changed even when one employs spectral methods to avoid the conceptual difficulty of having to work with differential equations. For, then, the number of the Fourier modes to be taken into account increases at the same rate.

The B-formalism, in contrast, is free from such difficulty owing to the statistical average taken in the process of generating distribution functions at the expense of dealing with multitude of such functions, infinite in number. The statistical average as meant here is either an ensemble average over repeated experiments, or an average over time that is long enough for the fractal ruggedness to be smoothed out, yet is short enough for fluid-dynamic unsteadiness, such as shedding period of Kármán vortices or aerodynamic flutter to be discernible. The ergodic theorem warrants their identity.

The objective of this paper is to demonstrate that the Reynolds average regime of the computational fluid dynamics can be founded on a firm first principle ground through the following processes:

i) Demonstration of how a closed set of kinetic equations is obtained out of an infinite chain of them of the B-formalism.

ii) Taking fluid moments of the kinetic equation for two-point fluctuation-correlations that is unique from the viewpoint of first principles.

iii) Rederivation of the whole set of equations thus obtained from phenomenological equations being used for DNS, namely, eliminating the process via statistical mechanics.
2. The Boltzmann and Klimontovich formalisms: A review

Any statistical theory rests on the axiom that a field quantity \( f(z) \) describing stochastic and possibly fractal physical phenomenon is equivalent to a set of quantities that are smooth, deterministic, and infinite in number,

\[
\begin{align*}
\bar{f} &\equiv \begin{cases} 
  f(\equiv \bar{f}) \\
  \bar{f} \hat{f} \\
  \bar{f} \hat{f} \hat{f} \\
  \vdots
\end{cases} \\
  (f' \equiv f - \bar{f}) \\
\end{align*}
\tag{1}
\]

where overbar stands for the statistical average as defined in the preceding section, and \( f = f(\hat{z}) \) is the same quantity at a different point \( \hat{z} \).

The Klimontovich formalism as defined here is a formalism where \( \bar{f} \) is identified with the microscopic density \[ \bar{f}(z) = \sum_{1 \leq n \leq N} \delta(z - z^{(n)}(t)) \tag{2} \]

In this expression \( z \equiv (x, v) \) is a point in the phase(\( \mu \)-)space, \( z^{(n)}(t) \) is the locus of \( n \)-th molecule in this space, \( N \) is the total number of molecules under consideration, and \( \delta \) denotes the six-dimensional delta function.

It has been shown \[ \text{[9]} \] that the equation governing \( \bar{f} \) is the unaveraged Boltzmann equation;

\[
B[\bar{f}] \equiv (\frac{\partial}{\partial t} + v \cdot \frac{\partial}{\partial x})\bar{f} - J(z|\hat{z})[\bar{f} \hat{f}] = 0 \tag{3}
\]

with \( J \) denoting the classical collision integral acting on molecule \( \hat{z} \). The key issue here is that Eq.(3) is a deterministic equation of continuity in the \( \mu \)-space, free from any statistical concepts\[ \text{[9]} \].

The Boltzmann formalism, on the other hand, deals with quantities to have appeared on the r.h.s. of (1), subject to statistical average, namely, the Boltzmann function

\[
f(z) \equiv \bar{f}
\tag{4}
\]

and the correlation functions of consecutive hierarchies

\[
\begin{align*}
\psi(z, \hat{z}) &\equiv f' \hat{f}' = \bar{f} \hat{f} - f \hat{f} \\
\psi(z, \hat{z}, \hat{\hat{z}}) &\equiv f' \hat{f}' \hat{\hat{f}}' = \bar{f} \hat{f} \hat{\hat{f}} - f \hat{f} \hat{\hat{f}} \quad \cdots
\end{align*}
\tag{5}
\]
Klimontovich variables such as instantaneous gas density $\rho$ and center-of-mass velocity $\mathbf{u}$ of the $N$-particle system are given by
\[
\rho(t) = m \int_{-\infty}^{\infty} f d\mathbf{v} = m \sum_{1 \leq n \leq N} \delta(\mathbf{x} - \mathbf{x}^{(n)}(t)) \quad (m \text{ : mass of a molecule})
\]
\[
\rho \mathbf{u}(t) = m \int_{-\infty}^{\infty} \mathbf{v} f d\mathbf{v} = m \sum_{1 \leq n \leq N} \mathbf{v}^{(n)}(t) \delta(\mathbf{x} - \mathbf{x}^{(n)}(t))
\]
The Reynolds-averaged version of those fluid variables are generated by taking average of expressions (6) and (7)
\[
\rho = m \int_{-\infty}^{\infty} f d\mathbf{v}
\]
\[
\overline{\rho \mathbf{u}} = \rho \mathbf{u} + \overline{\rho'} \mathbf{u}' = m \int_{-\infty}^{\infty} \mathbf{v} f d\mathbf{v}
\]

Two-point correlation $\psi(z, \hat{z})$ consists of two parts; short-range part due to direct molecular collisions that is irrelevant to turbulence and long-range part attributable to turbulence correlations. The latter part is expanded in a double series of Hermite polynomials where all the turbulent transport terms including Reynolds’ stress appear as expansion coefficients.

A set of equations governing those quantities standing on the l.h.s. of (3) is generated from Eq.(3) by taking moments and averaging. This procedure is not unique; in general there are infinite ways of constructing such moment equations. This arbitrariness is eliminated by invoking a postulate that the whole system be consistent with Liouville’s equation (the equation of continuity of $N$-particle probability density in $6N$-dimensional space; the master equation that is universally valid), or its corollary that the whole set of equations be identical with those of the BBGKY theory at each level of hierarchies. The only difference is that the BBGKY generates distribution functions in the direction of descending number of molecules through a series of integrations starting from $N \sim O(10^{20})$, whereas here are defined the same functions in ascending number of molecules. The kinematical information missing in the latter approach is identical in analogy with the fact that we cannot predict the functional form of $g(x, y)$ out of $f(x) = \int_{-\infty}^{\infty} g(x, y) dy$ . This is why we need the postulate.

The averaging process consistent with the postulate has led to following set of equations:

- **1 - particle level**
  \[
  \overline{B[f]} = 0 : \quad \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} \right) f - J(z, \hat{z})[f \hat{f} + \psi(z, \hat{z})] = 0
  \]
\( \dot{f}' B[f] + f' \dot{B}[f] = 0 \), \((\dot{B}[ ] \equiv \{B[ ]\}_{z \rightarrow \hat{z}})\):

\[
\begin{aligned}
&\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} + \hat{\mathbf{v}} \cdot \frac{\partial}{\partial \hat{\mathbf{x}}} \right) \psi(z, \hat{z}) - J(z|\hat{z}) \left[ f\psi(z, \hat{z}) + \hat{f}\psi(z, \hat{z}) + \psi(z, \hat{z}, \hat{\omega}) \right] = 0
\end{aligned}
\]
(11)

\[
\begin{aligned}
&\dot{f}' \dot{f}' B[f] + f' \dot{f}' \dot{B}[f] + \dot{f}' f' \dot{B}[f] = 0
\end{aligned}
\]
(12)

This system constitutes a chain of equations for the set of infinite number of variables \([f(z), \psi(z, \hat{z}), \psi(z, \hat{z}, \hat{\omega}), \cdots]\).

The issue that is most crucial to the quality of the proposed approach is the closure condition. It is how to truncate the infinite chain of equations to make the system tractable without violating physical soundness.

Early stage of development along this line has employed the following condition of tertiary chaos \cite{10}, \cite{11}:

\[
\psi(z, \hat{z}, \hat{\omega}) = 0
\]
(13)
a condition next to the simplest one known as Boltzmann’s (binary) molecular chaos hypothesis; \(\psi(z, \hat{z}) = 0\).

Eq.(11) under this closure condition is investigated in some depth: It is shown that assumption (13) allows Eq.(11) for separating variables into those for respective particles, thereby its fluid moment equation leads to linearized Navier-Stokes equation (the Orr-Sommerfeld equation, in particular.). It is also seen that this closure gives satisfactory description only for weak turbulence where the nonlinearity in turbulent intensity does not play major roles. Later, it has been superseded by alternative one that has wider range of applicability, yet preserving the variable-separability beyond linear regime \cite{12}: Namely, put

\[
\psi(z, \hat{z}) = \text{R.P.} \tau \int_{-\infty}^{\infty} \phi(z, \omega)\phi^*(\hat{z}, \omega) d\omega
\]
(14)

\[
\psi(z, \hat{z}, \hat{\omega}) = \text{R.P.} \tau^2 \int_{-\infty}^{\infty} \phi_3(z, \omega)\phi_3(\hat{z}, \hat{\omega})\phi_3(\hat{z}, \hat{\omega})\delta(\omega + \hat{\omega} + \hat{\omega}) d\omega d\hat{\omega}
\]
(15)

where \(\omega\) is the variable-separation parameter having the dimension of the frequency, \(\tau\) is a characteristic time, symbols(*) and R.P. denote the complex conjugate and the real part, respectively. Separated variable \(\phi\) is complex, subject to

\[
\phi^*(z, \omega) = \phi(z, -\omega)
\]
(16)
as will be justified a posteriori. (See Eq. (18) below.) The closure condition is introduced in the following form
\[ \phi_3 = \phi \]  
(17)

It makes Eq. (11) separated into two equations each for respective points \( z \) and \( \hat{z} \), in the form of complex conjugate to each other provided that condition (16) is met:
\[ (-i\omega + \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial x}) \phi - J(z|\hat{z})[\phi \hat{f} + f \hat{\phi} + \tau \int_{-\infty}^{\infty} \phi(\omega - \tilde{\omega})\hat{\phi}(\tilde{\omega})d\tilde{\omega}] = 0 \]  
(18)

If the nonlinear term of convolutional integral is deleted, the equation degenerates to the previous case with tertiary chaos closure.

Fluid moments of (18) together with (14) provide equations for turbulent transports such as Reynolds’ stress and turbulent heat flux density to obey. For actual derivation of these equations see [13].

3. Fluctuation equations in physical-plus-eddy space

The approach described in the previous section has shed some lights in turbulence research. In fact, for the cases tested agreement with experiments is satisfactory although the theory is free from any adjustable parameters [14, 15] as contrast with existing models such as eddy-viscosity model. The success, however, has been limited to cases where the flow geometry is governed by single variable. (Note that the velocity fluctuations are multi-dimensional.)

We will show that a small renovation of the theory sketched in the preceeding section can make turbulence with general three-dimensional geometry tractable. It is to replace the frequency \( \omega \), a scaler quantity having appeared in Eqs. (18) and (16), by the wave number \( \mathbf{k} \) that is a vector connected to the frequency through phase velocity \( \mathbf{c} \) by the dispersion formula
\[ \omega = \mathbf{c} \cdot \mathbf{k} \]  
(19)

Then, new separation rule to replace (14) is
\[ \psi(z, \hat{z}) = \text{R.P.} \int_{-\infty}^{\infty} \phi(z, \mathbf{k}) \phi^*(\hat{z}, \mathbf{k}) d\mathbf{k} \]  
(20)

where \( l \) is the characteristic length of the macroscopic phenomenon under consideration. Accordingly the governing equation for \( \phi \) to replace (18) is written as
\[ i\omega \phi = \Omega(\phi) \]

with
\[ \Omega(\phi) \equiv \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial x} \right) \phi - J(z|\hat{z}) \left[ f \hat{\phi} + \phi \hat{f} + \text{R.P.} \int_{-\infty}^{\infty} \phi(\mathbf{k} - \tilde{\mathbf{k}})\hat{\phi}(\tilde{\mathbf{k}})d\tilde{\mathbf{k}} \right] \]  
(21)
For practical purposes it is more convenient to separate out the spatially periodic factor from $\phi$ by putting

$$\phi(z, k) = e^{i k \cdot x} \Phi(z, k)$$  \hspace{1cm} (22)$$

and work with its amplitude $\Phi$. Owing to the fortuitous situation that the only nonlinear term in Eq.(21) has the form of convolitional integral, the factor $e^{i k \cdot x}$ is seen to drop off upon substituting expression (22) into Eq.(21). Since \( (\partial/\partial x_j)\phi = e^{i k \cdot x}(\partial/\partial x_j + i k_j)\Phi \) the equation for $\Phi$ should preserve the form of Eq.(21) with the only substitution

$$\frac{\partial}{\partial x_j} \rightarrow \frac{\partial}{\partial x_j} + i k_j$$  \hspace{1cm} (23)$$

Another favorable property of the nonlinear integral is that it reduces to a simple product through Fourier transform

$$\Phi(z, k) = \frac{1}{(2\pi l)^3} \int_{-\infty}^{\infty} e^{-i k \cdot s} F(z, s) \, ds$$  \hspace{1cm} (24)$$

such that

$$\int_{-\infty}^{\infty} \Phi(k - \tilde{k}) \hat{\Phi}(\tilde{k}) \, d\tilde{k} \rightarrow F \hat{F}$$  \hspace{1cm} (25)$$

Then Eq. (21), with (22) through (23) taken into account, reads

$$\left( \frac{\partial}{\partial t} - c_j \frac{\partial}{\partial s_j} + v_j \partial_j \right) F - J(z|\tilde{z}) \left[ f \hat{F} + \hat{f} F + F \hat{F} \right] = 0$$  \hspace{1cm} (26)$$

where $\partial_j$ is six-dimensional operator defined by

$$\partial_j \equiv \frac{\partial}{\partial x_j} + \frac{\partial}{\partial s_j}$$  \hspace{1cm} (27)$$

The Fourier variable $s$ introduced through the transform (24) has the dimension of length characterizing the size of eddies. Therefore $s$ might well be called the eddy variable.

Substituting (22) and (24) into (20) we have a remarkably simple formula for $\psi$ when written in terms of $F$,

$$\psi(z, \tilde{z}) = \frac{1}{(2\pi l)^3} \int_{-\infty}^{\infty} F(x, s, \nu) F(\tilde{x}, s + \tilde{\nu} - x, \tilde{\nu}) \, ds$$  \hspace{1cm} (28)$$

Note that here all the quantities of the integrand are real in contrast with those of (20).

Derivation of fluid equations from Eq.(26) is almost parallel to its low dimensional predecessor[13], so will not be repeated here. Minimum necessary steps to reach the final
form of fluid equations will be given in order: First we employ the same fluid-moment expansion for \( F(\mathbf{x}, \mathbf{s}, \mathbf{v}, t) \) in terms of Hermite’s polynomial \( \mathcal{H} \) in the \( \mathbf{v} \)-space after Grad [16]:

\[
F = \frac{e^{-\xi^2/2}}{(2\pi a^2)^{3/2}m} \left[ q_0 + \frac{q_i}{a} \mathcal{H}_j + \frac{q_{jk}}{2a^2} \mathcal{H}_{jk} + \frac{q_{jkk}}{10a^3} \mathcal{H}_{jrr} \right]
\]

with

\[
\begin{align*}
\mathcal{H} &= \mathcal{H}(\xi) \\
\xi &= \mathbf{w}/a = (\mathbf{v} - \mathbf{u}^\dagger)/a \\
u_j^\dagger &= m_j/\rho \\
m_j &= \rho u_j + \rho' u_j' \\
a^2 &= R_M T \quad (R_M \equiv \text{Avogadro no./molecular no.})
\end{align*}
\]

Note that this expansion differs from the classical 13-moment expansion in that \( q_j \neq 0, q_{jj} \neq 0 \). Second, we replace Eq. (26) by its moment equivalents

\[
m\int_{-\infty}^{\infty} M_\alpha[\text{Eq. (26)}] d\mathbf{v} = 0
\]

where \( F \) is substituted by (29) and \( M_\alpha \) stands for one of the 13 moment functions; \( 1, \mathcal{H}_j, \mathcal{H}_{jj}, \mathcal{H}_{jk}, \mathcal{H}_{jkk} \). These choices of moments correspond to equations of fluctuations of continuity, momentum, energy, stress tensor \( q_{jk} \) and heat flux density vector \( q_{jkk} \), respectively. The actual form of the equations are:

\[
\begin{align*}
Dq_0 + \partial_r q_r &= 0 \\
Dq_j + \partial_r q_{jr} + \partial_j q_{40} + \partial x_r q_{jr} - \frac{1}{\rho} \partial x_j q_0 &= 0 \\
\frac{3}{2} Dq_{40} + \partial_r q_{4jj} + \frac{5}{2} \partial_j (a^2 q_r) + \frac{\partial u_j^\dagger}{\partial x_r} q_{40} + \frac{\partial u_j^\dagger}{\partial x_r} q_{jr} - \frac{1}{\rho} \partial q_r &= 0 \\
q_{40} &= q_4 + a^2 q_0 \\
q_{jr} &= -\mu \left[ \partial_r \left( \frac{q_j}{\rho} \right) + \partial_j \left( \frac{q_r}{\rho} \right) - \frac{2}{3} \delta_{jr} \partial_k \left( \frac{q_k}{\rho} \right) \right] + \frac{1}{\rho} \left[ q_j q_r - \frac{1}{3} \delta_{jr} q_k^2 \right] \\
&\quad - \frac{1}{\rho R_M} \frac{d\mu}{dT} \left[ \frac{\partial u_j^\dagger}{\partial x_r} + \frac{\partial u_j^\dagger}{\partial x_j} - \frac{2}{3} \delta_{jr} \partial u_k^\dagger \partial x_k \right] q_4 \\
q_{rjj} &= -\frac{\lambda}{R_M} \partial_r \left( \frac{q_4}{\rho} \right) - \frac{1}{\rho R_M} \frac{d\lambda}{dT} \frac{\partial q_4}{\partial x_r} q_4 + \frac{5}{2} \frac{q_j q_4}{\rho} \\
\end{align*}
\]

where we have defined the following symbols:

\[
Dq = \frac{\partial q}{\partial t} - c_r \frac{\partial q}{\partial s_r} + \partial_r (u_r^\dagger q)
\]

In the above, \( \rho, p, T, \mu \) and \( \lambda \) denote density, pressure, temperature, viscosity and thermal conductivity coefficients, respectively.
It is readily seen that Eqs. (31) are exactly the same as those derived in ref. [13] (Eqs. (21) through (24)) if the following replacements are effected,

\[ i\omega \rightarrow c_j \frac{\partial}{\partial s_j} \]  

(32)

\[ \frac{\partial}{\partial x_j} \rightarrow \frac{\partial}{\partial x_j} + \frac{\partial}{\partial s_j} \]  

(33)

The set of Eqs. (31) describes evolution of five quantities \( (q_0, q_j, q_4) \) subject to homogeneous boundary conditions that all \( q \)’s vanish with \( |s| \rightarrow \infty \), on the solid surface, and wherever turbulent intensity is zero in the physical space. Therefore, the expected solution for those quantities must have the form of a solitary wave (not to be confused with a soliton).

Eqs. (31) are equations governing compressible turbulence. For incompressible flows \( (q_0 = 0) \) the energy fluctuation equation is decoupled, and a closed set of equations that results is

\[ \partial_j q_j = 0 \]  

(34)

\[ (D - \nu \partial^2)q_j + \partial_j q_{40} + \frac{\partial u_j}{\partial x_r} q_r + \frac{q_r}{\rho} \partial_r q_j = 0 \]  

(35)

where \( \nu \) is the kinematic viscosity, \( \partial_j \) and \( D \) have been defined by (27) and (31), respectively. It is readily seen that these equations represent the equation of continuity and the Navier-Stokes equation generalized to 6D space \( (x, s) \). In fact, if we suppress the eddy variables \( (\partial/\partial s_j = 0) \) this set degenerates to the usual Navier-Stokes equation for velocity \( u_j + \rho^{-1} q_j \) and pressure \( p + q_{40} \). If further, nonlinear terms are neglected in Eq. (35) and parallel flow \( (u_j = \delta_{j1} u(x_2)) \) is assumed, they reduce to the Orr-Sommerfeld equation to govern \( \rho^{-1} q_2 \) as it should.

4. Correspondence rule; relationships between solitary-wave functions and observables

It should be remarked that variables \( q \)’s do not correspond to any turbulent fluctuations that are tangible to macroscopic sensors. They are shown to be related to fluctuation correlations of turbulent quantities through the following deduction: From (8), (3) and (1) we have expression for instantaneous density fluctuation that is an observable:

\[ \rho' = m \int_{-\infty}^{\infty} f' \mathrm{d}v \]  

(36)
Similarly, by subtracting (9) from (7), we have
\[ \rho u_j' + \rho' u_j + (\rho' u_j' - \rho u_j') = m \int_{-\infty}^{\infty} v_j f' dv \]
This expression, upon substituting (36) for \( \rho' \), reduces to
\[ \rho u_j' = m \int_{-\infty}^{\infty} w_j f' dv + O(f'^3) \quad (37) \]
with
\[ O(f'^3) \equiv \rho^{-1} \rho' u_j' - (\rho' u_j' - \rho u_j') \]
from which we have, utilizing definition (5) for \( \psi \) and neglecting terms of \( O(f'^4) \)
\[ \rho \hat{\rho} u_j' \hat{u}_l' = m^2 \int_{-\infty}^{\infty} w_j \hat{w}_l \psi(z, \hat{z}) d\nu d\hat{\nu} \quad (38) \]
Furthermore, by substituting (28) for \( \psi \) and then (29) for \( F \), and carrying out integration over \((\nu, \hat{\nu})\) with orthonormal property of the Hermite polynomials incorporated, the following relationship results;
\[ \rho \hat{\rho} u_j' \hat{u}_l' = \frac{1}{(2\pi l)^3} \int_{-\infty}^{\infty} q_j(x, s) q_l(\hat{x}, s + \hat{x} - x) ds \quad (39) \]
Turbulent intensity or Reynolds’ stress is then given by putting \( \hat{x} = x \);
\[ \overline{u_j' u_l'} = \frac{1}{\rho^2(2\pi l)^3} \int_{-\infty}^{\infty} q_j(x, s) q_l(x, s) ds \quad (40) \]
a relationship expressing the observable turbulence intensities by an integral operation of the wave function. It is through this relationship that the Reynolds averaged Navier-Stokes equation is coupled with Eqs.(31) that govern \( q \)'s standing on the r.h.s. of (40).

In a similar fashion the wave function representing temperature fluctuation \( T' \) can be derived as follows: Since the ideal gas law \( p = R_M \rho T \) holds for instantaneous variables \( \rho \), we have
\[ R_M \rho T' = \rho' - R_M T \rho' = \frac{m}{3} \int_{-\infty}^{\infty} w_j f' dv - a^2 m \int_{-\infty}^{\infty} f' dv = \frac{ma^2}{3} \int_{-\infty}^{\infty} H_{jj} f' dv, \]
Accordingly, from (28)
\[ R_M^2 \rho T' \hat{T}' = \left( \frac{m}{3} \right)^2 a^2 \int_{-\infty}^{\infty} H_{jj} \hat{H}_{ll} \psi d\nu d\hat{\nu} \]
\[ = \frac{1}{(2\pi l)^3 \rho^2} \int_{-\infty}^{\infty} q_{jj}(x, s) q_{ll}(\hat{x}, s + \hat{x} - x) ds \]
where we have employed Hermite expansion (29). Thus we see that \( q_4 = (1/3)q_{jj} \) is the wave function to be responsible for the temperature fluctuation \( R_M \rho T' \).

Summarizing, the following correspondence rule holds between untangible wave function \( q_\alpha \) and corresponding observable fluctuation \( A'_\alpha \):

\[
q_\alpha = \begin{pmatrix}
q_0 \\
q_j \\
q_4 = \frac{1}{3}q_{jj} \\
q_{40}
\end{pmatrix}, \quad A'_\alpha = \begin{pmatrix}
\rho' \\
\rho u'_j \\
\rho R_M T' \\
p'
\end{pmatrix}
\] (41)

where the fourth quantity \( q_{40} \) in the column of \( q_\alpha \) is linearly dependent on \( q_0 \) and \( q_4 \). (See Eq. (31).) They are related to each other through the following fluctuation correlation formula:

\[
\overline{A'_\alpha A'_\beta} = \frac{1}{(2\pi l)^3} \int_{-\infty}^{\infty} q_\alpha(x, s) q_\beta(\tilde{x}, s + \tilde{x} - x) ds
\] (42)

In particular, for example, turbulent heat flux density is given as follows, using (41) and (42) with \( \tilde{x} = x \):

\[
c_p \rho^2 \overline{T'u_j} = \frac{5}{2} \int_{-\infty}^{\infty} q_4 q_j ds
\] (43)

where \( c_p \) is the specific heat under constant pressure.

5. Reformulation within phenomenologies

Once the correspondence rule (41) has been established we are able to reconstruct Eq. (31) using phenomenologies alone. This is what is anticipated because the present (Boltzmann) formalism is the averaged version of the Klimontovich formalism describing \( A'_\alpha \) directly, where the identity of phenomenologies and first-principle approach is warranted.

To effect this we shall base on the assertion that turbulent compressible flow of inert gas is governed by the following set of equations:

\[
\Lambda_0 \equiv \frac{\partial \rho_j}{\partial t} + \frac{\partial m_r}{\partial x_r} = 0 \quad (44)
\]

\[
\Lambda_j \equiv \frac{\partial \rho_j}{\partial t} + \frac{\partial m_r}{\partial x_r} \left[ \frac{m_r m_r}{\rho} + p\delta_{jr} + (p_{jr})_{NS} \right] = 0 \quad (45)
\]

\[
\Lambda_4 \equiv \frac{\partial}{\partial t} \left( E + \frac{m_j^2}{2\rho} \right) + \frac{\partial}{\partial x_r} \left[ \frac{m_r}{\rho} \left( H + \frac{m_j^2}{2\rho} \right) + \frac{m_r}{\rho} (p_{jr})_{NS} + (Q_{jr})_F \right] = 0 \quad (46)
\]
where

\[ m_j \equiv \rho u_j \]  \hspace{1cm} (47)\]

\[ E \equiv \rho e = \frac{p}{\gamma - 1} \quad (\gamma; \text{specific heats ratio}) \]  \hspace{1cm} (48)\]

\[ H \equiv \rho h = \frac{p}{\gamma - 1} \left[ \frac{\gamma}{\gamma - 1} \right] \]  \hspace{1cm} (48)\]

\[ (p_{jr})_{NS} \equiv -\mu \left[ \frac{\partial}{\partial x_r} \left( \frac{m_j}{\rho} \right) + \frac{\partial}{\partial x_j} \left( \frac{m_r}{\rho} \right) \right] - \frac{2}{3} \delta_{jr} \frac{\partial}{\partial x_k} \left( \frac{m_k}{\rho} \right) \]  \hspace{1cm} (49)\]

\[ (Q_r)_F = -\frac{\lambda}{R_M} \frac{\partial}{\partial x_r} \left( \frac{p}{\rho} \right) \]  \hspace{1cm} (49)\]

\[ p_{jr} = (p_{jr})_{NS} + \rho u'_j u'_r \]  \hspace{1cm} (50)\]

\[ (p_{jr})_{NS} = (p_{jr})_{F} + \rho c_p T' u'_r \]  \hspace{1cm} (50)\]

\[ (Q_r)_F = (Q_r)_{F} \]  \hspace{1cm} (50)\]

\[ \Lambda_\alpha = 0 \quad (\alpha = 0, j, 4) \]  \hspace{1cm} (51)\]

\[ \Lambda_0 \equiv \frac{\partial \rho}{\partial t} + \frac{\partial m_r}{\partial x_r} = 0 \]  \hspace{1cm} (51)\]

\[ \Lambda_j \equiv \frac{\partial m_j}{\partial t} + \frac{\partial}{\partial x_r} \left( \frac{m_j m_r}{\rho} + p \delta_{jr} + p_{jr} \right) = 0 \]  \hspace{1cm} (52)\]

\[ \Lambda_4 \equiv \frac{\partial}{\partial t} \left( E + \frac{m_j^2}{2\rho} \right) + \frac{\partial}{\partial x_r} \left( \frac{m_r H}{\rho} + \frac{1}{\rho} m_r m_j^2 + \frac{m_j}{\rho} p_{jr} + Q_r \right) = 0 \]  \hspace{1cm} (53)\]

\[ Q_r = (Q_r)_F + \rho c_p T' u'_r \]  \hspace{1cm} (53)\]

A few remarks are in order:

i) These equations are exact to \( O(A^2) \).
ii) They are written in terms of quantities that are \textit{proportional to the density}, for example, mean mass-flux density

\[ m_j \equiv \overline{m}_j = \rho u_j + \rho' u'_j \]

to replace mean fluid velocity \( u_j \), also mean internal energy \( E \) per unit of volume

\[ E \equiv \overline{E} = 1/\gamma - 1 (p + R_M \rho' T') \]

to replace the specific internal energy \( e \).

iii) Item ii) is the key that enables to express Reynolds-averaged equations (52) and (53) in \textit{compressibility invariant} forms, in other words, \textit{single term turbulence correction} to each of stress \( p_{jr} \) and heat flux density \( Q_r \) suffices even under presence of density fluctuation such as turbulent combustion.

iv) Otherwise, lengthy additional terms for turbulence correction would appear, or we would need the so-called mass averaging (say \( \overline{u}_j \), for instance) that suffers from a conceptual difficulty \((\overline{u}'_j \neq 0)\) in processing experimental data.

Next step, the main issue of this section, is to show the identity of Eqs. (31) with the following phenomenological equations

\[ A'_\alpha \bar{\Lambda}^\beta + \bar{A}'_\beta \Lambda^\alpha = 0, \ (\alpha, \beta; 1, j, 4) \] (54)

where \( A'_\alpha \) is defined in (41). These equations consist of terms of double \((O(A'^2))\) and triple \((O(A'^3))\) correlations for which we employ the separation rule exactly parallel to those of the previous section [Eq. (20) through Eq. (28)]:

Put

\[
\begin{align*}
\overline{A}'_\alpha \bar{A}'_\beta &= \text{R.P.} \ i^3 \int_{-\infty}^{\infty} g_\alpha(x, k) g_\beta(x', k') \ d\mathbf{k} \\
\overline{A}'_\alpha \overline{A}'_\beta \Lambda^\gamma &= \text{R.P.} \ i^6 \int_{-\infty}^{\infty} g_\alpha(x, k) g_\beta(x', k') \ g_\gamma(x, k - k') \ d\mathbf{k} d\mathbf{k}'
\end{align*}
\] (55)

and substitute into Eq. (54), then we are led to the equation that allows for the separation of variables:

\[
\int_{-\infty}^{\infty} d\mathbf{k} \ g_\alpha(x, k') \left[ \frac{\bar{\Lambda}^\dagger_\alpha}{g_\alpha} + \left( \frac{\bar{A}'_\beta}{g_\beta} \right)^* \right] \left[ \frac{\Lambda^\dagger_\alpha}{g_\alpha} + \left( \frac{\Lambda^\dagger_\beta}{g_\beta} \right)^* \right] = 0
\]

\[
\| \frac{\Lambda^\dagger_\alpha}{g_\alpha} + \left( \frac{\Lambda^\dagger_\beta}{g_\beta} \right)^* \| = 0
\] (56)
In the above $\Lambda^\dagger_\alpha$ is the fluctuating part of $\Lambda_\alpha$ in which $A'_\alpha$ is replaced with $g_\alpha$, also $A'_\alpha A'_\gamma$ with convolution integral $\int_{-\infty}^{\infty} g_\alpha(k') g_\gamma(k-k') d\mathbf{k}'$, and $\partial/\partial x_r$ with $\partial/\partial x_r + ik_r$. The separated equation thus obtained, namely,

$$-i\omega g_\alpha + \Lambda^\dagger_\alpha = 0 \quad (57)$$

is then rewritten in Fourier-analyzed form after

$$g(x, k) = \frac{1}{(2\pi l)^3} \int_{-\infty}^{\infty} e^{-i\mathbf{k} \cdot \mathbf{s}} q(x, s) \, ds \quad (58)$$

to lead to the same equations as Eqs.(31) except for the energy fluctuation equation which takes the form,

$$\frac{1}{\gamma - 1} D q_{40} + \partial_r q_{c, ij} + \frac{\gamma}{\gamma - 1} \partial_r (a^2 q_r) + \frac{\partial u^\dagger_1}{\partial x_r} q_{40} + \frac{\partial u^\dagger_2}{\partial x_r} q_{40} - \frac{1}{\rho} \frac{\partial p}{\partial x_r} q_r = 0 \quad (59)$$

This equation reduces in the case of monatomic gases ($\gamma = 5/3$) to the third of Eqs.(31) as it should.

6. A solitary-wave solution for mixing layer turbulence

A preliminary computation checking whether the present approach is physically sound has been carried out for turbulent mixing shear layer of an incompressible flow [18]. Eqs.(34) and (35) are employed assuming the average flow profile $[u(\eta), v(\eta), 0]$ with $\eta \equiv x_2/\alpha x_1$ as prescribed. The flow is self-similar in this sense as confirmed by experiment [19], which is an indicative of molecular viscosity playing no roles in the equation. (See ref.[18].) Then we have the following set of equations:

$$\begin{align*}
\partial_1 q_1 + \partial_2 q_2 + \partial_3 q_3 / \partial s_3 &= 0 \\
NL q_1 + \partial_1 q_{40} - \alpha \eta u' q_1 + u' q_2 &= 0 \\
NL q_2 + \partial_2 q_{40} - \alpha \eta v' q_1 + v' q_2 &= 0 \\
NL q_3 + \partial q_{40} / \partial s_3 &= 0
\end{align*} \quad (60)$$

where $u' \equiv du/d\eta$, and

$$\begin{align*}
\partial_1 &\equiv (1 - \alpha s_1) \partial / \partial s_1 - \alpha (\eta \partial / \partial \eta + s_2 \partial / \partial s_2 + s_3 \partial / \partial s_3) \\
\partial_2 &\equiv \partial / \partial \eta + \partial / \partial s_2 \\
NL &\equiv \partial / \partial t - c \partial / \partial s_1 + (u + q_1) \partial_1 + (v + q_2) \partial_2 + q_3 \partial / \partial s_3
\end{align*} \quad (61)$$

with $s$ redefined using the shear mixing layer thickness $l = \alpha x_1$, namely, $s/l \rightarrow s$.

The set of equations has five independent variables $(s, \eta, t)$, therefore no existing tools are immediately available. At this preliminary stage of checking physical soundness of the proposed approach it is advisable to suppress variable $s_2$ by assuming $\partial / \partial \eta >>$
\( \partial / \partial s_2 \). The set of equations is solved for arbitrary chosen initial values for \( q_\alpha \) and boundary conditions

\[
q_j \rightarrow 0, \ (j = 1, 2, 3) \text{ as } |s|, |\eta| \rightarrow \infty \\
q_{40} \rightarrow 0 \text{ as } |s| \rightarrow \infty, \ \partial q_{40} / \partial \eta \rightarrow 0 \text{ as } \eta \rightarrow \infty 
\]

(62)

The form of solution to be expected from these homogeneous boundary conditions must be a solitary wave generated by the shearing motion and kept sustained by nonlinearity.

In Figs.1 are shown such standing waves that build up and reach steady state with elapse of time for different choices of the wave speeds; (a) experimentally observed one \( c = u_0 = [u(\infty) + u(-\infty)]/2 \), and (b) Taylor's hypothesis \( c = u(\eta) \). Reynolds' stress [Eq.(40)] is calculated using this solution and compared with existing experiment \([19]\) in Fig.2. Agreement is more than reasonable considering that the theory involves no empirical constants to fit with experiments.

7. Comparison with classical statistical theory and current turbulence models

Consistency with classical statistical theory

Kármán and Howarth \([20]\), the founders of classical statistical theory of turbulence, have derived Eq.(54) for incompressible flows \((\alpha, \beta; 0, 1, 2, 3)\) correctly on intuitive basis, with no reference to first principles. Obviously these 6-D equations are not tractable in this form, so homogeneity/isotropy assumptions have been introduced. Here we have employed the method of separation of variables, thereby the classical limitation on flow geometry is eliminated. It is effected, however, at the expense of introducing additional independent variable \( s \) in the Navier-Stokes equation as we have seen through Eqs.(34) and (35).

The classical assumptions of homogeneity and isotropy are often referred to as an oversimplification of reality. In fact, also here, this model is shown to lead to an unphysical solution: For the equation of continuity

\[
\frac{\partial q_j}{\partial s_j} = 0
\]

(63)

which is the homogeneous version \((\partial / \partial x_j = 0)\) of Eq.(54), coupled with the isotropy requirement (Robertson's theorem \([21]\))

\[
q_j = s_j q(s), \ (s \equiv |s|)
\]

(64)

gives

\[
3 q + s \frac{dq}{ds} = 0
\]

(65)
Solution of this equation, namely, \( q \sim s^{-3} \) causes the integral (40) for turbulence intensity to diverge. To be noted is the fact that this is a direct consequence of the equation of continuity, a kinematical relationship universally valid, therefore independent of any closure condition employed.

*Inconsistency with \( k - \epsilon \) models*

We have seen that formulation in 6-D space \((x, \hat{x})\) [Eq.(54)] is the only one that is consistent with Liouville’s equation, namely, with first principles of nonequilibrium statistical mechanics. Turbulent transports such as (10) and (13) that are quantities in 3-D space are obtained from the solution in the 6-D space by putting \( \hat{x} = x \) after the equations have been solved. Suppressing variables in the equations as is often employed is a pathological process. The following simple example would help extract what is meant by this trivial-looking warning: Let a steady-state temperature distribution of a three-dimensional body, say, a column with rectangular cross-section in the \( x-y \) plane be asked, but the information only on the diagonal plane \( x = y \) is required. Needless to say that proper process is to work with 3-D Laplace equation for the solution \( T(x, y, z) \), and put \( x = y \) to have \( T(x, x, z) \). The improper process mentioned here corresponds to solving pathological equation \((2\partial^2/\partial x^2 + \partial^2/\partial z^2)T = 0\).

Majority of turbulence models currently prevailing do not concur, in the simplest case of the homogeneous and isotropic turbulence, with the Kármán-Howarth theory as a consequence of the hasty reduction in independent variables as sketched here.

Summarizing, the proposed approach shares the common basis with \( k - \epsilon \) models only at the lowest level of description, namely, the Reynolds-averaged Navier-Stokes equation, but differs substantially at next level of the Reynolds’ stress equation.

8. Concluding remarks

On the basis of the Boltzmann formalism, namely, nonequilibrium statistical mechanics designed for turbulence, two sets of equations are derived to comprise a closed set. The one is the group of equations governing Reynolds-averaged fluid quantities, and the other is the variable-separated version of the fluctuation-correlation equations that reduces to the classical Kármán-Howarth equation in the homogeneous and isotropic limit. The two sets of equations are coupled through turbulent transports such as Reynolds’ stress and turbulent heat-flux density.

The key role of the first principle lies in that

(i) for the Reynolds averaged equations, it gives a firmer basis than via phenomenologies, whereas,

(ii) for the turbulent-transport equations, it reveals a hidden kinematical prerequisite for any turbulence governing equations to fulfill, thereby enabling to single out the
unique form. It is also shown that once their unique form has been established the whole sets of equations are able to be reconstructed a posteriori using phenomenologies alone.

The latter set of equations is converted into a variable-separated form, leading to those governing solitary-wave function through which all the turbulent-transport properties are calculated.

The equations are solved for a self-similar turbulent mixing layer, leading to a solitary-wave type solution in the physical-plus-eddy space. Reynolds stress is obtained through a simple integration of the solution over the eddy space in a form free from any empirical parameters, yet showing satisfactory agreement with existing experiment.

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Figure captions

Fig.1 Solitary wave $q_1(s_1, s_3, 0)$ on the plane of $\eta = 0$ for two choices of the phase velocity $c$;

a) $c = u_0$, where $u_0 = [u(\infty) + u(-\infty)]/2$ is the propagation velocity of eddies as observed by flow visualization,

b) $c = u$ (Taylor’s hypothesis).

Fig.2 Reynolds’ stress as calculated from Eq.(40) [18] using the solitary-wave solutions (Figs.1a and 1b), and compared with existing experiment[19].
$C = u$
