

A simple model for nonequilibrium fluctuations in a fluid

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(Received 16 November 1995; accepted 27 February 1996)

In equilibrium systems, thermal fluctuations are correlated in time (fluctuation–dissipation theorem) yet their instantaneous values are uncorrelated in space over macroscopic distances. Out of equilibrium, long range spatial correlations are predicted by theory and have been observed in both laboratory experiments and computer simulations. In this paper, we present a simple model, called the train model, that illustrates this phenomenon. The theoretical analysis of the model and its connection with fluctuating hydrodynamics are outlined. © 1996 American Association of Physics Teachers.

I. INTRODUCTION

Equilibrium systems are usually considered to be homogeneous, yet at small scales spontaneous fluctuations are observed. This phenomenon is seen daily in the Rayleigh scattering that makes the sky blue.¹ The Brownian motion of large particles suspended in a fluid (e.g., pollen in water) and the thermal noise found in electrical circuits (Johnson effect) are examples of fluctuation phenomena that are easily observed in the laboratory. Perhaps more important than the effects produced by fluctuations is their role in the theoretical development of statistical physics. By using a probabilistic formulation, the connection between mechanics and thermodynamics was established by Gibbs, Boltzmann, Maxwell, and Einstein. The utility of their approach was the prediction of macroscopic quantities as the average (or most probable value) of a distribution function. Yet the validation of the construction of this distribution came from the prediction of its variance i.e., the fluctuation spectrum. For this reason, the theory of equilibrium fluctuations occupies a chapter in most statistical mechanics textbooks.²

The key to the formulation of the equilibrium probability distribution is the existence of thermodynamic potentials, for example the free energy for a closed, noninsulated system. Consider the thermodynamic variable q ; let q_{eq} be its macroscopic value at equilibrium. The probability of observing a fluctuation $\delta q = q - q_{\text{eq}}$ is given by

$$P(\delta q) \propto e^{-\Delta F(\delta q)/k_B T}, \quad (1)$$

where ΔF is the change in the free energy resulting from the fluctuations δq . Macroscopic variations in the free energy are much larger than $k_B T$ so $P(\delta q)$ is sharply peaked, giving us the good fortune of living in a deterministic (if sometimes chaotic) world. There are, however, some exceptions to this rule which occur whenever the system is close to a “phase coexistence” region. A well known visible example is provided through the phenomenon of “critical opalescence” that illustrates the coexistence of liquid droplets with the vapor phase.³ Except for such pathological situations, one can expand ΔF around its minimum. To dominant order in δq , $P(\delta q)$ reduces to a Gaussian distribution from which the average square fluctuation, $\langle \delta q^2 \rangle$, can easily be obtained.

One may define local values of thermodynamic variables

by dividing the system into a set of coupled, equilibrium subsystems. Instantaneous fluctuations are uncorrelated at different points in space; that is

$$\langle \delta q(\mathbf{r}, t) \delta q(\mathbf{r}', t) \rangle \propto \delta(\mathbf{r} - \mathbf{r}'), \quad (2)$$

where \mathbf{r} is the location of a subsystem. Note that fluctuations are, in general, not δ -correlated in time; if a point is spontaneously hot (or dense), it takes time for the heat (or matter) to diffuse.

Let us now consider a system maintained out of equilibrium through appropriate external constraints. Some examples are a fluid under a constant temperature gradient, under a constant shear, and in the presence of a constant external force (see Fig. 1). Much work has been done on the generalization of thermodynamics to nonequilibrium systems.⁴ Extending the equilibrium theory of fluctuations to nonequilibrium steady states is not simple because, unfortunately, there seems to be no general way to formulate a “thermodynamic potential” for nonequilibrium systems.⁵

Among the many techniques used in the study of nonequilibrium fluctuations, two commonly used methods are: the extension of macroscopic theories using the separation of fast and slow scales and the construction of simple models for specific problems. An example of the first approach is the formulation of the fluctuating Navier–Stokes equations of fluid mechanics. In a fluid, conserved quantities (mass, momentum, and energy) can only change locally by fluxing from one location to another. These fluxes have a reversible component (inertia and pressure contributions) and an irreversible component (dissipative contributions such as viscosity and thermal conductivity). The reversible component is microscopically exact but the irreversible part of the flux is estimated as a linear response. For example, the heat flux, \mathbf{Q} , is given by the Fourier law, $\mathbf{Q} = -\kappa \nabla T$, where κ is the thermal conductivity; Newton’s law gives a similar relationship between velocity gradients and the dissipative (viscous) component of the momentum flux.

Landau realized that spontaneous fluctuations in a fluid add a stochastic contribution to the dissipative component of the fluxes. For example, consider two adjacent points, A and B , in a fluid, with temperatures T_A and T_B . If $T_A = T_B$ then the Fourier law tells us that no heat will flow from A to B . While this is true macroscopically, a fluctuation *can* cause heat to spontaneously flow from A to B , even if $T_A < T_B$. To

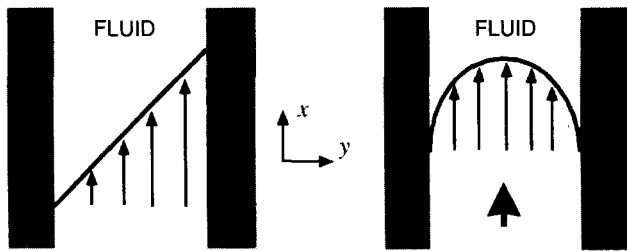


Fig. 1. Illustration of nonequilibrium steady states for a fluid. On the left, a fluid between parallel walls is subject to a constant shear (one wall is moving relative to the other). On the right, the fluid is subject to a constant external force acting upwards. In the Couette system the velocity profile is linear while it is parabolic in the Poiseuille system.

take this into account, Landau proposed modifying the Fourier law to the form, $Q = -\kappa \nabla T + Q^*$, where Q^* is a stochastic process. Since Q is not a conserved quantity, its fluctuating component is short-lived, which, in turn, implies that it is also short-ranged; Landau proposed that it takes the form of a noise with zero mean and with variance,

$$\langle Q_i^*(\mathbf{r}, t) Q_j^*(\mathbf{r}', t') \rangle = A_{ij} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t'), \quad (3)$$

so Q^* is “white” in space and time. The amplitude A_{ij} of the noise is found by matching the fluctuation amplitude given by equilibrium statistical mechanics;⁶ the extension of the theory to nonequilibrium problems was developed by Keizer⁷ and others.⁸

As we already stated, at thermodynamic equilibrium instantaneous fluctuations of hydrodynamic quantities (density, velocity, etc.) are uncorrelated at macroscopic length scales. Some years ago, however, it was realized that this was not true for nonequilibrium systems at steady states⁹⁻¹¹ where long-range correlations were predicted (for a review up to 1983, see Ref. 12; more advanced theories are reviewed in Ref. 13). This property was measured, indirectly, in light scattering experiments on fluids subject to a temperature gradient in which modifications to the Brillouin and Rayleigh lines are observed.^{14,15} It is also expected that the scattered spectrum is modified in a fluid with a velocity gradient, yet technological limitations make the laboratory experiment impractical.¹⁶ However, computer simulations of both the velocity and temperature gradient scenarios show good agreement with fluctuating hydrodynamics calculations.¹⁷⁻¹⁹ Unfortunately, nonequilibrium fluctuations are rarely discussed in textbooks since theory, experiment, and simulation are all difficult for realistic physical systems.

This brings us to another approach in the study of nonequilibrium fluctuations: the formulation of simple models. A useful model should contain those elements that must be present for the existence of a phenomenon while shedding all nonessential details. For equilibrium systems, the Ising model of a ferromagnet is the classic paradigm in critical phenomena. For nonequilibrium systems, some examples would be the drunkard’s walk to model Brownian motion, birth–death models for chemical reactions problems, and lattice gas models of fluids. Simple models have the pedagogical advantage of being easy to understand from basic principles.

In this paper, we present a simple stochastic model, called the train model, to illustrate nonequilibrium fluctuations in a fluid. In this model particles perform a random walk between adjacent fluid layers (the caricature is that of passengers

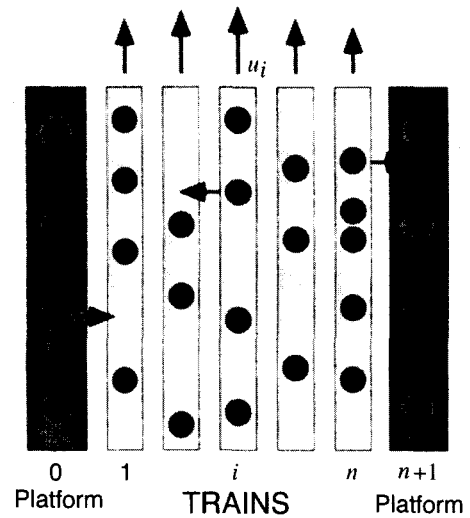


Fig. 2. Cartoon illustrating the train model. Passengers (indicated by filled circles) are shown jumping from the left platform onto the first train, off the last train onto the right platform and from train i to train $i-1$ (transferring momentum mu_i).

jumping between trains). The mechanism of momentum transfer can be expressed in terms of elementary transitions that are easily described and for which the physics is very clear. The model contains many of the qualitative features of a nonequilibrium fluid and it can easily be simulated on the computer. We also present the model’s theoretical development to illustrate its connection to fluctuating hydrodynamic theory.

II. THE STOCHASTIC TRAIN MODEL

Consider a set of n flat-car trains running on parallel tracks between two platforms (see Fig. 2). The trains have no engines, rather they roll down a frictionless inclined plane tilted at angle θ , thus $a = g \sin \theta$ is the acceleration of a train when it rolls freely downhill. Train i moves with velocity u_i and has N_i travelers (of mass m) who jump, at random time intervals Δt , onto the adjacent trains $i+1$ or $i-1$. Every passenger on every train has an equal probability to jump onto either of the adjacent trains (or platforms) regardless of the relative positions of the trains (i.e., the travelers execute a random walk process in the direction perpendicular to the tracks). When a traveler moves from one train to another, the total momentum and number of passengers change, in a discontinuous manner, for both trains. For simplicity, the mass of a train’s cars is assumed to be negligible as compared to the mass of its passengers (giving the train cars a nonzero mass somewhat complicates the analysis yet adds no new qualitative features to the model). Passengers remain at rest in the frame of reference of their train (i.e., they do not run up or down the length of their train). The numbers of travelers on each platform, N_0 , is constant so the platforms act as reservoirs of passengers.

The above prescriptions lead to a very simple stochastic model, based on Maxwell’s original formulation of elementary kinetic theory.^{20,21} The stochasticity in the trains’ velocities arises from the random walk process of the passengers. We assume that the probability of a jump occurring at some given time t is entirely determined by the state of the system at that time t , i.e., the evolution of the system is governed by

its present state and is totally independent of the past. Such a stochastic process is traditionally referred to as a Markov process. Given the Markov assumption, the waiting times Δt between successive jumps are exponentially distributed. Specifically, the probability for the waiting time Δt to be *at least* equal to t_w is

$$P(\Delta t \geq t_w) = \exp(-t_w/\tau), \quad (4)$$

where

$$\tau = \frac{1}{D \left(N_0 + \sum_{i=1}^n N_i \right)} \quad (5)$$

is the mean waiting time between jumps and the parameter D stands for jump frequency of each passenger. The mean waiting time would be inversely proportional to the total number of passengers in the system except that the passengers on the platforms jump half as frequently as passengers on the trains since the former have only one direction to jump (off the platform) instead of two. For this reason, the denominator in Eq. (5) has the total number of passengers on the trains plus half the total number of passengers on both platforms. Note that when the trains and platforms are stationary (with $a=0$), the model reduces to the Ehrenfest dog-flea model.²²

III. COUETTE AND POISEUILLE FLOW

We consider two basic scenarios for the motion of the trains. In the first, we set the incline angle to zero (so $a=0$) but take the right platform to have constant velocity u_c (like a moving sidewalk). The left platform is stationary so the boundary conditions are $u_0=0$ and $u_{n+1}=u_c$ (see Fig. 2). A passenger jumping from a train (or platform) onto an adjacent train will change the velocity of the latter, thanks to the conservation of linear momentum. For example, suppose the trains are initially at rest with N passengers on each train; when a passenger jumps off the moving right platform onto the rightmost train n , that train acquires momentum mu_c and starts to move with a velocity $u_c = u_n/(N+1)$. The random walk of the passengers leads thus to a perpetual exchange of the linear momentum between adjacent trains or platforms. As time passes, this process will eventually reach a stationary regime where the average velocity of each train will be nearly equal to the average velocities of its nearest neighbor trains. Given the boundary conditions, we expect an average linear velocity profile, so the model mimics Couette flow (see Fig. 1). Moreover, the rate at which the system approaches the stationary regime will clearly be governed by the jump frequency D of passengers, i.e., the larger the jump frequency, the sooner the linear profile will be established. In the train model, the jump frequency D thus plays a role similar to that of the viscosity in the corresponding "real" fluid. Maxwell presented a similar model to illustrate why a dilute gas has nonzero viscosity.²⁰

For our second flow scenario, we fix both platforms to be at rest but have the system on an inclined plane (so $\theta \neq 0$ and $a \neq 0$). By the same mechanism of momentum transfer described above, in time the system will reach a stationary regime, but now the average velocity will be higher for trains running near the center than for those running near the sides (remember that in this case $u_0 = u_{n+1} = 0$). The average velocity profile is thus expected to be parabolic and the model

mimics Poiseuille flow (see Fig. 1). A rigorous derivation of the above intuitive results will be presented in the later sections.

IV. NUMERICAL SIMULATION OF THE TRAIN MODEL

One of the major attractions of the train model is that it can be easily simulated on a computer. The outline of the algorithm is as follows.

- (1) Initialize the number of passengers N_i , and the velocity u_i , of trains and platforms.
- (2) Select a passenger at random as the next jumper; determine the jumper's point of origin. Since the passengers on the platforms jump half as frequently as those on the trains, for the purpose of selecting a random jumper, take the number of passengers on each platform to be $N_0/2$.
- (3) Decrement N_i on jumper's train of origin; if the passenger is jumping from a platform, add a replacement passenger to the platform.
- (4) If jumping from a train, select the jumper's destination (to the left or right of the point of origin) at random.
- (5) Reset the N_i and u_i for the jumper's destination. If a passenger jumps to a platform, remove that passenger from the system.
- (6) Compute the time until the next jump as $\Delta t = \tau[-\ln(\mathcal{R})]$ where τ is the mean time between jumps, defined in Eq. (5); and \mathcal{R} is a uniformly distributed random number.²³
- (7) Accelerate the trains to their new velocities as $u_i^{\text{new}} = u_i^{\text{old}} + a\Delta t$, for $i = 1, \dots, n$.
- (8) Periodically measure the state of the system to accumulate statistical samples.
- (9) Loop to step 2 until desired number of samples are taken.

A FORTRAN program to simulate the train model is available on request from the authors.

The average train velocity, as obtained by computer simulation, is shown in Fig. 3 for the two flow scenarios (Couette and Poiseuille) described in the previous section. The fluctuations measured in the simulations are described at the end of the next section.

V. THEORETICAL ANALYSIS OF THE TRAIN MODEL

Let us now consider the theoretical analysis for fluctuations in the stochastic train model. We first construct the evolution equation for the probability distribution associated with the state variables of the system. Suppose that at some time t the system is in the state $\{N_1, J_1; \dots; N_n, J_n\} \equiv \{N, J\}$ where $J_i = mu_i N_i$ is the momentum of the i th train. Obviously, the system will leave this state at the next jump so the probability that the system is in the state $\{N, J\}$ at time $t + dt$, given that it was in that state at time t , is $(1 - \text{the probability of having a jump during } dt)$. Now, the probability that a jump occurs from train i during the time interval dt , equals $DN_i dt$ plus terms that vanish more rapidly as $dt \rightarrow 0$. On the other hand, suppose all the trains are in the state $\{N, J\}$ at time t , except for two adjacent trains that are in the state $(N_i + 1, J_i + mu_i)$ and $(N_{i\pm 1} - 1, J_{i\pm 1} - mu_i)$. If a jump occurs from the former to the latter train during dt , then the system will reach $\{N, J\}$ at $t + dt$. Combining the above possibilities, one finds that, in the limit $dt \rightarrow 0$,

$$\begin{aligned} \frac{\partial}{\partial t} P(\{N, J\}) = & \frac{D}{2} \sum_{i=1}^n [-2N_i P(\{N, J\}) + (N_i + 1) P(\{\dots; N_i + 1, J_i + mu_i; N_{i+1} - 1, J_{i+1} - mu_i; \dots\}) \\ & + (N_i + 1) P(\{\dots; N_{i-1} - 1, J_{i-1} - mu_i; N_i + 1, J_i + mu_i; \dots\})] + \frac{D}{2} [N_0 P(\{N_1 - 1, J_1 - mu_0; \dots\}) \\ & + N_0 P(\{\dots; N_n - 1, J_n - mu_{n+1}\}) - (N_1 + N_n) P(\{N, J\})] \\ & - \sum_{i=1}^n \frac{\partial}{\partial J_i} ma N_i P(\{N, J\}). \end{aligned} \quad (6)$$

The one-half factor comes from the fact that each traveler has an equal probability to jump to the left or to the right and the last term takes into account the ‘‘continuous’’ change of the trains’ velocities due to the acceleration field. In the absence of the acceleration field ($a=0$), this equation reduces to the so-called *birth and death Master equation*; the corresponding stochastic process is called a *birth and death process*. For $a \neq 0$, we have a combination of a birth and death process and a time continuous deterministic process, which is known as a Feller process.²⁴

In what follows, we shall be mainly interested in the asymptotic behavior of the Master equation [Eq. (6)], in the limit $N_0 \rightarrow \infty$, known as the *thermodynamic limit*. To this end, we first introduce the intensive variables,

$$\rho_i = \frac{N_i}{N_0}, \quad p_i = \frac{J_i}{N_0}, \quad (7)$$

which correspond to number and momentum densities, respectively. We also note that, by definition, the trains’ velocities can be written as

$$u_i = \frac{p_i}{m\rho_i}. \quad (8)$$

It is now easy to check that in the thermodynamic limit the solution of the Master equation (6), expressed in terms of number and momentum densities, reduces to

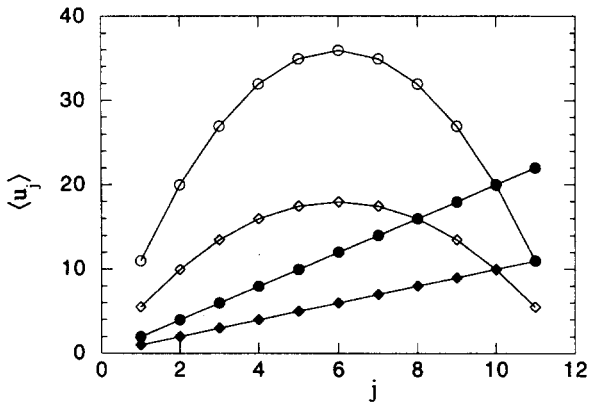


Fig. 3. Average train velocity $\langle u_j \rangle$ for Couette and Poiseuille flows. Data points are from a computer simulation of the train model with $n=11$ trains, $N_0=50$ passengers per platform and jump frequency $D=1$. The simulations were run for 10^7 jumps, which requires about a minute on a workstation. Simulation results are in perfect agreement with Eqs. (12) and (13). Filled symbols: Couette flow (diamonds, $\gamma=1$; circles, $\gamma=2$); open symbols: Poiseuille flow (diamonds, $a=0.5$; circles, $a=1.0$).

$$\lim_{N_0 \rightarrow \infty} P\left(\left\{\frac{N_i}{N_0}, \frac{J_i}{N_0}\right\}\right) = \prod_{i=1}^n \delta(\rho_i - \bar{\rho}_i) \delta(p_i - \bar{p}_i), \quad (9)$$

if the initial probability is a δ -function (i.e., the initial state is uniquely specified). The ‘‘macroscopic’’ variables, $\bar{\rho}_i$ and \bar{p}_i obey the following ‘‘deterministic’’ equations:

$$\frac{\partial}{\partial t} \bar{\rho}_i = \frac{D}{2} (\bar{\rho}_{i+1} + \bar{\rho}_{i-1} - 2\bar{\rho}_i), \quad (10)$$

$$\frac{\partial}{\partial t} \bar{p}_i = \frac{D}{2} (\bar{p}_{i+1} + \bar{p}_{i-1} - 2\bar{p}_i) + ma\bar{p}_i. \quad (11)$$

As $t \rightarrow \infty$, $\bar{\rho}_i$ and \bar{p}_i approach their steady-state values, $\hat{\rho}_i$ and \hat{p}_i . For Couette flow, $a=0$, $u_0=0$, and $u_{n+1}=u_c$. The steady-state solution of (10) is $\hat{\rho}_i=1$, that is, all trains have, on average, the same number of passengers as the platforms. The steady-state solution of (11) reads

$$\hat{u}_i = \frac{\hat{p}_i}{m\hat{\rho}_i} = i \frac{u_c}{n+1} \equiv i\gamma, \quad (12)$$

so the Couette velocity profile is linear with gradient γ (see Figs. 1 and 3). For Poiseuille flow, $u_0=u_{n+1}=0$ but the acceleration $a \neq 0$. As with Couette flow, the steady-state density is constant. The steady-state solution of (11) gives

$$\hat{u}_i = \frac{a}{D} i(n+1-i), \quad (13)$$

so the velocity profile is parabolic (see Figs. 1 and 3).

Let us now consider the fluctuations about the macroscopic state, defined as

$$\delta\rho_i(t) = \rho_i(t) - \bar{\rho}_i(t), \quad (14)$$

$$\delta p_i(t) = p_i(t) - \bar{p}_i(t). \quad (15)$$

As mentioned above [cf. Eq. (9)], in the thermodynamic limit the set of random variables $\{\rho_i, p_i\}$ converges, *in probability*, to the corresponding macroscopic values $\{\bar{\rho}_i, \bar{p}_i\}$. In other words, the probability for the fluctuations $\{\delta\rho_i(t), \delta p_i(t)\}$ to take on values other than zero, becomes negligible as $N_0 \rightarrow \infty$. Extracting the form of the fluctuations thus requires higher order corrections to the macroscopic behavior. The singular nature of the solution (9), however, clearly indicates that any perturbative expansion in the inverse power of N_0 is bound to fail.²⁵ To overcome this difficulty, we introduce the scaled variables, $\xi_i(t) \equiv \sqrt{N_0} \delta\rho_i$ and $\eta_i(t) \equiv \sqrt{N_0} \delta p_i$. It is a matter of simple algebra to check that, in the thermodynamic limit, $N_0 \rightarrow \infty$, the Master equation, expressed in terms of the above scaled variables, reduces to the following *Fokker-Planck* equation:

$$\begin{aligned} \frac{\partial}{\partial t} P(\{\xi, \eta\}) = & -\frac{D}{2} \sum_{i=1}^n \left\{ \frac{\partial}{\partial \xi_i} (\xi_{i+1} + \xi_{i-1} - 2\xi_i) \right. \\ & \left. + \frac{\partial}{\partial \eta_i} [(\eta_{i+1} + \eta_{i-1} - 2\eta_i) + ma\xi_i] \right\} \\ & \times P(\{\xi, \eta\}) + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \left\{ Q_{ij}^{pp} \frac{\partial^2}{\partial \xi_i \partial \xi_j} \right. \\ & \left. + 2Q_{ij}^{pu} \frac{\partial^2}{\partial \xi_i \partial \eta_j} + Q_{ij}^{uu} \frac{\partial^2}{\partial \eta_i \partial \eta_j} \right\} P(\{\xi, \eta\}), \end{aligned} \quad (16)$$

where

$$\begin{aligned} Q_{ij}^{pp} = & \frac{D}{2} ([2\bar{\rho}_i + \bar{\rho}_{i+1} + \bar{\rho}_{i-1}] \delta_{i,j}^{Kr} - [\bar{\rho}_{i+1} + \bar{\rho}_i] \delta_{i+1,j}^{Kr} \\ & - [\bar{\rho}_{i-1} + \bar{\rho}_i] \delta_{i-1,j}^{Kr}), \\ Q_{ij}^{pu} = & \frac{D}{2} ([2\bar{\rho}_i + \bar{\rho}_{i+1} + \bar{\rho}_{i-1}] \delta_{i,j}^{Kr} - [\bar{\rho}_{i+1} + \bar{\rho}_i] \delta_{i+1,j}^{Kr} \\ & - [\bar{\rho}_{i-1} + \bar{\rho}_i] \delta_{i-1,j}^{Kr}), \\ Q_{ij}^{uu} = & \frac{D}{2} ([2\bar{\rho}_i^2/\bar{\rho}_i + \bar{\rho}_{i+1}^2/\bar{\rho}_{i+1} + \bar{\rho}_{i-1}^2/\bar{\rho}_{i-1}] \delta_{i,j}^{Kr} \\ & - [\bar{\rho}_{i+1}^2/\bar{\rho}_{i+1} + \bar{\rho}_i^2/\bar{\rho}_i] \delta_{i+1,j}^{Kr} - [\bar{\rho}_{i-1}^2/\bar{\rho}_{i-1} \\ & + \bar{\rho}_i^2/\bar{\rho}_i] \delta_{i-1,j}^{Kr}), \end{aligned} \quad (17)$$

and $\delta_{i,j}^{Kr}$ is the Kronecker delta function. Now, the Fokker-Planck equation governs the evolution of the probability density of Markov processes with continuous realizations, which are known as *diffusion processes*. The scaled variables $\{\xi_i(t), \eta_i(t)\}$ thus converge, in the thermodynamic limit, to a diffusion process.²⁶

Thanks to its linearity, the Fokker-Planck equation (16) can be solved exactly and the result is a propagating multi-Gaussian distribution around the macroscopic path. The explicit form of the solution, however, is quite involved and thus is not presented here. Instead, we concentrate on the stationary regime of the system, which can be completely specified in terms of the covariance matrices of the associated time-independent multi-Gaussian distribution. To do so, all we need is to compute the “static” (equal time) correlation functions of the system.²⁷

For density, the probability distribution turns out to be a multi-Poissonian distribution, in agreement with equilibrium statistical mechanics predictions.²⁸ In particular, the static density-density correlation function is given by

$$\langle \delta\rho_i \delta\rho_j \rangle = \frac{1}{N_0} \delta_{i,j}^{Kr}. \quad (18)$$

Taking into account this result, the density-momentum static correlation function is readily found to be

$$\langle \delta\rho_i \delta p_j \rangle = \frac{\hat{p}_i}{N_0} \delta_{i,j}^{Kr}. \quad (19)$$

On the other hand, using the relations (14) and (15) and the definition (8), one finds to dominant order in $1/N_0$ the following relation for the velocity fluctuations:

$$\delta u_i(t) = \frac{\delta p_i(t)}{\hat{\rho}_i} - \frac{\hat{p}_i}{\hat{\rho}_i^2} \delta p_i(t) = \delta p_i(t) - \hat{p}_i \delta p_i(t), \quad (20)$$

where we have used the fact that $\hat{\rho}_i = 1$ for both Couette and Poiseuille cases. One can then easily check that

$$\langle \delta\rho_i \delta u_j \rangle = 0, \quad (21)$$

which shows that the instantaneous density and velocity fluctuations are not correlated.

Let us now consider the static velocity-velocity correlation function which is readily found to obey the following equation:

$$\begin{aligned} \langle \delta u_{i+1} \delta u_j \rangle + \langle \delta u_{i-1} \delta u_j \rangle + \langle \delta u_i \delta u_{j+1} \rangle + \langle \delta u_i \delta u_{j-1} \rangle \\ - 4\langle \delta u_i \delta u_j \rangle = -\frac{f_i}{N_0} \delta_{i,j}^{Kr} \end{aligned} \quad (22)$$

with $\langle \delta u_0 \delta u_i \rangle = \langle \delta u_{n+1} \delta u_i \rangle = 0$ and

$$f_i = (\hat{u}_{i+1} - \hat{u}_i)^2 + (\hat{u}_{i-1} - \hat{u}_i)^2 \propto |\nabla u_i|^2 \quad (23)$$

indicating that the static correlation of velocity fluctuations is proportional to the square of the local velocity gradient.

To solve Eq. (22) we introduce the discrete Fourier sine transform:

$$C_{pq} = \sum_{i=1}^n \sum_{j=1}^n \sin \frac{\pi p i}{n+1} \sin \frac{\pi q j}{n+1} \langle \delta u_i \delta u_j \rangle, \quad (24)$$

so that the solution of (22) may be written as

$$\langle \delta u_i \delta u_j \rangle = \frac{4}{(n+1)^2} \sum_{p=1}^n \sum_{q=1}^n \sin \frac{\pi p i}{n+1} \sin \frac{\pi q j}{n+1} C_{pq}, \quad (25)$$

where

$$C_{pq} = -\frac{1}{2N_0 \lambda_{pq}} \sum_{k=1}^n \sin \frac{\pi p k}{n+1} \sin \frac{\pi q k}{n+1} f_k \quad (26)$$

and

$$\lambda_{pq} = \cos \frac{\pi p}{n+1} + \cos \frac{\pi q}{n+1} - 2. \quad (27)$$

Note that $\{\lambda_{pq}\}$ are the eigenvalues of the finite difference operator.

For Couette flow, the steady state velocity profile is linear, $\hat{u}_i = \gamma i$, so $f_i = 2\gamma^2$ and

$$C_{pq} = -\frac{(n+1)\gamma^2}{2N_0 \lambda_{pq}} \delta_{p,q}^{Kr}. \quad (28)$$

In this case, the sums may be evaluated explicitly to obtain,

$$\langle \delta u_i \delta u_j \rangle = \frac{\gamma^2}{N_0(n+1)} \begin{cases} i(n+1-j), & \text{if } i \leq j, \\ j(n+1-i), & \text{if } j < i. \end{cases} \quad (29)$$

This function is plotted in Fig. 4 along with the results from a computer simulation of the train model. The piecewise linear function in (29) is similar to the amplitude of a plucked string since (22) is similar to the discretized Green's problem for the one-dimensional Laplace equation with Dirichlet boundary conditions. In general, the sums in (25) cannot be evaluated analytically but they are simple to compute numerically. Figure 5 compares the results from a computer simulation of the train model with the numerical evaluation of (25) for Poiseuille flow.

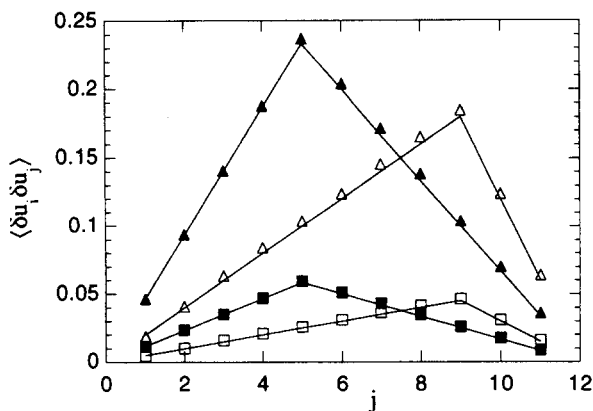


Fig. 4. Couette flow results for the static correlation $\langle \delta u_i \delta u_j \rangle$ for two different values of platform speed. Data points are from a computer simulation of the train model with $n=11$ trains, $N_0=50$ passengers per platform, and jump frequency $D=1$. The simulations were run for 10^7 jumps, which requires about a minute on a workstation (filled symbols: $i=5$; open symbols: $i=9$; squares: $\gamma=1$; triangles: $\gamma=2$). The solid line is given by Eq. (29).

VI. COMPARISON WITH FLUCTUATING HYDRODYNAMICS

Our main goal in this section is to describe the connection between the train model and the fluctuating hydrodynamic theory of fluids. As was stated in the Introduction, the analysis of fluctuations in nonequilibrium systems is not simple, especially when boundary effects have to be included, as is precisely the case for Couette and Poiseuille flows. For this reason, only a brief sketch of the fluctuating hydrodynamics calculation will be presented here; the interested reader is invited to consult Ref. 18 for a detailed exposition.

Consider a simple fluid confined between a pair of rigid, no-slip, perfectly conducting walls located at $y=0$ and L . For simplicity, the system is assumed to be periodic in the x and z directions with cross-section area S (see Fig. 1). The motion of the fluid may be produced by having the right wall moving in the $+x$ direction (Couette case) or by applying an accelerating field in the $+x$ direction, maintaining the containing walls at rest (Poiseuille case).

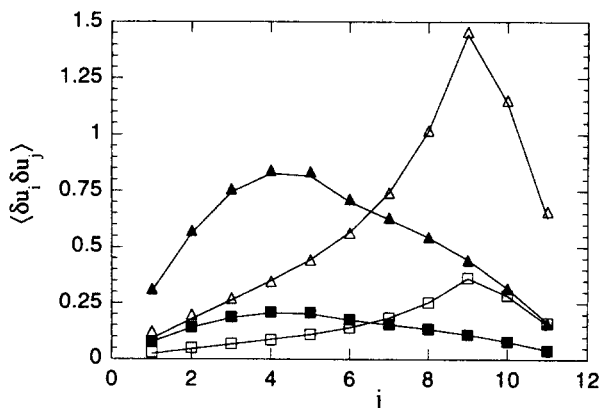


Fig. 5. Poiseuille flow results for the static correlation $\langle \delta u_i \delta u_j \rangle$ for two different values of acceleration. Data points are from a computer simulation of the train model with $n=11$ trains, $N_0=50$ passengers per platform, and jump frequency $D=1$. The simulations were run for 10^7 jumps, which requires about a minute on a workstation (filled symbols: $i=5$; open symbols: $i=9$; squares: $a=1$; triangles: $a=2$). The solid line is found by numerically evaluating the summations in Eq. (25).

We first consider the stationary solution of the macroscopic hydrodynamic equations. If the applied constraint (e.g., the acceleration field in the Poiseuille flow) is large, the stationary “laminar” regime may become unstable with the flow developing complex structures, such as eddies, or even becoming turbulent. In such cases, the analysis of the fluctuations, without resorting to computer calculations, is prohibitively difficult. For this reason we will limit our attention to fluids in laminar flow. Note that the thermal fluctuations described in this paper arise from the atomistic nature of a fluid, unlike the statistical variance of velocity arising from the chaotic properties of a nonlinear, turbulent flow.

Another complication comes from the fact that, in general, the temperature is not uniform throughout the fluid. Because of the internal friction between adjacent layers of the fluid, mechanical energy is not conserved. The heat released through this energy dissipation diffuses throughout the system, thanks to the mechanism of heat conduction, eventually reaching the containing walls which act as thermal reservoirs. The balance between energy dissipation, known as “viscous heating,” and heat conduction give rise to a temperature profile (the temperature is higher in the middle of the system than near the boundaries), which also induces a density profile in the system. The amplitude of the temperature profile, however, is proportional to the square of the velocity gradient and can thus be neglected if the applied constraints on the system are weak. Furthermore, when this viscous heating effect is incorporated into numerical calculations of the fluctuation spectrum, no significant qualitative changes in the results are observed. For these reasons, we will take the macroscopic density and temperature to be constant throughout the system (as is the case in the train model).

Given the above conditions, the x component of the macroscopic fluid velocity, \bar{u} , obeys the simplified Navier-Stokes equation,⁶

$$\frac{\partial}{\partial t} \bar{u}(y, t) = \nu \frac{\partial^2 \bar{u}}{\partial y^2} - a, \quad (30)$$

where ν is the kinematic viscosity for the fluid. Using the standard discretization of the spatial variable, $y=i\Delta y$ with $\Delta y=L/(n+1)$ and $i=0, 1, \dots, n+1$, and the centered difference,²³

$$\frac{\partial^2}{\partial y^2} \bar{u} \rightarrow \frac{\bar{u}_{i+1} + \bar{u}_{i-1} - 2\bar{u}_i}{\Delta y^2}, \quad (31)$$

one finds

$$\frac{\partial}{\partial t} \bar{u}_i = \frac{\nu}{\Delta y^2} (\bar{u}_{i+1} + \bar{u}_{i-1} - 2\bar{u}_i) - a. \quad (32)$$

Comparing the above equation with Eq. (11) of the train model, one finds that the two are equivalent if $D=2\nu/\Delta y^2$. The velocity profiles for Couette and Poiseuille flow are then given by (12) and (13), respectively.

Let us now consider the statistical properties of the system. To do so, first we have to linearize the hydrodynamic equations about the macroscopic stationary state. Next, as sketched in the Introduction, in the resulting equations one must use the *fluctuating Newton law*, relating the shear and bulk stress to the velocity gradient, and the *fluctuating Fourier law*, describing thermal conduction. This procedure leads to a set of stochastic partial differential equations, known as the “Landau-Lifshitz fluctuating hydrodynamic

equations," which govern the evolution of the fluctuation of hydrodynamic variables. Unfortunately, the analysis of these equations, in their general form, proves to be extremely difficult in our case. Besides the finite size effects, the main source of difficulty arises from the coupling of energy (or temperature) fluctuations with velocity and density fluctuations. Associating a "temperature" with the train model is problematic since there is random motion in the y -direction (passengers jump between trains) yet none in the x direction (passengers remain at rest in the frame of reference of their train). In real fluids, we can neglect the coupling with thermal fluctuations when the thermal expansivity coefficient is negligibly small (e.g., water near 4 °C) and this scenario received a considerable amount of attention in the late 1970s (for a review, see Ref. 29). But even in this case, only the Couette problem can be handled analytically;¹⁸ the density and y -velocity fluctuations assume their equilibrium form, very much as in the train model. The nonequilibrium contribution to the x -velocity (static) correlation function is given by

$$\begin{aligned} \langle \delta u(y) \delta u(y') \rangle &= \frac{k_B \hat{T}}{\hat{\rho} S} \delta(y-y') \\ &= \gamma^2 \frac{k_B \hat{T}}{\hat{\rho} L c^2} \left\{ y'(L-y) - \frac{\lambda L}{2 \sinh(L/\lambda)} \right. \\ &\quad \left. \times \left[\cosh\left(\frac{y-y'-L}{\lambda}\right) - \cosh\left(\frac{y+y'-L}{\lambda}\right) \right] \right\} \end{aligned} \quad (33)$$

with $y > y'$ (for $y < y'$, exchange y and y') and

$$\lambda \equiv \frac{\sqrt{\nu(\zeta + 7\nu/3)}}{c}. \quad (34)$$

In this relation, \hat{T} and $\hat{\rho}$ are the steady state (constant) temperature and density, respectively, k_B is Boltzmann's constant, c is the (isothermal) sound speed, and ζ is the kinematic bulk viscosity coefficient. Note that the macroscopic velocity gradient γ is constant (independent of space), since the velocity profile is linear.

The parameter λ , which has the units of length, can be associated with an acoustic absorption scale. For instance, the ratio λ/L is approximately the same as the Knudsen number in a dilute gas. Now, the validity of hydrodynamics can only be guaranteed for length scales larger than λ , since otherwise there will be no clear separation between microscopic processes, giving rise to sound generation, and macroscopic effects at the origin of dissipation, such as, for example, the phenomenon of sound viscous damping. Such small scale phenomena are described through the so-called "generalized hydrodynamics,"³⁰ whose discussion is beyond the scope of the present work. Accordingly, we shall consider the limit $L \gg \lambda$, in which case the relation (33) reduces to

$$\begin{aligned} \langle \delta u(y) \delta u(y') \rangle &= \frac{k_B \hat{T}}{\hat{\rho} S} \delta(y-y') \\ &\approx \gamma^2 \frac{k_B \hat{T}}{\hat{\rho} L c^2} \begin{cases} y(L-y'), & \text{if } y \leq y', \\ y'(L-y), & \text{if } y > y'. \end{cases} \end{aligned} \quad (35)$$

The second term on the left-hand side of (35) represents the local equilibrium contribution to the velocity fluctuation. In the train model, the equilibrium velocity fluctuation is zero since in the absence of nonequilibrium constraints the trains remain at rest. The right-hand side of (35) is a piecewise

linear function with amplitude proportional to the square of the velocity gradient, just as in Eq. (29) of the train model. We thus arrive at the conclusion that the fluctuating hydrodynamics theory leads basically to the same type of long range correlations as the train model, a striking result given the simplicity of the model.

VII. CONCLUSION

In this paper, we present a simple model that illustrates the long-range correlation of fluctuations in nonequilibrium systems. This correlation is found to be approximately piecewise linear with an amplitude that is proportional to the square of the imposed gradient. Remarkably, the fluctuating hydrodynamic calculations lead basically to the same result. Besides the references discussed in the Introduction, similar results are also found for the nonequilibrium temperature correlations in a high Prandtl number liquid³¹ and for the nonequilibrium density autocorrelation function in a cellular automata model.³²

While the theoretical analysis of the model requires some knowledge of stochastic processes, the physics of the model is no more difficult to understand than the standard random walk ("drunkard's walk") model. A computer simulation of the model can easily be written by undergraduate students and significant results can be obtained using a personal computer. We hope that this model can serve as a pedagogical introduction to the theory of nonequilibrium fluctuations.

ACKNOWLEDGMENTS

The authors wish to thank Professor B. Alder, Professor F. Alexander, Professor G. Nicolis, and Professor J. W. Turner for helpful discussions. This work has been partially supported by the Belgian Federal Office for Technical and Cultural Affairs.

¹J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), 2nd ed., Sec. 9.7.

²F. Reif, *Fundamentals of Statistical Mechanics and Thermal Physics* (McGraw-Hill, New York, 1965), Chap. 15; R. K. Pathria, *Statistical Mechanics* (Pergamon, Oxford, 1977), Chap. 13; L. E. Reichl, *A Modern Course in Statistical Physics* (University of Texas, Austin, 1980), Chap. 15.

³J. J. Binney, N. J. Dowrick, A. J. Fisher, and M. E. J. Newman, *The Theory of Critical Phenomena* (Clarendon, Oxford, 1992).

⁴P. Glandsdorff and I. Prigogine, *Thermodynamics of Structure, Stability, and Fluctuations* (Wiley-Interscience, New York, 1971); D. Jou, J. Casas-Vasquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer-Verlag, Berlin, 1993).

⁵In some cases, potentials may be crafted; for some examples see R. Graham, "Macroscopic potentials, bifurcations and noise in dissipative systems," in *Noise in Nonlinear Dynamical Systems*, edited by F. Moss and P. McClintock (Cambridge U. P., Cambridge, 1989), Vol. 1, pp. 225-278.

⁶L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon, Oxford, 1959).

⁷J. Keizer, "A theory of spontaneous fluctuations in viscous fluids far from equilibrium," *Phys. Fluids* **21**, 198-208 (1978); J. Keizer, *Statistical Thermodynamics of Nonequilibrium Processes* (Springer-Verlag, New York, 1987).

⁸G. Nicolis, I. Prigogine, and R. Fox, *Self-Organization in Nonequilibrium Systems* (Wiley, New York, 1977). "Master equation derivation of Keizer's theory of nonequilibrium thermodynamics with critical fluctuations," *J. Chem. Phys.* **70**, 4660-4663 (1979); H. Grabert, "Fokker-Planck equation approach to fluctuations about nonequilibrium steady states," *J. Stat. Phys.* **26**, 113-135 (1981).

⁹I. Procaccia, D. Ronis, and I. Oppenheim, "Light scattering from nonequilibrium stationary states: The implication of broken time-reversal symmetry," *Phys. Rev. Lett.* **42**, 287-290 (1979).

- ¹⁰T. R. Kirkpatrick, E. G. D. Cohen, and J. R. Dorfman, "Kinetic theory of light scattering from a fluid not in equilibrium," *Phys. Rev. Lett.* **42**, 862–865 (1979).
- ¹¹J. Keizer and M. Medina-Noyola, "Spatially nonlocal fluctuation theories: Hydrodynamic fluctuations for simple fluids," *Physica A* **115**, 301–338 (1982).
- ¹²A. M. Tremblay, "Theories of Fluctuations in Nonequilibrium Systems," in *Recent Developments in Nonequilibrium Thermodynamics*, edited by J. Casas-Vasquez, D. Jou, and G. Lebon (Springer-Verlag, Berlin, 1984).
- ¹³R. Schmitz, "Fluctuations in nonequilibrium fluids," *Phys. Rep.* **171**, 1–58 (1988).
- ¹⁴D. Beysens, Y. Garrabos, and G. Zalczer, "Experimental evidence for Brillouin asymmetry induced by a temperature gradient," *Phys. Rev. Lett.* **45**, 403–406 (1980); G. H. Wegdam, N. M. Keulen, and J. C. F. Michielsen, "Small angle Rayleigh scattering in CCl_4 subjected to a temperature gradient," *Phys. Rev. Lett.* **55**, 630–633 (1985).
- ¹⁵B. M. Law and J. V. Sengers, "Fluctuations in fluids out of thermal equilibrium," *J. Stat. Phys.* **57**, 531–547 (1989); B. M. Law, P. N. Segré, R. W. Gammon, and J. V. Sengers, "Light-scattering measurements of entropy and viscous fluctuations in a liquid far from thermal equilibrium," *Phys. Rev. A* **41**, 816–824 (1990).
- ¹⁶J. Machita, I. Procaccia, and I. Oppenheim, "Light scattering and pair-correlation functions in fluids with nonuniform velocity fields," *Phys. Rev. Lett.* **42**, 1368–1371 (1979).
- ¹⁷M. Malek Mansour, A. L. Garcia, G. Lie, and E. Clementi, "Fluctuating hydrodynamics in a dilute gas," *Phys. Rev. Lett.* **58**, 874–877 (1987).
- ¹⁸A. L. Garcia, M. Malek Mansour, G. Lie, M. Mareschal, and E. Clementi, "Hydrodynamic fluctuations in a dilute gas under shear," *Phys. Rev. A* **36**, 4348–4355 (1987).
- ¹⁹M. Mareschal, M. Malek Mansour, G. Sonnino, and E. Kestemont, "Dynamic structure factor in a nonequilibrium fluid: A molecular-dynamics approach," *Phys. Rev. A* **45**, 7180–7183 (1992).
- ²⁰J. C. Maxwell, "Illustrations of the dynamical theory of gases.-Part I. On the motions and collisions of perfectly elastic spheres," *Philos. Mag.* **19**, 19–32 (1860); "Illustrations of the dynamical theory of gases.-Part II. On the process of diffusion of two or more kinds of moving particles among one another," *Philos. Mag.* **20**, 21–37 (1860).
- ²¹E. H. Kennard, *Kinetic Theory of Gases* (McGraw-Hill, New York, 1938).
- ²²P. Ehrenfest and T. Ehrenfest, "Ueber eine Aufgabe aus der Wahrscheinlichkeitsrechnung die mit kinetischen Deutung der Entropievermehrung zusammenhängt," *Math. Naturw. Blätter* **3** (1906), in *Paul Ehrenfest, Collected Scientific Papers*, edited by M. J. Klein (North-Holland, Amsterdam, 1959), pp. 128–130.
- ²³A. L. Garcia, *Numerical Methods for Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1994).
- ²⁴C. W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences* (Springer-Verlag, Berlin, 1983).
- ²⁵N. G. Van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
- ²⁶T. G. Kurtz, "Limit Theorems and Diffusion Approximations for Density Dependent Markov Chains," *Math. Progr. Stud.* **5**, 67–78 (1976); "Strong approximation theorems for density dependent Markov chains," *Stoch. Proc. Appl.* **6**, 223–240 (1978).
- ²⁷A. L. Garcia, M. Malek Mansour, G. C. Lie, and E. Clementi, "Numerical integration of the fluctuating hydrodynamic equations," *J. Stat. Phys.* **47**, 209–228 (1987).
- ²⁸L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, Oxford, 1980), Part I.
- ²⁹M. Malek Mansour, J. W. Turner, and A. Garcia, "Correlation functions for simple fluids in a finite system under nonequilibrium constraints," *J. Stat. Phys.* **48**, 1157–1186 (1987).
- ³⁰W. E. Alley and B. J. Alder, "Generalized transport coefficients for hard spheres," *Phys. Rev. A* **27**, 3158–3173 (1983); W. E. Alley, B. J. Alder, and S. Yip, "The neutron scattering function for hard spheres," *Phys. Rev. A* **27**, 3174–3186 (1983).
- ³¹G. Nicolis and M. Malek Mansour, "Onset of spatial correlations in nonequilibrium systems: A master-equation description," *Phys. Rev. A* **29**, 2845–2853 (1984); A. Garcia, "Thermal fluctuations in a Knudsen flow system," *Phys. Lett. A* **119**, 379–382 (1987).
- ³²H. Spohn, "Long range correlations for stochastic lattice gases in a nonequilibrium steady state," *J. Phys. A* **16**, 4275–4291 (1983).

Using qualitative problem-solving strategies to highlight the role of conceptual knowledge in solving problems

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(Received 4 October 1995; accepted 7 March 1996)

We report on the use of qualitative problem-solving strategies in teaching an introductory, calculus-based physics course as a means of highlighting the role played by conceptual knowledge in solving problems. We found that presenting strategies during lectures and in homework solutions provides an excellent opportunity to model for students the type of concept-based, qualitative reasoning that is valued in our profession, and that student-generated strategies serve a diagnostic function by providing instructors with insights on students' conceptual understanding and reasoning. Finally, we found strategies to be effective pedagogical tools for helping students both to identify principles that could be applied to solve specific problems, as well as to recall the major principles covered in the course months after it was over. © 1996 American Association of Physics Teachers.

I. INTRODUCTION

Two primary goals in teaching introductory physics are to help students learn major concepts and principles, and to help students learn how to apply them to solve problems. In

traditionally taught courses we assign many problems with the assumption that solving the problems will help develop in students an understanding of concepts and principles, as well as an appreciation of the role they play in solving problems. Yet, research findings demonstrate that problem solv-