Burgers's turbulence model as a stochastic dynamical system: Master equation and simulation

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By means of Burgers's equation a stochastic description of turbulent fluid flows is explained which is based on a discrete master equation. The latter governs the dynamics of a discrete multivariate stochastic process representing the random velocity field of the fluid. From the characteristic function corresponding to this stochastic process, the Hopf functional equation of turbulence is obtained. This implies that the infinite hierarchy of correlation functions can be derived from the master equation. The master-equation description naturally leads to a simple stochastic simulation algorithm which is well suited to numerical implementation. Stochastic simulations of the Burgers model of turbulence are performed and are shown to yield very accurate results.

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I. INTRODUCTION

It is well known that stochastic concepts provide a natural tool for the description of turbulent fluid motion [1, 2]. In order to obtain a statistical theory one considers an ensemble of initial velocity fields, each member of which evolves deterministically in time according to the Navier-Stokes equation. Recently a different stochastic approach to the description of turbulent fluid flows has been proposed [3]. Within this approach the velocity field is regarded as a discrete stochastic process defined by a multivariate master equation [4, 5]. The latter governs the time evolution of the joint probability distribution of the stochastic process and replaces the deterministic dynamics of the Navier-Stokes equation. Thus, within this approach turbulent fluids are interpreted as stochastic dynamical systems.

The motivation for this master-equation formulation of turbulent fluid dynamics is twofold. First, one of the leading ideas of a statistical approach to the problem of turbulence is to abandon the attempt to follow single trajectories in time and instead to concentrate on the time development of an ensemble of trajectories. Therefore it is tempting to try to formulate an inherently probabilistic dynamical theory which describes the probabilistic time evolution of an ensemble of initial velocity fields. Second, the formulation of a probabilistic dynamics for the velocity field defined by a multivariate master equation makes possible the use of stochastic simulation methods which are particularly well suited for the numerical treatment of dynamical systems with many degrees of freedom. The last statement is made evident by the experience gained in the stochastic simulation of complex chemical reactions [6, 7]. Therefore promising computational approaches to the study of turbulence can be expected from the interpretation of the fluid as a stochastic dynamical system.

It is the aim of the present paper to analyze in detail the connection between the stochastic process defined by our master equation and the usual statistical description of turbulence. In order to keep things as simple as possible, we will perform this analysis by employing the (1+1)-dimensional Burgers model of turbulence [8, 9].

A rigorous mathematical formulation of a statistical theory of turbulence was given by Hopf [10–12]. He investigated the characteristic functional of the probability measure in the space of velocity fields which completely characterizes the statistical properties of the ensemble under consideration. From the Navier-Stokes equation Hopf derived a functional differential equation for this characteristic functional. Employing the (1+1)-dimensional Burgers model of turbulence, we will demonstrate that the characteristic functional corresponding to our multivariate master equation obeys in the continuum limit the Hopf functional equation. This implies that our stochastic approach correctly represents the infinite hierachy of n-point correlation functions of the turbulent velocity field. We illustrate this fact by performing some stochastic simulations of the Burgers model which yield, for example, the correct power-law behavior of the energy spectrum.

Deriving the Hopf equation from our multivariate master equation, the limit of continuous space has to be taken. A systematic expansion reveals that the next to leading-order term represents a random momentum flux induced by the thermal fluctuations in the fluid. Thus the stochastic process defined by our master equation models hydrodynamic as well as thermodynamic degrees of freedom.

The paper is organized as follows. In Sec. II we present the master-equation formulation of Burgers's equation. The equation governing the time evolution of the first moments of our multivariate stochastic process is derived and shown to yield Burgers's equation in the continuum limit. In Sec. III, which is the central part of this paper, we investigate the characteristic functional obtained from our master equation. There it is shown that this characteristic functional leads in the continuum limit to

the Hopf functional equation of turbulence. Section IV is devoted to the method of stochastic simulation. We demonstrate that our stochastic formulation leads to a very efficient and simple numerical simulation algorithm. The latter is applied to Burgers's model of turbulence. Numerical results, such as the energy spectrum and the dissipation rate are discussed. Finally, in Sec. V we draw our conclusions and outline the subjects of future work.

II. FLUIDS AS STOCHASTIC DYNAMICAL SYSTEMS

It is the aim of this section to present in detail a recently proposed stochastic description of the dynamics of fluids. At this stage we restrict the discussion of the master-equation formulation of fluid dynamics to stable flow situations. Our approach will be explained with the help of Burgers's equation which may be regarded as a one-dimensional version of the Navier-Stokes equation (without pressure term),

$$\frac{\partial}{\partial t}v(x,t)+v(x,t)\frac{\partial}{\partial x}v(x,t)=\nu\frac{\partial^2}{\partial x^2}v(x,t) \quad , \tag{1}$$

where $v(x,t)$ is the velocity field and ν the kinematic viscosity. In analogy to the Navier-Stokes equation, Burgers's equation contains a nonlinear inertial term and a dissipative viscosity term. In this paper we study Burgers's equation on the interval $[0,L]$ imposing periodic boundary conditions $v(x+L,t)=v(x,t)$.

A. The multivariate master equation

The stochastic dynamical system we are going to construct is defined on a discrete phase space. In order to construct the latter we first divide physical space, i.e. the interval $[0,L]$, into a sufficiently large number $M+1$ of cells of width $\delta l = L/(M+1)$ centered at points $x_\lambda = \delta l \lambda$, which are labeled by the integer valued index $\lambda = 0,1,\ldots,M$. The discretization of the velocity space is achieved in the following way: We introduce a mesoscopic velocity scale δu representing the size of the smallest change of the velocity in a given cell. Thus we measure the velocity in integer multiples of δu. This means that in each cell λ the velocity is described by an integer variable $N_\lambda \in \mathbb{Z}$. Within this description the state of the fluid is completely fixed by specifying the set of numbers $\{N_\lambda\}$. Formally, the resulting discrete phase space Γ may be written as

$$\Gamma = \left\{ \{N_\lambda\}_{\lambda=0,1,\ldots,M} \mid N_\lambda \in \mathbb{Z} \right\}. \tag{2}$$

The central idea of our stochastic formulation of fluid dynamics is the following one: The numbers N_λ introduced above are considered to be time-dependent random numbers. Consequently, the set of variables $\{N_\lambda\}$ is regarded as a multivariate stochastic process. The connection to Burgers's equation is provided by interpreting the velocity field $v(x_\lambda,t)$ as the expectation value of this integer valued stochastic process, that is, we require

$$v(x_\lambda,t) \equiv v_\lambda(t) = \delta u \langle N_\lambda \rangle \quad , \tag{3}$$

where the angular brackets denote the time-dependent expectation value (see below). In this section we will define an appropriate dynamics for the stochastic process $\{N_\lambda\}$ in such a way that $v_\lambda(t)$ as defined in Eq. (3) obeys a discretized version of Burgers's equation. In other words, within our stochastic approach Burgers's equation is regarded as the *macroscopic* dynamical equation of an underlying *mesoscopic* stochastic process.

Having introduced the discrete phase space Γ we now have to define the dynamics of the stochastic process $\{N_\lambda\}$. To this end we introduce the joint probability distribution $P(\{N_\lambda\},t)$, which gives the probability at time t of finding the set of numbers $\{N_\lambda\}$ and completely characterizes the stochastic process once an initial condition has been specified. Of course, the joint probability distribution $P(\{N_\lambda\},t)$ is normalized,

$$\sum_{\{N_\lambda\}} P(\{N_\lambda\},t) = 1 \quad , \tag{4}$$

where $\sum_{\{N_\lambda\}}$ denotes a $(M+1)$-fold sum over all integers N_λ, $\lambda = 0,1,2,\ldots,M$. Once the joint probability distribution $P(\{N_\lambda\},t)$ is known one can evaluate expectation values for arbitrary functions

$$\mathcal{F} = \mathcal{F}(\{N_\lambda\}) \tag{5}$$

of the stochastic variables $\{N_\lambda\}$ according to

$$\langle \mathcal{F} \rangle \equiv \sum_{\{N_\lambda\}} \mathcal{F}(\{N_\lambda\})\ P(\{N_\lambda\},t) \quad . \tag{6}$$

As will be explained in Sec. III B, it is reasonable to postulate $\{N_\lambda\}$ to be a multivariate Markov process. Therefore the time evolution of the joint probability distribution $P(\{N_\lambda\},t)$ is governed by a multivariate master equation which we formally write as

$$\frac{\partial}{\partial t}P(\{N_\lambda\},t) = \mathcal{A}P(\{N_\lambda\},t) \quad , \tag{7}$$

where we introduced the generator $\mathcal{A}$ of the time evolution of P. In the following, $\mathcal{A}$ is regarded as an operator which acts (to the right) on functions of the stochastic variables $\{N_\lambda\}$. Correspondingly, the time derivative of the expectation value of an arbitrary function may be written as

$$\begin{aligned}\frac{\partial}{\partial t}\langle \mathcal{F} \rangle &= \sum_{\{N_\lambda\}} \mathcal{F}(\{N_\lambda\})\ \frac{\partial}{\partial t}P(\{N_\lambda\},t) \\ &= \sum_{\{N_\lambda\}} \mathcal{F}(\{N_\lambda\})\ \mathcal{A}P(\{N_\lambda\},t) \\ &\equiv \langle \mathcal{F}\mathcal{A} \rangle \quad . \end{aligned} \tag{8}$$

Once a time evolution operator $\mathcal{A}$ is given the dynamics of the stochastic process $\{N_\lambda\}$ is completely specified. The operator $\mathcal{A}$ given below has originally been constructed [4, 5] in order to fulfill the requirement that the time evolution equation of the expectation value $\delta u \langle N_\lambda \rangle$

obeys in the limit $\delta u \longrightarrow 0$, i.e., in the limit of large numbers N_λ, a discretized version of Burgers's equation which leads in the continuum limit $\delta l \longrightarrow 0$ to the partial differential equation (1).

In a previous series of publications [3–5, 13] it was shown that the stochastic process $\{N_\lambda\}$ defined by the following multivariate master equation satisfies this requirement:

$$\frac{\partial P}{\partial t} = \frac{\nu}{\delta l^2}\sum_{\lambda=0}^{M}\left[\left(\mathbf{E}_{\lambda-1}^{-1}\mathbf{E}_\lambda - \mathbf{1}\right)N_\lambda^+ + \left(\mathbf{E}_{\lambda+1}^{-1}\mathbf{E}_\lambda - \mathbf{1}\right)N_\lambda^+\right]P - \frac{\nu}{\delta l^2}\sum_{\lambda=0}^{M}\left[\left(\mathbf{E}_{\lambda-1}\mathbf{E}_\lambda^{-1} - \mathbf{1}\right)N_\lambda^- + \left(\mathbf{E}_{\lambda+1}\mathbf{E}_\lambda^{-1} - \mathbf{1}\right)N_\lambda^-\right]P$$
$$+\frac{1}{2}\frac{\delta u}{\delta l}\sum_{\lambda=0}^{M}\left(\mathbf{E}_{\lambda+1}^{-1}\mathbf{E}_\lambda - \mathbf{1}\right)\frac{1}{2}\left\{N_\lambda^2 + N_{\lambda+1}^2\right\}P \equiv \mathcal{A}P. \tag{9}$$

Let us explain the compact notation used to formulate the above equation. First, we have defined the shift operators $\mathbf{E}_\lambda^{\pm 1}$ by

$$\mathbf{E}_\lambda^{\pm 1}\mathcal{F}(\{\ldots, N_\lambda, \ldots\}) = \mathcal{F}(\{\ldots, N_\lambda \pm 1, \ldots\}) \quad . \tag{10}$$

Furthermore, since the velocity can take positive as well as negative values, the positive part N_λ^+ and the negative part N_λ^- of the stochastic process N_λ have been introduced through the relations

$$N_\lambda = N_\lambda^+ + N_\lambda^-, \quad |\, N_\lambda \,| = N_\lambda^+ - N_\lambda^-. \tag{11}$$

Since we want to investigate the stochastic formulation of Burgers's equation with periodic boundary conditions we have to fix the boundary conditions of the stochastic process accordingly. Recalling that we divided the interval $[0, L]$ into $M+1$ cells of equal width the periodic boundary condition imposed on the stochastic process reads

$$N_{M+1} \equiv N_0 \quad . \tag{12}$$

Now it is evident that all sums in Eq. (9) run from $\lambda = 0$ to $\lambda = M$.

The above master equation (9) is the fundamental equation of our approach. It defines our formulation of the fluid as a stochastic dynamical system and will be the starting point of the theoretical and numerical investigations in this paper.

B. The time evolution equation for the first moments

Having presented the master equation defining the time evolution of the stochastic process $\{N_\lambda\}$ we now demonstrate that our requirement explained in Sec. II A is satisfied, i.e., we show that the expectation value of the stochastic process $\delta u\langle N_\lambda\rangle$ indeed obeys a discrete form of Burgers's equation.

More generally, let us first derive an appropriate form for the time evolution equation of the expectation value of an arbitrary function $\mathcal{F}(\{N_\lambda\})$ of the stochastic variables. To this end, we consider an expression of the form $\langle \mathbf{E}_{\lambda+1}^{-1}\mathbf{E}_\lambda \mathcal{F}\rangle$. Recalling that the expectation value involves a multiple sum over all integers N_λ, it is easy to show with the help of the definition of the operators $\mathbf{E}_\lambda^{\pm}$, Eq. (10), and by shifting the summation indices appropriately that the following equation holds:

$$\langle \mathbf{E}_{\lambda+1}^{-1}\mathbf{E}_\lambda \mathcal{F}\rangle = \langle \mathcal{F}\rangle \quad . \tag{13}$$

This equation is true, of course, for any other product of shift operators appearing in our master equation (9). Thus these products of shift operators when acting on a function of the stochastic variables have no influence on its expectation value and can, within the angular brackets, always be replaced by the identity. Since the time evolution operator $\mathcal{A}$ contains the above products of shift operators only in the form $(\mathbf{EE}-\mathbf{1})$, Eq. (13) implies that

$$\langle \mathcal{A}\,\mathcal{F}\rangle = \sum_{\{N_\lambda\}} \mathcal{A}\,\mathcal{F}P = 0 \quad . \tag{14}$$

Introducing the commutator (the function $\mathcal{F}$ being regarded as a multiplication operator)

$$[\mathcal{F}, \mathcal{A}] \equiv \mathcal{F}\mathcal{A} - \mathcal{A}\,\mathcal{F} \tag{15}$$

and exploiting relation (14), Eq. (8) takes the form

$$\frac{\partial}{\partial t}\langle \mathcal{F}\rangle = \langle [\mathcal{F}, \mathcal{A}]\rangle \quad . \tag{16}$$

Thus the time derivative of the expectation value of a function $\mathcal{F}$ of the stochastic variables is equal to the expectation value of the commutator $[\mathcal{F}, \mathcal{A}]$.

For the special case of the first moments of the stochastic process $\delta u N_\lambda$ we have

$$\delta u \frac{\partial}{\partial t}\langle N_\lambda\rangle = \delta u\ \langle [N_\lambda, \mathcal{A}]\rangle \quad . \tag{17}$$

In order to determine the commutator $[N_\lambda, \mathcal{A}]$ we proceed by evaluating the commutator

$$\left[N_\lambda, \mathbf{E}_{\lambda'\pm 1}^{-1}\mathbf{E}_{\lambda'}\right] = \mathbf{E}_{\lambda'\pm 1}^{-1}\mathbf{E}_{\lambda'}\left(\delta_{\lambda'\pm 1,\,\lambda} - \delta_{\lambda',\,\lambda}\right). \tag{18}$$

Inserting the expression for the time evolution operator $\mathcal{A}$ into Eq. (17) and using (18) for the determination of $[N_\lambda, \mathcal{A}]$ and (13) for evaluating the expectation value we finally obtain

$$\delta u\,\frac{\partial}{\partial t}\langle N_\lambda\rangle = \nu\frac{\delta u}{\delta l^2}\langle N_{\lambda+1}^+ - 2N_\lambda^+ + N_{\lambda-1}^+ + N_{\lambda+1}^- - 2N_\lambda^- + N_{\lambda-1}^-\rangle - \frac{\delta u^2}{4\delta l}\langle N_{\lambda+1}^2 - N_{\lambda-1}^2\rangle \quad . \tag{19}$$

Recalling that $N_\lambda = N_\lambda^+ + N_\lambda^-$, the time evolution equation of the first moment of the stochastic process N_λ can

be written as

$$\delta u \frac{\partial}{\partial t}\langle N_\lambda\rangle = \nu\frac{\delta u}{\delta l^2}\langle N_{\lambda+1} - 2N_\lambda + N_{\lambda-1}\rangle - \frac{\delta u^2}{4\delta l}\langle N_{\lambda+1}^2 - N_{\lambda-1}^2\rangle. \quad (20)$$

As should have been expected, the system of dynamic equations for the first moments is not closed. In fact, as a consequence of the nonlinear transition rates occurring in the master equation (9) the second moments $\langle N_\lambda^2\rangle$ enter the above equations. Correspondingly, the equations for the nth moments contain the $(n+1)$th moments and so on. Thus the master equation leads to an infinite hierarchy of coupled moment equations and an appropriate approximation scheme is required in order to obtain a finite-dimensional system of equations.

As we already stated, the discrete Burgers equation should be obtained as the macroscopic equation for the stochastic process $\delta u N_\lambda$ in the limit $\delta u \longrightarrow 0$. In this limit the numbers N_λ become infinitely large and, therefore, one expects that fluctuations are small. Thus it is plausible to assume that the approximation

$$\langle N_\lambda^2\rangle \approx \langle N_\lambda\rangle^2 \quad (21)$$

holds to a sufficient degree of accuracy. It is then possible to close the system of equations (20) for the first moments. In fact, invoking (21) one immediately obtains the discretized Burgers equation

$$\frac{\partial}{\partial t}v_\lambda(t) = \nu\frac{v_{\lambda+1} - 2v_\lambda + v_{\lambda-1}}{\delta l^2} - \frac{1}{2}\frac{v_{\lambda+1}^2 - v_{\lambda-1}^2}{2\,\delta l}\quad , \quad (22)$$

which, in turn, leads to Burgers's equation (1) in the continuum limit $\delta l \longrightarrow 0$.

Thus we have obtained Burgers's equation as a macroscopic equation of the stochastic process $\{N_\lambda\}$. This has been achieved by employing the crude approximation (21), which completely disregards the fluctuations. However, one can obtain [14, 15] the macroscopic equation (22) of the underlying stochastic process governed by the master equation (9) in a systematic way by means of van Kampen's Ω expansion [16]. Furthermore, the Ω expansion leads to a linear noise approximation which can be shown [14, 15] to be equivalent to the theory of fluctuating hydrodynamics [17–19].

The analysis of the master equation presented in this section was based on the assumption that the stochastic process N_λ describes small fluctuations around a stable macroscopic solution of Burgers's equation. These considerations were done in order to motivate the ideas which lead to the master-equation formulation of Burgers's equation. However, in this paper we want to study the Burgers model of (spatially) homogeneous turbulence which describes a completely different situation: While the macroscopic velocity field vanishes identically, $v_\lambda \equiv 0$, fluctuations become important. We therefore have to follow a different strategy in order to demonstrate that our approach may be applied to turbulent situations as well. This will be done in the next section.

III. THE MASTER EQUATION APPROACH TO BURGERS'S MODEL OF TURBULENCE

In this section we will analyze the relation of the master equation description presented in Sec. II to the usual statistical approach to turbulent fluid motion which leads to the functional Hopf equation. In order to keep the presentation as simple as possible we restrict ourselves to the discussion of the (1+1)-dimensional Burgers model of turbulence and investigate the Hopf equation for the latter.

A. The Hopf functional formulation

Let us first precisely state the statistical approach to the problem of turbulence which has been used by Hopf in order to derive an equation for the characteristic functional [10–12]. Within this approach an ensemble of velocity fields is defined by specifying an initial probability distribution $P_0^H[v_0(x)]$ in the phase space, i.e., the space of velocity fields $v_0(x)$ which obey the correct boundary conditions (in this section we use the index H to indicate all quantities which refer to the stochastic process defined by the Hopf functional). Once an initial velocity field $v_0(x)$ has been chosen according to this probability distribution $P_0^H[v_0(x)]$ a corresponding solution of Burgers's equation,

$$v(x,t) = \Phi^t v_0(x) \quad , \quad (23)$$

is uniquely defined. In the above equation, Φ^t denotes the phase flow corresponding to Burgers's equation, i.e., the time evolution operator which maps any solution $v(x,s)$ of Burgers's equation at time s to its value $v(x,s+t)$ at time $t+s$. In particular, we have

$$\Phi^s\Phi^t = \Phi^{s+t}\ , \quad \Phi^0 = \text{identity} \quad . \quad (24)$$

Since $v_0(x)$ is a random initial field, the velocity field $v(x,t)$ as defined by Eq. (23) may be regarded as a stochastic process. Accordingly, the probability distribution $P^H[v(x),t]$ which represents the probability density for the velocity field to take the value $v(x)$ at time t is obtained from the Liouville equation [10]

$$P^H[v(x),t] = \int Dv_0\, P_2^H\,[v_2(x),t_2 \mid v_1(x),t_1] \times P_0^H[v_0(x)], \quad (25)$$

where $\int Dv_0$ denotes the functional integral over the (function) space of initial velocity fields. The transition probability P_2^H is defined by

$$P_2^H\,[v_2(x),t_2 \mid v_1(x),t_1] = \delta[\Phi^{t_2-t_1}v_1(x) - v_2(x)] \quad , \quad (26)$$

where $\delta[v(x)]$ denotes the functional delta function

$$\delta[v(x)] \equiv \prod_x \delta(v(x)) \quad , \quad (27)$$

$\delta(v(x))$ being the ordinary delta function.

According to its general definition,

$$P_2^H\,[v_2(x),t_2 \mid v_1(x),t_1]$$

is the conditional probability that at time t_2 the velocity field $v_2(x)$ is realized provided the velocity field at time t_1 is given by $v_1(x)$. Thus Eq. (26) expresses the fact that each realization of the stochastic process is a solution of Burgers's equation: P_2^H is nonzero if and only if the field $v_2(x)$ evolves from $v_1(x)$ according to Burgers's equation during the time interval from t_1 to t_2, i.e., if and only if the phase flow $\Phi^{t_2-t_1}$ maps $v_1(x)$ to $v_2(x)$.

It is a well-known result of the theory of stochastic processes that the Liouville equation (25) together with some transition probability P_2^H uniquely defines a Markov process $v(x,t)$ provided the Chapman-Kolmogorov equation

$$\begin{aligned} &P_2^H\,[v_3(x),t_3 \mid v_1(x),t_1] \\ &= \int Dv_2\; P_2^H\,[v_3(x),t_3 \mid v_2(x),t_2] \\ &\quad \times P_2^H\,[v_2(x),t_2 \mid v_1(x),t_1] \end{aligned} \tag{28}$$

is fulfilled. It is easy to see that Eq. (28) is an immediate consequence of (26) and the property (24) of the flow. Moreover, we see that the Markov process $v(x,t)$, although being nonstationary in general, is homogeneous in time since its transition probability (26) obviously depends only on the time difference $t_2 - t_1$. Thus we conclude that $v(x,t)$ is a homogeneous (in time) Markov process. We emphasize that this property holds for each stochastic process which is obtained from a deterministic autonomous dynamical system by imposing random initial conditions [20, 21].

Now the Hopf functional equation corresponding to Burgers's equation can be written down. To this end, we introduce the characteristic functional

$$\begin{aligned} M^H\,[z(x),t] &\equiv \left\langle \exp\left\{ i \int dx\; z(x) v(x) \right\} \right\rangle \\ &\equiv \int Dv\; \exp\left\{ i \int dx\; z(x) v(x) \right\} \\ &\quad \times P^H[v(x),t], \end{aligned} \tag{29}$$

from which arbitrary equal time moments of the random velocity field can be obtained by evaluating functional derivatives with respect to $z(x)$. Inserting Eq. (25) into the definition (29) of the characteristic functional and employing the equation of motion, i.e., Burgers's equation, one arrives at the following equation for the characteristic functional:

$$\begin{aligned} &\frac{\partial}{\partial t} M^H\,[z(x),t] \\ &= \int dx\; z(x) \left\{ \frac{i}{2} \frac{\partial}{\partial x} \left(\frac{\delta^2 M^H}{\delta z(x)^2} \right) + \nu \frac{\partial^2}{\partial x^2} \left(\frac{\delta M^H}{\delta z(x)} \right) \right\} . \end{aligned} \tag{30}$$

This is Hopf's functional equation for Burgers's model of turbulence.

B. The master-equation formulation

We now turn to the master-equation formulation of the problem. As we have seen in Sec. III A the statistical formulation of Burgers's model of turbulence naturally leads to the stochastic Markov process $v(x,t) = \Phi^t v_0(x)$. It is therefore reasonable to postulate this same Markov character for the stochastic process $\delta u N_\lambda(t)$ as was done in Sec. II by constructing a multivariate master equation. It should be noted that the Markov character of $v(x,t)$ and $\delta u N_\lambda(t)$ is only guaranteed if the full phase space of velocity fields is taken into account. Stated differently, reducing the number of degrees of freedom would immediately destroy the Markov property.

Being a Markov process, $\delta u N_\lambda(t)$ is characterized by the joint probability distribution $P(\{N_\lambda\},t)$ and a transition probability P_2,

$$P_2 = P_2\left(\{N_\lambda^{(2)}\}, t_2 \mid \{N_\lambda^{(1)}\}, t_1 \right) . \tag{31}$$

Moreover, since the operator $\mathcal{A}$ constructed in Sec. II does not depend explicitly on time, the transition probability depends only on the difference $t_2 - t_1$ of the time arguments. The consistency condition connecting the probability distribution and the transition probability reads

$$\begin{aligned} P(\{N_\lambda\},t) &= \sum_{\{N_\lambda^{(0)}\}} P_2\left(\{N_\lambda\}, t \mid \{N_\lambda^{(0)}\}, 0 \right) \\ &\quad \times P_0\left(\{N_\lambda^{(0)}\} \right) , \end{aligned} \tag{32}$$

where $P_0\left(\{N_\lambda^{(0)}\}\right)$ denotes the initial probability distribution. It is this equation that is the master-equation analog of the Liouville equation (25). Comparing both equations we see that the stochastic processes $v(x,t)$ and $\delta u N_\lambda(t)$ are both specified by an initial distribution in the corresponding phase space. However, each realization of the random process $v(x,t)$ is a smooth solution of Burgers's equation; in contrast, the process $\delta u N_\lambda(t)$ is a discrete jump process each realization of which changes discontinuously by finite steps. As a consequence of this fact, turning from the random process $v(x,t)$ to $\delta u N_\lambda(t)$, the δ-functional transition probability P_2^H whose time evolution is induced by the phase flow Φ^t is replaced by the discrete transition probability P_2 the time evolution of which is governed by the discrete master equation.

Since both stochastic processes introduced above are homogeneous (in time) and since the initial probability distributions P_0^H and P_0 are completely arbitrary, it suffices to analyze the relation between the time-dependent probability distributions P^H and P given by Eqs. (25) and (32). Thus it is the aim of the present section to investigate the connection between these distributions and to make precise the mathematical and physical meaning of the transition from P^H to P.

Of course, one could try to investigate this relation by comparing directly these probability distributions. However, it is much more convenient to work with the characteristic functionals of both processes and to compare their equations of motion. Thus the strategy we are going to follow may be summarized as follows. In a first

step, we derive the equation of motion for the characteristic functional $M(\{z_\lambda\},t)$ pertaining to the stochastic process $\delta u N_\lambda(t)$,

$$M(\{z_\lambda\},t) \equiv \left\langle \exp\left\{ i\delta u \delta l \sum_\lambda z_\lambda N_\lambda \right\} \right\rangle \equiv \langle \mathcal{F}(\{N_\lambda\}) \rangle \,, \tag{33}$$

where we have introduced the function

$$\mathcal{F}(\{N_\lambda\}) \equiv \exp\left\{ i\delta u \delta l \sum_\lambda z_\lambda N_\lambda \right\} \quad . \tag{34}$$

The equation of motion for M contains, of course, the small mesoscopic scales δu and δl introduced within our discrete master-equation formulation. This is due to the fact that the phase space Γ underlying our master-equation formulation is discrete in space as well as velocity space. We therefore assume that in the limit of small δu the stochastic process

$$u_\lambda(t) \equiv \delta u N_\lambda(t) \tag{35}$$

represents a process which, to leading order, does not depend on δu. Thus the second step consists of an expansion of the equation of motion for M with respect to this mesoscopic velocity scale δu. In a third step we then perform the continuum limit $\delta l \longrightarrow 0$. The leading-order term of this expansion turns out to be identical to the functional Hopf equation. Furthermore, the physical origin of the next to leading-order term is discussed and the mesoscopic scales are related to physical quantities.

In order to derive the equation governing the time evolution of the characteristic function M we have to evaluate, according to Eq. (16), the expectation value of the commutator $[\mathcal{F},\mathcal{A}]$. This can be done easily by use of

$$\left[\mathcal{F}(\{N_\lambda\}) \,, \mathbf{E}_{\lambda'\pm 1}^{-1}\mathbf{E}_{\lambda'}\right] = \mathbf{E}_{\lambda'\pm 1}^{-1}\mathbf{E}_{\lambda'} \left(e^{i\delta u \delta l (z_{\lambda'\pm 1} - z_{\lambda'})} - 1 \right) \mathcal{F}(\{N_\lambda\}) \quad . \tag{36}$$

Invoking Eq. (16) we find

$$\begin{aligned}
\frac{\partial M}{\partial t} = {} & \frac{\nu}{\delta l^2} \sum_{\lambda'} \left(e^{i\delta u \delta l (z_{\lambda'-1} - z_{\lambda'})} - 1 \right) \left\langle (N_{\lambda'}^+ - N_{\lambda'-1}^-)\, \mathcal{F}(\{N_\lambda\}) \right\rangle \\
& + \frac{\nu}{\delta l^2} \sum_{\lambda'} \left(e^{i\delta u \delta l (z_{\lambda'+1} - z_{\lambda'})} - 1 \right) \left\langle (N_{\lambda'}^+ - N_{\lambda'+1}^-)\, \mathcal{F}(\{N_\lambda\}) \right\rangle \\
& + \frac{\delta u}{4\delta l} \sum_{\lambda'} \left(e^{i\delta u \delta l (z_{\lambda'+1} - z_{\lambda'})} + e^{i\delta u \delta l (z_{\lambda'} - z_{\lambda'-1})} - 2 \right) \left\langle N_{\lambda'}^2\, \mathcal{F}(\{N_\lambda\}) \right\rangle .
\end{aligned} \tag{37}$$

This is an exact equation for the time derivative of the characteristic functional M. We now expand the exponentials containing the differences $z_{\lambda'\pm 1} - z_{\lambda'}$ in powers of $\delta u \delta l$ up to second order. Employing Eq. (11) we obtain

$$\begin{aligned}
\frac{\partial M}{\partial t} = {} & \frac{\nu}{\delta l^2} \sum_{\lambda'} i\delta u \delta l \, \left[z_{\lambda'+1} + z_{\lambda'-1} - 2z_{\lambda'} \right] \left\langle N_{\lambda'}\, \mathcal{F}(\{N_\lambda\}) \right\rangle \\
& + \frac{\nu}{\delta l^2} \sum_{\lambda'} \frac{(i\delta u \delta l)^2}{2} \left[(z_{\lambda'+1} - z_{\lambda'})^2 + (z_{\lambda'-1} - z_{\lambda'})^2 \right] \langle\!| \, N_{\lambda'} \, | \, \mathcal{F}(\{N_\lambda\}) \rangle \\
& + \frac{\delta u}{4\delta l} \sum_{\lambda'} i\delta u \delta l \left[z_{\lambda'+1} - z_{\lambda'-1} \right] \left\langle N_{\lambda'}^2\, \mathcal{F}(\{N_\lambda\}) \right\rangle \\
& + \frac{\delta u}{4\delta l} \sum_{\lambda'} \frac{(i\delta u \delta l)^2}{2} \left[(z_{\lambda'+1} - z_{\lambda'})^2 + (z_{\lambda'} - z_{\lambda'-1})^2 \right] \left\langle N_{\lambda'}^2\, \mathcal{F}(\{N_\lambda\}) \right\rangle .
\end{aligned} \tag{38}$$

Expressing $N_{\lambda'}$ and $N_{\lambda'}^2$ by derivatives with respect to $z_{\lambda'}$, the equation for M can be written in the following form which is appropriate to infer the structure of the continuum limit:

$$\begin{aligned}
\frac{\partial M}{\partial t} = {} & \nu \sum_\lambda \delta l \, \frac{z_{\lambda+1} + z_{\lambda-1} - 2z_\lambda}{\delta l^2} \frac{1}{\delta l} \frac{\partial M}{\partial z_\lambda} \\
& - \frac{i}{2} \sum_\lambda \delta l \left(\frac{z_{\lambda+1} - z_{\lambda-1}}{2\delta l} + \frac{i\delta u \delta l}{4} \left\{ \frac{(z_{\lambda+1} - z_\lambda)^2}{\delta l} + \frac{(z_\lambda - z_{\lambda-1})^2}{\delta l} \right\} \right) \frac{1}{\delta l^2} \frac{\partial^2 M}{\partial z_\lambda^2} \\
& - \frac{\nu \delta u \delta l}{2} \sum_\lambda \delta l \left(\frac{(z_{\lambda+1} - z_\lambda)^2}{\delta l^2} + \frac{(z_{\lambda-1} - z_\lambda)^2}{\delta l^2} \right) \langle\!| \, u_\lambda \, | \, \mathcal{F} \rangle \, .
\end{aligned} \tag{39}$$

It is now easy to perform, at least formally, the continuum limit of this equation. In the limit $\delta l \longrightarrow 0$ the set of numbers z_λ turns into a function $z(x)$. Correspondingly, $M(\{z_\lambda\};t)$ becomes a functional $M[z(x),t]$ and ordinary derivatives with respect to z_λ translate into functional derivatives:

$$\frac{1}{\delta l}\frac{\partial}{\partial z_\lambda} \longrightarrow \frac{\delta}{\delta z(x)} \quad . \tag{40}$$

Moreover, we assume that the process $u_\lambda(t)$ converges in the continuum limit to a well-defined stochastic process $u(x,t)$. Hence we obtain to leading order in δl

$$\frac{\partial}{\partial t}M[z(x),t] = \nu\int dx\,\frac{\partial^2 z}{\partial x^2}\frac{\delta M}{\delta z(x)} - \frac{i}{2}\int dx\,\frac{\partial z}{\partial x}\frac{\delta^2 M}{\delta z(x)^2} - \nu\delta u\delta l\int dx\,\left(\frac{\partial z}{\partial x}\right)^2 \times\left\langle \mid u(x)\mid e^{i\int dy\, z(y)u(y)}\right\rangle . \tag{41}$$

Performing an integration by parts finally yields

$$\frac{\partial}{\partial t}M[(z(x),t] = \int dx\, z(x)\left\{\frac{i}{2}\frac{\partial}{\partial x}\left(\frac{\delta^2 M}{\delta z(x)^2}\right)+\nu\frac{\partial^2}{\partial x^2}\left(\frac{\delta M}{\delta z(x)}\right)\right\} - \nu\delta u\delta l\int dx\,\left(\frac{\partial z}{\partial x}\right)^2 \times\left\langle \mid u(x)\mid \exp(i\int dy\, z(y)u(y))\right\rangle \quad . \tag{42}$$

Equation (42) represents, including terms of order $\delta u\delta l$, the equation of motion for the characteristic functional M of the stochastic process defined by our multivariate master equation. Comparing Eq. (42) with (30) we conclude that the leading-order terms in Eq. (42) are identical to the Hopf functional equation. The next-to-leading-order term, which may formally be written as

$$c[z(x),t] = -\nu\delta u\delta l\int dx\,\left(\frac{\partial z}{\partial x}\right)^2\left|\frac{1}{i}\frac{\delta}{\delta z(x)}\right| M[z(x),t], \tag{43}$$

is of order δu and, therefore, vanishes as $\delta u \longrightarrow 0$. Note that including the case of external random stirring forces Novikov derived a generalization [22] of Hopf's functional equation in which an additional term appears which is of similar structure as $c[z(x),t]$. However, in our formulation the functional $c[z(x),t]$ does not represent the effect of external random forces. We shall see below that it has a different physical interpretation.

Equation (42) constitutes the central result of this section. It leads to the conclusion that in the limit $\delta u \longrightarrow 0$ the stochastic process $\delta u N_\lambda(t)$ underlying our master equation is equivalent to the stochastic process $v(x,t)$ of the Hopf formulation.

From a mathematical point of view this conclusion has to be taken with caution since we did not actually prove that the probability distribution P converges to P^H in a rigorous mathematical sense. In order to give such a proof one would first have to construct an embedding of the phase space of smooth velocity fields into the discrete phase space Γ underlying our master equation. Second, a measure in the space of probability distributions is required which allows for a precise definition of convergence. A mathematical investigation along these lines must show, in particular, how the two limiting procedures $\delta u \to 0$ and $\delta l \to 0$ have to be performed in order to guarantee certain smoothness properties of the stochastic process $u(x,t)$.

However, in spite of these mathematical questions we can give the above statement concerning the relation between the random processes $\delta u N_\lambda(t)$ and $v(x,t)$ the following meaning. On a purely formal level, the Hopf equation (30) as well as Eq. (42) for the characteristic functional of our multivariate stochastic process may be regarded as a condensed way of writing the hierachy of dynamic moment equations. In fact, functional differentiating M^H and M with respect to $z(x)$ one may derive the differential equations for the (equal time) n-point correlation functions for both processes. It is clear from the structure of the functional equations (30) and (42) that the resulting equations for the two stochastic processes differ from each other by the corresponding functional derivatives of the correction term $c[z(x),t]$. As one can see from the definition of $c[z(x),t]$ all nth-order functional derivatives of $c[z(x),t]$, taken at n different points, exist. Thus the equations for the n-point correlation functions differ by a term which vanishes as $\delta u \longrightarrow 0$. This is the precise formulation of the conclusion we draw from our investigation.

It should be clear that the functional derivatives of $c[z(x),t]$ induce δ-function-type singularities. This is due to the fact that for small but finite δu the continuum limit ($\delta l \longrightarrow 0$) of $\delta u N_\lambda$ does not lead to a smooth stochastic process. We will see below that this is to be expected physically.

As an example, we derive the equation for the two-point correlation function

$$\langle u(y,t)\,u(x,t)\rangle = \frac{1}{i^2}\frac{\delta^2}{\delta z(y)\delta z(x)}M[z,t]\Big|_{z=0} \quad . \tag{44}$$

Following the usual procedure we obtain

$$\frac{\partial}{\partial t}\langle u(y,t)\,u(x,t)\rangle + \frac{1}{2}\left\langle u(y,t)\frac{\partial}{\partial x}u^2(x,t)\right\rangle + \frac{1}{2}\left\langle u(x,t)\frac{\partial}{\partial y}u^2(y,t)\right\rangle = \nu\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\langle u(y,t)\,u(x,t)\rangle - \frac{\delta^2}{\delta z(y)\delta z(x)}c[z,t]\Big|_{z=0} \quad . \tag{45}$$

Apart from the last term the above equation is identical to that one which is obtained from the functional Hopf equation, of course. The functional derivatives of $c[z,t]$

yield the expression ($\tilde{v} \equiv \langle | u | \rangle$)

$$-\frac{\delta^2}{\delta z(y)\delta z(x)} c[z,t]\Big|_{z=0} = -2\nu\delta u\delta l \frac{\partial}{\partial x}\tilde{v}\frac{\partial}{\partial x}\delta(y-x), \tag{46}$$

which is obviously of order δu.

From a physical point of view there is another reason why mathematical considerations concerning the continuum limit of $\delta u N_\lambda(t)$ are only of secondary importance. The reason is that the functional $c[z(x),t]$ can be given a clear physical meaning. As we will now show interpreting this term as the influence of thermal fluctuations one is forced to fix the product $\delta u \delta l$ to a *finite value.* Thus questions about the existence of the continuum limit are only of mathematical interest.

We now demonstrate that the term (46) can be interpreted as a random stress induced by thermal fluctuations. To this end, we assume in the following that the stochastic process is spatially homogeneous; in particular this implies $\tilde{v} = \text{const}$. Introducing the Fourier transformation of the velocity,

$$u(x,t) = \frac{1}{L}\sum_k e^{ikx} u_k(t) \quad , \tag{47}$$

where $k = 2\pi n/L$ and $n \in \mathbb{Z}$, we obtain from Eq. (45)

$$\frac{\partial}{\partial t}\langle u_k^* u_k\rangle + \frac{1}{L}\sum_q iq\langle u_{k+q}^* u_k u_q\rangle + \text{c.c.}$$

$$= -2\nu k^2\langle u_k^* u_k\rangle + 2\nu\tilde{v}\delta u\delta l L k^2 \quad . \tag{48}$$

Recall that $\langle u_k^* u_k\rangle$ is proportional to the kinetic energy E_k (per unit mass) pertaining to the mode k,

$$E_k = \frac{1}{2L}\langle u_k^* u_k\rangle \quad . \tag{49}$$

The convolution sum on the left-hand side of Eq. (48) results from the inertial term of Burgers's equation and obviously couples the different modes. The first term on the right-hand side represents the decay of the hydrodynamic modes due to viscous friction whereas the last term is the Fourier transform of (46). At small scales, that is for large k, the influence of the inertial term may be neglected. It is then easy to see that the effect of the last term in (48) is to slow down the exponential decay of the energy of the mode k until, finally, the stationary value

$$E_k^s = \frac{1}{2}\tilde{v}\delta u\delta l \tag{50}$$

is reached. One can go one step further by requiring that the kinetic energy E_k^s of each stationary mode is equal to its thermodynamic equilibrium value at temperature T. This requirement leads to the relation $E_k^s = \frac{1}{2}k_B T/\rho$ (ρ denotes the fluid density and k_B the Boltzmann constant) which implies

$$\tilde{v}\delta u\delta l = \frac{k_B T}{\rho} \quad . \tag{51}$$

The fluctuation-dissipation-type relation (51) fixes $\delta u\delta l$ to a finite value. This means that from a physical viewpoint the continuum limit makes no sense. This fact should have been clear from the begining since below a certain length scale the assumption of thermodynamic equilibrium and, thus, a description by macroscopic variables only is no longer possible.

It should be clear that performing stochastic simulations of our master equation (see Sec. IV) it is by no means necessary to choose parameters in such a way that the fluctuation-dissipation relation (51) is satisfied. In other words, it is not necessary to take into account all scales ranging from the hydrodynamic to the thermodynamic degrees of freedom. On the contrary, in view of practical applications another interpretation of the finite mesoscopic scales δl and δu is possible. This interpretation is based on the fact that any experimental measurement is characterized by some finite resolution in velocity space as well as position space. It is therefore natural to assume that

$$\delta l = \Delta l \ , \quad \tilde{v}\delta u = \sigma^2 \quad ,$$

where Δl denotes the spatial resolution and σ^2 the variance of the error of velocity measurements. Fixing the mesoscopic parameters in this way, it might be possible to simulate directly that velocity field which is actually measured.

IV. STOCHASTIC SIMULATIONS

In the preceding section we have demonstrated that the master equation formulation of homogeneous turbulence indeed leads to the infinite hierarchy of correlation functions which is expected from the Hopf statistical theory of turbulence. In fact we showed that in the continuum limit the equation for the characteristic functional derived from our multivariate master equation is the well-known Hopf functional equation. It is the aim of the present section to show that the power of this approach lies in its practical relevance. Namely, this approach to fluid dynamics makes possible the formulation of very stable and efficient numerical algorithms for computational investigations of turbulence.

In this section we describe how stochastic simulation algorithms for the random process $\{N_\lambda\}$ can be derived starting from our master equation. First, by means of Burgers's model of turbulence we review briefly the stochastic simulation method. In Sec. IV B we then present and discuss some results of stochastic simulations which have been performed for the Burgers model of homogeneous turbulence.

A. The stochastic simulation algorithm

Basically, by means of the stochastic simulation method [23] an ensemble of realizations of $\{N_\lambda\}$ is generated. From this ensemble the physical quantities of interest can then be evaluated as ensemble averages. Let us first summarize the important facts which will be needed

in order to explain how a realization of the stochastic process is generated.

Recall that the master equation (9) defines all possible transitions and the corresponding transition rates of the stochastic process $\{N_\lambda\}$. In each transition exactly two numbers, say N_λ, and one of its neighbors $N_{\lambda\pm1}$, change by $+1$ or -1. The probability per unit time w_λ that N_λ and one of its neighbors change can be read off from the master equation

$$w_\lambda = \frac{2\nu}{\delta l^2} \mid N_\lambda \mid + \frac{\delta u}{4\delta l}\left\{N_\lambda^2 + N_{\lambda+1}^2\right\} \quad . \tag{52}$$

Obviously, the total transition rate W which describes the rate of a transition to occur somewhere in the system can easily be computed as the sum of all w_λ,

$$W(\{N_\lambda\}) = \sum_{\lambda=0}^{M} w_\lambda \quad . \tag{53}$$

Now, the generation of a realization proceeds along the following lines

(i) Let us assume that at time t the state of the system is given by $\{N_\lambda(t)\}$. In the first step, the time $t+\tau$ of the next transition is determined. Our algorithm uses a stochastic time step τ to be evaluated as follows. The quantity $W(\{N_\lambda(t)\})d\tau$ is obviously the probability for the next transition to occur somewhere in the system within the infinitesimal time step $d\tau$. Therefore the probability $pd\tau$ of the next transition to take place in the time interval $[\tau, \tau + d\tau]$ is given by

$$pd\tau = W \exp(-W\tau)\, d\tau \quad .$$

Thus the total transition rate W determines the waiting time distribution, i.e., the probability distribution of the time τ the system remains in the state $\{N_\lambda(t)\}$. In the stochastic simulation the random number τ which determines the time for the next transition to occur can be obtained by the inversion method with the help of the following formula

$$\tau = -\frac{1}{W\left(\{N_\lambda(t)\}\right)} \ln \eta \quad , \tag{54}$$

where η is a uniformly distributed random number in the interval $[0, 1]$.

(ii) Having determined the transition time we have to perform a specific transition, i.e., we have to determine the new state $\{N_\lambda(t+\tau)\}$ of the system. To this end, one chooses according to the relative probabilities w_λ/W a certain cell. Once a definite cell λ, say, has been chosen, the new state of the system is to be selected from the following possibilities: (a) Diffusive transitions:

$$\left.\begin{matrix} N_\lambda \to N_\lambda - s \\ N_{\lambda+1} \to N_{\lambda+1} + s \end{matrix}\right\} \text{probability} = \frac{\nu}{\delta l^2}\frac{\mid N_\lambda \mid}{w_\lambda}, \tag{55}$$

$$\left.\begin{matrix} N_\lambda \to N_\lambda - s \\ N_{\lambda-1} \to N_{\lambda-1} + s \end{matrix}\right\} \text{probability} = \frac{\nu}{\delta l^2}\frac{\mid N_\lambda \mid}{w_\lambda}, \tag{56}$$

where

$$s = \begin{cases} +1 & \text{for } N_\lambda > 0 \\ -1 & \text{for } N_\lambda < 0; \end{cases}$$

(b) convective transitions:

$$\left.\begin{matrix} N_\lambda \to N_\lambda - 1 \\ N_{\lambda+1} \to N_{\lambda+1} + 1 \end{matrix}\right\} \text{probability} = \frac{\delta u}{4\delta l}\frac{N_\lambda^2 + N_{\lambda+1}^2}{w_\lambda}. \tag{57}$$

Note that each of these transitions corresponds to one of the five terms in our master equation (9) and that the sum of transition probabilities given above add up to 1. Performing one of these transitions yields the new state $\{N_\lambda(t+\tau)\}$.

(iii) The complete trajectory of the stochastic process can be determined by repeating the above scheme until a desired final time is reached. Finally, by generating a large number S of realizations of the stochastic process $\{N_\lambda(t)\}^j$, $j = 1, \ldots, S$, one can evaluate the interesting quantities as ensemble averages.

The simplicity of the above scheme makes clear that the numerical simulation of a stochastic process defined by a master equation is straightforward. In fact, in the description of complex polymerization reactions involving a very large number of reacting particles, stochastic simulation algorithms have been shown to be more efficient than the integration of the corresponding macroscopic differential equations [6, 7]. As has been demonstrated in previous work [3–5] the stochastic simulation algorithm derived from our master equation turns out to be very stable. For instance, in the simulation of shock waves at high Reynolds numbers such effects like numerical viscosity and the Gibbs phenomenon, observed in the integration by other conventional schemes, are strongly suppressed [13].

B. Stochastic simulations of the Burgers model of turbulence

In this subsection we will apply the stochastic simulation method described above to Burgers's model of homogeneous turbulence. Let us first precisely define the initial conditions and the physical quantities which have been used in our calculations.

Within our discrete description the two-point correlation function is defined by

$$Q(\mu, t) \equiv \frac{1}{L}\sum_{\lambda=0}^{M} \delta l\, \delta u^2 \langle N_{\lambda+\mu} N_\lambda \rangle,$$

$$\mu = 0, 1, 2, \ldots, M \quad , \tag{58}$$

where, assuming spatial homogeneity, a space average has been taken. The expectation value is, as explained in Sec. IV A, evaluated by averaging over the ensemble which is generated by the stochastic simulation. Computing the Fourier transform of the correlation function we obtain the energy spectrum E_k defined in Eq. (49). The total

kinetic energy E is evaluated by means of the expression

$$E(t) = \frac{1}{2L} \sum_{\lambda} \delta l \, \delta u^2 \langle N_\lambda^2 \rangle \quad , \tag{59}$$

which leads to the energy dissipation rate $\varepsilon(t) = -\dot{E}$. The initial random velocity is given by a superposition of $N = 1000$ randomly chosen modes,

$$u_0(x) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (A_i \cos k_i x + B_i \sin k_i x) + w(x) \quad . \tag{60}$$

Here, $k_i = 2\pi n_i$ (we choose $L = 1$) and the n_i denote identically distributed random integers with distribution function $P(n) = P(-n)$. The amplitudes A_i and B_i are also identically distributed and independent real random numbers with zero mean and with variance

$$\langle A_i A_j \rangle = \langle B_i B_j \rangle = A^2 \delta_{ij} \quad .$$

Furthermore, we add a small fluctuating field $w(x)$ with zero mean and correlation function $\langle w(y)\, w(x) \rangle = w^2 \delta l \delta(y - x)$, where $w^2 = \tilde{v} \delta u$. It follows from these conditions that the initial field (60) is homogeneous and that the initial energy spectrum is given by $E_k(0) = A^2 P(k/2\pi)/2 + \tilde{v} \delta u \delta l/2$. In our calculations we used $A^2 = 1/3$ and a Poisson-distributed initial spectrum

$$P(n+1) = \frac{1}{2} \frac{\mu^n}{n!} e^{-\mu} \quad , \tag{61}$$

where $n = 0, 1, 2, 3, \ldots, (M+1)/2$, and $P(0) = 0$. We shall characterize this initial condition by two Reynolds numbers: First, we define an integral Reynolds number based on the total length $L = 1$ and rms velocity $U = \langle u^2 \rangle^{1/2}$,

$$R_L \equiv \frac{UL}{\nu} \quad . \tag{62}$$

Second, we introduce a Taylor-Reynolds number by

$$R_\Lambda \equiv \frac{U\Lambda}{\nu} \quad , \tag{63}$$

where the Taylor microscale Λ is defined by

$$\left(\frac{2\pi}{\Lambda}\right)^2 \equiv \frac{\varepsilon(0)}{2\nu E(0)} = \frac{\sum k^2 E_k(0)}{\sum E_k(0)} = \left(\frac{2\pi}{L}\right)^2 [(\mu+1)^2 + \mu] \quad . \tag{64}$$

The following simulations have been performed along the lines described in Sec. IV A employing the parameters $\delta u = 5 \times 10^{-4}$ and $M + 1 = 1024$. The random initial configuration is given by

$$N_\lambda(0) = \text{int}\left(\frac{u_0(x_\lambda)}{\delta u}\right) \quad . \tag{65}$$

In Fig. 1 we depict one realization of the stochastic process $u_\lambda = \delta u N_\lambda$ for three different times and $\nu = 5000^{-1}$. As can be seen from the figure, the initial field develops a typical sawtooth structure consisting of smooth increasing ramps followed by sharp shocks.

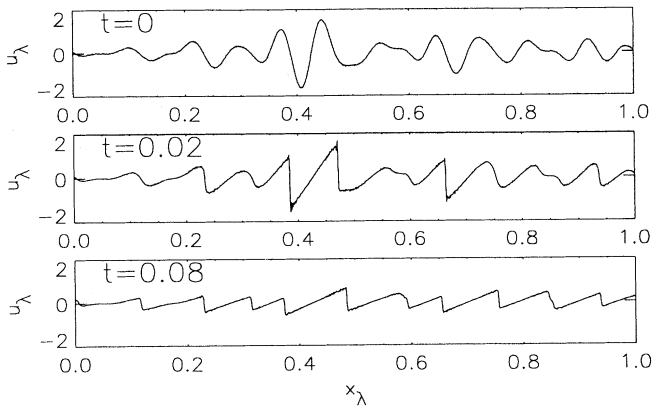

FIG. 1. One realization of the stochastic process $u_\lambda = \delta u N_\lambda$ defined by the master equation (9) and the random initial condition given by (60) and (65) for $\nu = 5000^{-1}$ and three different times $t = 0$, $t = 0.02$, and $t = 0.08$. The parameter μ of the initial configuration was chosen to be $\mu = 10$. The stochastic simulation has been performed with the parameters $\delta u = 5 \times 10^{-4}$, $M + 1 = 1024$.

In Fig. 2 we show the energy dissipation rate ε as function of time for $\nu = 3000^{-1}$ ($R_L = 1733$, $R_\Lambda = 156$) and $\nu = 5000^{-1}$ ($R_L = 2821$, $R_\Lambda = 253$). In both cases the results have been obtained by averaging over 100 realizations. Figure 2 clearly demonstrates the characteristic features of the dissipation: During a short initial period in which the dissipation rate is small, shocks form and the resulting steep velocity gradients lead to a strong enhancement of the dissipation rate. The latter reaches a maximum at a characteristic time $t \approx 0.02$. During the post shock period the dissipation rate can be clearly seen to become independent of the viscosity as is predicted by analytical considerations [24, 25].

Finally, we shall discuss the energy spectrum. Fig-

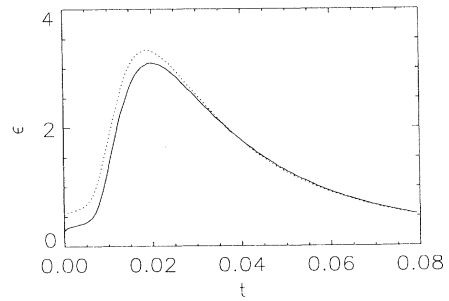

FIG. 2. The energy dissipation rate ε as a function of time for two different kinematic viscosities $\nu = 3000^{-1}$ (dotted line) and $\nu = 5000^{-1}$ (continuous line). The stochastic simulation has been performed with the same random initial condition and the same parameters as in Fig. 1. The energy dissipation rate has been estimated by averaging over 100 realizations of the stochastic process.

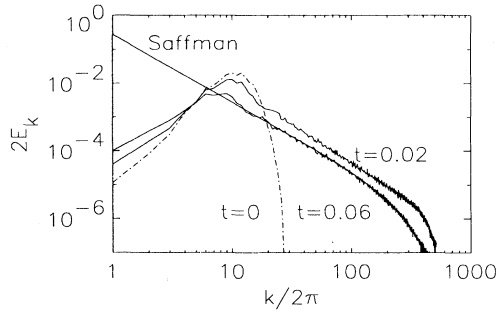

FIG. 3. The energy spectrum $E_k(t)$ obtained by Fourier transforming the correlation function (58) for three different times $t = 0$, $t = 0.02$, and $t = 0.06$. The correlation function has been estimated by averaging over 100 realizations. The stochastic simulation has been performed with the same random initial condition and with the same parameters as in Fig. 1. The kinematic viscosity is $\nu = 5000^{-1}$. The continuous line represents the Saffman curve (66) for the parameters $W = 0.85 \times 10^{-5}$ and $d = 0.0078$.

ure 3 shows E_k as obtained from the Fourier transform of the correlation function $Q(\mu, t)$. Again, the expectation value has been evaluated by averaging over 100 realizations of the stochastic process. We show the energy spectrum for three different times and for the viscosity $\nu = 5000^{-1}$ ($R_L = 2821$, $R_\Lambda = 253$). As can be seen, a k^{-2} power-law behavior appears which represents the universal inertial range of Burgers's model. In order to demonstrate the accuracy of the stochastic simulation method over the whole range of wavenumbers we compare the spectrum at time $t = 0.06$ with the analytical result given by Saffman [25]

$$E_k = W \sinh^{-2}(dk/2\pi) \quad . \tag{66}$$

Saffman derived this expression for the Burgers model by assuming that the small-scale structure is given by periodic trains of shocks. Note that E_k as given by (66) approaches for $dk/(2\pi) \ll 1$ the form $E_k \approx 4\pi^2 W/(dk)^2$. The energy scale W and the dissipation length d which depend on the large scale properties of the initial condition have been determined from our data by comparison with the limiting behavior of the Saffman result for large wave numbers [$E_k \approx 4W \exp(-dk/\pi)$]. We find $W = 0.85 \times 10^{-5}$ and $d = 0.0078$. As demonstrated in Fig. 3 the agreement between the analytical result (66) with our stochastic simulation is excellent over the whole range of wave numbers.

V. CONCLUSIONS

It has been demonstrated in this paper that a recently proposed stochastic formulation of fluid dynamics leads to an approach to turbulence. The basic idea of our approach has been explained by means of Burgers's equation which represents a simplified, paradigmatic version of the Navier-Stokes equation. Discretizing position as well as velocity space by means of a length scale δl and a velocity scale δu we have constructed a discrete phase space Γ. Each point in this space is given by a set $\{N_\lambda\}$ of integers which completely fixes the velocity of the fluid. The probabilistic dynamics is introduced by regarding $\{N_\lambda\}$ as a multivariate stochastic process governed by a master equation for the joint probability distribution P. The master equation that we propose has been investigated in this paper by different techniques. First, we have shown that neglecting higher moments the time evolution equation for the first moments $\delta u \langle N_\lambda \rangle$ is nothing but a discretized version of Burgers's equation. A systematic Ω expansion reveals that, in fact, Burgers's equation is the macroscopic equation corresponding to our multivariate master equation [14].

This result is only valid, of course, under the assumption that the stochastic process $\{N_\lambda\}$ describes a stable flow on which small fluctuations are superimposed. Thus, in order to prove that our stochastic theory is applicable to turbulent situations which are characterized by large fluctuations, we have investigated the characteristic functional pertaining to $\{N_\lambda\}$. It has been demonstrated that the time evolution equation for this characteristic functional obeys in the continuum limit the well-known Hopf functional equation which characterizes the statistical properties of an ensemble of turbulent velocity fields. Furthermore, the next-to-leading-order term in an expansion in δu and δl has the structure of a random stress. The latter has a clear physical interpretation. By relating the mesoscopic scales to thermodynamic state variables it represents the effect of thermal fluctuations in the fluid. From a pragmatic point of view the mesoscopic scales may also be interpreted as representing the finite resolution in position and velocity of experimental observations.

These theoretical investigations constitute the basis of a stochastic simulation method for turbulent flows. In fact, by a simple simulation algorithm derived from our master equation an ensemble of realizations of the stochastic process $\{N_\lambda\}$ is generated and physical quantities are estimated as ensemble averages. This method is illustrated by stochastic simulations of Burgers's model of turbulence. The simulations are shown to yield very accurate results.

We emphasize that this stochastic simulation method is completely different from direct numerical simulation methods [9, 26–28] which generate trajectories by solving the Navier-Stokes equation. Furthermore, the stochastic simulation method presented in this paper should be distinguished from the method given by Hosokawa and Yamamoto [29, 30]. In order to reduce the number of degrees of freedom these authors use a space of randomly sampled Fourier modes and a modified Navier-Stokes operator which acts in this space. The important point to note here is that in this method the time evolution is, in contrast to our approach, given by a deterministic differential equation.

It should be clear that the theoretical considerations and the simulation technique presented in this paper are not restricted to (1+1)-dimensional flows. In fact, it is straightforward to write down a master equation for a multivariate stochastic process which describes (3+1)-

dimensional flows. A stochastic counterpart of the pressure gradient which is absent in Burgers's equation may be constructed as well. This point was the subject of another publication [5]. Furthermore, it can be shown that the equation of continuity and the equation expressing the conservation of energy may be treated by the same tools. Of course, these considerations are beyond the scope of the present work.

[1] G. K. Batchelor, *The Theory of Homogeneous Turbulence* (Cambridge University Press, Cambridge, 1982).

[2] W. D. McComb, *The Physics of Fluid Turbulence* (Clarendon, Oxford, 1990).

[3] H. P. Breuer and F. Petruccione, J. Phys. A **25** L661 (1992).

[4] H. P. Breuer and F. Petruccione, *Hydrostochastics: The Stochastic Approach to Fluid Dynamics* (Istituto Italiano per gli Studi Filosofici, Naples, 1991).

[5] H. P. Breuer and F. Petruccione, Continuum Mech. Thermodyn. **4**, 247 (1992).

[6] H. P. Breuer, J. Honerkamp, and F. Petruccione, Chem. Phys. Lett. **190**, 199 (1992).

[7] H. P. Breuer, J. Honerkamp, and F. Petruccione, Comput. Polymer Sci. **1**, 233 (1991).

[8] J. M. Burgers, in *Statistical Models and Turbulence*, edited by J. Ehlers, K. Hepp, and H. A. Weidenmüller, Lecture Notes in Physics Vol. 12 (Springer-Verlag, Berlin, 1972).

[9] W. C. Meecham and A. Siegel, Phys. Fluids **7**, 1178 (1964).

[10] E. Hopf, J. Rat. Mech. Anal. **1**, 87 (1952).

[11] E. Hopf, Proc. Symp. Appl. Math. **7**, 41 (1957).

[12] E. Hopf, Proc. Symp. Appl. Math. **13**, 157 (1962).

[13] H. P. Breuer and F. Petruccione, Phys. Lett. A **172**, 49 (1992).

[14] H. P. Breuer and F. Petruccione, Physica A (to be published).

[15] H. P. Breuer and F. Petruccione, Transp. Theor. Stat. Phys. (to be published).

[16] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[17] R. F. Fox, Phys. Rep. **48**, 179 (1978).

[18] H. Grabert, *Projection Operator Techniques in Nonequilibrium Statistical Physics*, Springer Tracts in Modern Physics Vol. 95 (Springer-Verlag, Berlin, 1982).

[19] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon, London, 1959).

[20] L. Arnold, *Stochastic Differential Equations* (Wiley, New York, 1974).

[21] C. W. Gardiner, *Handbook of Stochastic Methods*, 2nd ed. (Springer-Verlag, Berlin, 1985), Sec. 3.5.3.

[22] E. A. Novikov, Zh. Eksp. Teor. Fiz. **47**, 1919 (1964) [Sov. Phys. JETP **20**, 1290 (1965)].

[23] J. Honerkamp, *Stochastische Dynamische Systeme* (VCH, Weinheim, 1990).

[24] R. H. Kraichnan, Phys. Fluids **11**, 265 (1968).

[25] P. G. Saffman, in *Topics in Nonlinear Physics*, edited by N. J. Zabusky (Springer-Verlag, Berlin, 1968).

[26] D. K. Lilly, Phys. Fluids Suppl. **II**, 240 (1969).

[27] S. A. Orzag and G. S. Patterson, Phys. Rev. Lett. **28**, 76 (1972).

[28] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang, *Spectral Methods in Fluid Dynamics* (Springer-Verlag, New York, 1988).

[29] I. Hosokawa and K. Yamamoto, Phys. Fluids **13**, 1683 (1970).

[30] I. Hosokawa and K. Yamamoto, J. Phys. Soc. Jpn. **56**, 521 (1987).