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Cell Hydrodynamics: An Information-Conserving Theory

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A formulation of hydrodynamics in terms of discrete cell variables is given, which is as exact as possible in the sense that, for given initial measurements on a system, it gives the maximum possible information on future measurements. An apparently rapidly convergent successive-approximation scheme is described, which requires data obtainable from short-time computer simulation on small systems. The lowest approximation gives the linearized Navier–Stokes and energy flow equations, yielding explicit expressions for transport coefficients.

KEY WORDS: Hydrodynamics; molecular dynamics; transport coefficients.

1. INTRODUCTION

This paper is concerned with the problem of hydrodynamics, i.e., of predicting the motion of a macroscopic fluid, given the microscopic equations of motion of its constituent particles and suitable information about its initial state.

This problem has usually been approached by the method of continuum hydrodynamics.(1) This involves writing partial differential equations [the continuum equations (68) and (69)] describing the time evolution of certain "averaged hydrodynamic variables" [density, energy density, and momentum density: $n(\mathbf{r}, t)$, $\epsilon(\mathbf{r}, t)$, $\mathbf{p}(\mathbf{r}, t)$]. These equations can be used to predict the results of an experiment on a real system, as follows. First we devise smooth functions $n(\mathbf{r}, 0)$, $\epsilon(\mathbf{r}, 0)$, and $\mathbf{p}(\mathbf{r}, 0)$ which somehow represent the distribution of discrete particles in the initial state of the system. Then we compute the time evolution of these functions from the equations of continuum hydrodynamics, typically by discretizing the functions on a grid and approximating the differential equation by a difference equation. The resulting approximation

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to the function $n(\mathbf{r}, t)$ can be used to predict the results of a measurement, say the number of particles in some volume at time t.

The purpose of this paper is to inquire whether the frequent translation back and forth between discrete and continuous variables required by continuum hydrodynamics is really necessary or useful. The answer is found to be "no." I develop below an alternative, totally discrete formulation of hydrodynamics (to be referred to as "cell hydrodynamics"), which is superior in many ways to continuum hydrodynamics: (1) It can be formulated in a precise way from the microscopic equations of motion of the fluid, whereas the continuum equations are essentially phenomenological (derivations from microscopic equations have been attempted,(2–4) but seem always to bog down in heuristic appeals to "coarse-graining"). Well-defined successive approximations to the cell theory can be given, which give (in the limit) all possible information about the behavior of the system, consistent with one's initial knowledge. (2) From the point of view of actual computation, exact solutions to the (already approximate) continuum equations can be obtained from difference-equation approximations only by allowing the cell size to approach zero (in practice, this is usually the most serious limitation on accuracy). The "equations of change" of cell hydrodynamics are intrinsically difference equations, and approach exactness at fixed, *nonzero* cell size.

The plan of this paper is as follows: In Section 2, I use epistemological considerations to argue that a discrete theory is more natural than a continuum one, and that it should be based on a conditional probability. Such a theory is formulated precisely in Section 3. In Section 4 I present a complete parametrization of the conditional probability, which plausible physical arguments suggest to be rapidly convergent. The resulting hydrodynamic equations of change are determined in Section 5. Section 6 describes an algorithm for determining the parameters from easily calculable equilibrium correlations, by successive approximations. The method is simplified by symmetry considerations in Section 7. I work out the parameters explicitly in Section 8 for a simple but nontrivial approximation. The resulting equations of change, taken in the continuum limit, turn out to be the usual continuity, energy flow, and Navier–Stokes equations; explicit formulas appear for the thermal conductivity and shear viscosity [Eqs. (75a) and (75b)].

2. HEURISTIC DESCRIPTION OF CELL HYDRODYNAMICS

Consider a classical fluid, i.e., a large box containing many particles interacting according to classical[2] equations of motion. I want to study the

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[2] Although this paper treats only the classical case, everything but Section 6 can be adapted to quantum systems.

dynamics of this system from an epistemological point of view; that is, to ask what can be determined about the future behavior of the system from the knowledge of its present state that can be obtained by measurement. If this knowledge were complete, so we knew the exact state of the system (positions and momenta of all particles), the microscopic equations of motion would exactly determine its state at any future time. Useful predictions cannot be made this way, both because our measuring instruments will not tell us the exact state and because we could not solve the equations of motion if they did. Consistently with my epistemological point of view, I regard the limitation on knowledge as being more fundamental than the computational limitation. I therefore concentrate on determining the form of our information about the system, and worry later about computing its evolution.

In continuum theories, this initial information consists of "smoothed" distributions of the conserved variables: $n(\mathbf{r}, 0)$, $\epsilon(\mathbf{r}, 0)$, $\mathbf{p}(\mathbf{r}, 0)$. But this is clearly inappropriate for an epistemological approach; our instruments are not going to give us five continuous functions of four real variables. At best they will give us some discrete numbers, which I must accept as the fundamental variables of the theory. Clearly, similar considerations apply to the information I want to predict at later times; this should also involve discrete variables.

The fundamental discrete variables may be chosen in many different ways, and for many of these ways theories similar to that described below can be constructed. For simplicity, I shall develop the theory for variables chosen by partitioning the box into equal cubical cells (indexed by l). At discrete times $t = -m\tau$ (m an integer) we measure each cell's content of each conserved quantity[3]: $N_l(-m\tau)$, $E_l(-m\tau)$, $P_l(-m\tau)$. For conciseness I will call these contents $c_{\alpha lm}$, where $\alpha = N, E, P_x, P_y$, or P_z. Since I will frequently have occasion to refer collectively to all the contents at a particular time (i.e., $c_{\alpha lm}$ for all α and l but fixed m), I will use the symbol c_m for this.

The objective of the cell hydrodynamic theory is now to predict the contents at, say, $t = 0$ (i.e., c_0) given the previous contents. Of course I cannot expect an exact prediction—I have only partial information about the system. The best I can hope to do is calculate a probability distribution for the values of c_0, given the previous contents. One might suppose that this should depend only on the immediately preceding contents (c_1, at $t = -\tau$). This would be true if c_1 described the system exactly. But since it does not, one is throwing away relevant information by ignoring c_2 (at $t = -2\tau$), etc. Put differently, the ensemble of fixed c_1, c_2 is smaller than the ensemble of fixed c_1, and therefore pinpoints the actual system we are looking

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[3] There is ambiguity in the assignment of the potential energy of a pair of particles to the E_l if they lie in different cells, which is usually resolved by assigning half to each.

at (which is contained in both ensembles) more precisely.[4] This leads me to introduce a conditional probability distribution

$$Q(c_0|c_1, c_2, c_3, \ldots) \tag{1}$$

which is the probability of finding the cell contents at $t = 0$ to be c_0 in the ensemble of fixed $c_1, c_2, \ldots$.[5] This conditional probability Q is the basis of the new hydrodynamic theory, and is used to predict the evolution of a system. If we start with some initial information $c_1, c_2, \ldots$ (at $t = -\tau, -2\tau, \ldots$), Q determines the distribution of contents at $t = 0$, $c_{\alpha l 0}$. If this distribution is a narrow one about some mean values $\bar{c}_{\alpha l}(c_1, c_2, \ldots)$ (functions of all previous contents), we may take these means as the contents $c_{\alpha l 0}$ at $t = 0$. Then the mean value at $t = \tau$ is $\bar{c}_{\alpha l}(c_0, c_1, \ldots)$, which we take as $c_{\alpha, l, -1}$. This procedure can clearly be iterated to follow the hydrodynamic evolution of the system indefinitely.

Of course if $\bar{c}_{\alpha l}(c_1, \ldots)$ is really a function of an infinite number of variables, this is not going to work. But intuition suggests it depends strongly on only a few variables, near in space and time to the variable $c_{\alpha l 0}$ being predicted. One can argue, for example, that $c_{\alpha l 0}$ will not depend on a quantity measured in the distant past because that quantity's short-wavelength components will have returned to equilibrium, and its long-wavelength components will be reflected in the more recent c's, which are properly taken into account. And spatially distant (but recent) variables cannot have an effect because such an effect cannot propagate faster than the sound speed. One could also note that my variables are closely related to those used in numerical solutions of the continuum equations discretized on a grid (roughly, I average the density over a cell instead of evaluating it at the center). The success of such solutions in describing real systems suggests that for large cells, only nearest neighbor (in time and space) variables are necessary for predicting the time evolution.

The foregoing argument has ignored fluctuations (i.e., assumed the

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[4] This is an extremely important point. It is impossible to get a complete (information-preserving) hydrodynamic theory while assuming that the evolution of a system is determined by its hydrodynamic state at a single time. For example, the Boltzmann equation makes an assumption of this sort (that a contracted description at one time determines the evolution) and the Enskog treatment of hydrodynamics based on the Boltzmann equation makes the assumption again in further contracting the description. The assumption is necessary to get a differential equation out, of course, but is justified only in the limit that the time variation of the system is infinitely slow. The inconsistency of the assumption has been called the Hilbert paradox (see Ref. 2).

[5] The mere existence of this ensemble shows an advantage over continuum theory, in which nonequilibrium ensembles of fixed n, ϵ, and p are very hard to define (see Ref. 5). This Q is defined precisely in Section 3. The number of times involved is not really infinite, but extends back as far as our measurements do.

conditional distribution Q of predicted $c_{\alpha l 0}$ is very narrow), which is justified in many hydrodynamic problems. In general, though, the distribution of each variable $c_{\alpha l 0}$ will have some width, and Q (which is a *joint* distribution of many variables in different cells l) may impose correlations between variables. However, the arguments used above would suggest that these correlations are short-ranged[6] and that the width and correlations involving a particular $c_{\alpha l 0}$ depend only on $c_{\alpha' l' m'}$ with $l' \sim l$ and $m' \sim 0$. That is, in a certain sense (which will be clear when I parametrize it) the conditional distribution Q is a reasonably simple function, short-ranged in space and time. Then, by using Q as the basis of the theory, the possibility exists of describing phenomena in which fluctuations are not negligible (turbulence, critical dynamics). This also produces a theory which is in principle exact, in the following sense: Take $c_1, c_2, \ldots$ as initial information about a state and consider $Q(c_0 | c_1, c_2, \ldots)$. Instead of finding the mean value $\bar{c}_{\alpha l 0}$ as before, I retain Q and call it H^1, the first in a series of functions H^S giving the conditional probability of S consecutive states. Then

$$H^2(c_{-1}, c_0 | c_1, \ldots) \equiv Q(c_{-1} | c_0, \ldots) Q(c_0 | c_1, \ldots) \tag{2}$$

which is the conditional probability, given the initial information, that the system will evolve through the hydrodynamic states $c_{\alpha l 0}$ and $c_{\alpha, l, -1}$ (at $t = 0$ and $t = \tau$). Clearly I can repeat this, defining inductively

$$H^S(c_{1-S}, c_{2-S}, \ldots, c_0 | c_1, \ldots) \equiv Q(c_{1-S} | c_{2-S}, \ldots) H^{S-1}(c_{2-S}, \ldots | c_1, \ldots) \tag{3}$$

This gives the probability of an entire *history* of the system from $t = 0$ to $t = (S-1)\tau$, given our initial measurements $c_1, c_2, \ldots$. But this is clearly the maximum information any theory could possibly predict about future measurements on the system, consistently with our epistemological constraints, namely our incomplete initial knowledge $c_1, c_2, \ldots$. Of course we are not likely to want to know H^S completely (it is not a simple function), but its existence proves that whatever partial information we *do* want [such as average contents at $t = (S-1)\tau$] we can get from Q.

In fact, a function like H^S (with some unwanted variables integrated out) is the most direct possible link between theory and experiment (it predicts the distribution of experimental outcomes, given the initial conditions), so it should really be taken as the basic goal of any calculation.

To summarize the results of this section: I have found that by using discrete cell variables $c_{\alpha l m}$, I can define a conditional probability $Q(c_0 | c_1, c_2, \ldots)$ which determines the exact probability distribution for the current hydrodynamic variables in terms of the past ones. I have reason to believe that Q is not intractably complicated, but it nonetheless determines an exact (i.e., perfectly information-preserving) hydrodynamic theory. Thus encouraged,

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[6] But see Section 3.

I construct a precise definition of Q in the next section, and try to parametrize it in the following one.

3. EXACT FORMULATION

I now seek exact definitions of the functions discussed in Section 2. It turns out that the conditional probability $Q(c_0|c_1, c_2,...)$ of Section 2 is not as simple as was hoped; the values of $c_{\alpha l0}$ are correlated over long distances. It is easy to see that this is a consequence of the conservation laws obeyed by the contents $c_{\alpha l0}$. If I fix c_1 (thus fixing the total number of particles at $t = -\tau$, $N = \sum_l c_{Nl1}$, for example), then the variables c_{Nl0} are constrained to add up to N, giving long-ranged correlations.[7] So I must look for variables at $t = 0$ that obey no conservation law, but determine the $c_{\alpha l0}$. It is natural to choose the discrete analogs of the fluxes used in continuum theory, namely the *transfers* $x_{\alpha f}$, defined as the amount of α (i.e., number, energy, or momentum) passing through the face f during the time interval $(-\tau, 0)$. This requires indexing all the square faces separating the cells of the system, and establishing for each a conventional direction of "positive" flow. (In this paper I assume that for a face with normal in the x direction, flow toward increasing x is positive, etc.) The definition of $x_{\alpha f}$ is obvious for the properties carried by the particles: For each time a particle of total energy E and momentum $\mathbf{p}$ crosses face f (positively) we must add 1, E, p_x, p_y, and p_z, respectively, to x_{Nf}, x_{Ef}, x_{Pxf}, x_{Pyf}, and x_{Pzf}, with these quantities to be subtracted for each negative crossing. But there are also contributions to $\mathbf{x}_{Pf}$ and x_{Ef} due to the interatomic potential: For each pair of particles and each face f intersected by the line segment[8] connecting them, we must add $\int \mathbf{F}\, dt$ to $\mathbf{x}_{Pf}$ and $\int \mathbf{F}\cdot\mathbf{v}\, dt$ to x_{Ef}, where $\mathbf{F}$ is the force due to the particle on the negative side of f acting on the particle on the positive side, and $\mathbf{v}$ is the center-of-mass velocity of the pair. The integral is taken over the subinterval(s) of $(-\tau, 0)$ during which the segment intersects f.

If the box containing my system has real boundaries, these will transfer energy and momentum in ways not included in the above description. To avoid this complication, and ensure complete energy and momentum conservation, I assume a cubical box with periodic boundary conditions. Then *every* face separates two cells of the system; those at the apparent boundaries actually connect two cells on opposite sides of the system.

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[7] These vanish in the infinite-system limit, but this appears to be insufficient to rescue the theory.

[8] One can avoid the artificiality of using line segments by letting f index all pairs of cells; then each particle pair contributes to only one x_{Pf}. But this greatly increases the number of variables and it is not clear what real benefit it confers.

The transfers can now be used to determine the $t = 0$ contents $c_{\alpha l0}$:

$$c_{\alpha l0} = c_{\alpha l1} + \sum_f \sigma(f, l) x_{\alpha f} \tag{4}$$

where the sign factor σ is $+1$ if l is on the positive side of f, -1 if on the negative side, and may be taken to vanish if f is not a face of l. Clearly the transfers contain more information than the contents $c_{\alpha l0}$; a theory which predicts them is at least as good as one which predicts $c_{\alpha l0}$.

I would like to define probability distributions for the variables $x_{\alpha f}$, $c_{\alpha lm}$ in terms of the microscopic variables of the system at $t = 0$, namely N, $\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \ldots, \mathbf{p}_N$. Evidently $N, \mathbf{r}_1, \ldots$ determine the microscopic variables at all times $t = -m\tau$ (through the classical equations of motion); hence they determine the cell contents $c_{\alpha lm}$ uniquely. This defines a function $c^N_{\alpha lm}(\mathbf{r}_1, \ldots, \mathbf{p}_N)$. Similarly we can calculate the trajectory from $t = 0$ to $t = -\tau$ and define the transfers which take place as $x^N_{\alpha f}(\mathbf{r}_1, \ldots, \mathbf{p}_N)$. I will approach defining the desired conditional probability Q (Section 2) by first defining a general probabilty distribution P_M for all the content variables $c_{\alpha lm}$ at M times $t = -\tau, \ldots, -M\tau$, in addition to the transfer variables $x_{\alpha f}$ (referred to collectively as x). This requires only the fundamental assumption of equal a priori probability in phase space.$^{(4)}$ Set

$$P_M(x; c_1, \ldots, c_M) \equiv \int d\mathbf{r}_1 \cdots d\mathbf{p}_N \prod_{\alpha f} \delta[x_{\alpha f} - x^N_{\alpha f}(\mathbf{r}_1, \ldots, \mathbf{p}_N)] \times \prod_{\alpha l} \prod_{m=1}^{M} \delta[c_{\alpha lm} - c^N_{\alpha lm}(\mathbf{r}_1, \ldots, \mathbf{p}_N)] \tag{5}$$

where

$$N \equiv \sum_l c_{NlM} \tag{6}$$

(recall c_{NlM} is the number content of cell l at $t = -M\tau$). Since this distribution is unnormalized (and unnormalizable!), it will only be used to determine *relative* probabilities. To avoid an explosion of notation, the same notation is used for Dirac and Kronecker delta functions; the index α determines uniquely which is meant. Similarly, integrals (below) over $x_{\alpha f}$ or $c_{\alpha lm}$ are to be interpreted as sums if $\alpha = N$. Subscripts will be dropped when the meaning is obvious; for example, $\int dx$ means integration over all the $x_{\alpha f}$.

Now I can define a conditional probability

$$Q_M(x \mid c_1, \ldots, c_M) \equiv P_M(x; c_1, \ldots, c_M) \Big/ \int P_M(x'; c_1, \ldots, c_M)\, dx' \tag{7}$$

which differs from the Q discussed in Section 2 in that the period of observation is made explicit by the index M. Since Q_M is expected to be "short-ranged" (hence to depend on $c_{\alpha lm}$ only for small m), the index M is often irrelevant. To be precise, for any choice of $c_{\alpha lm}$ ($m = 1, \ldots, \infty$), the limit

$$Q(x \mid c_1, c_2, \ldots) \equiv \lim_{M \to \infty} Q_M(x \mid c_1, \ldots, c_M) \tag{8}$$

exists and is approached rapidly. This is the Q of Section 2, except that the transfers, rather than the contents directly, are predicted.

I want to show that the conditional probability Q_M indeed determines an information-conserving theory. As suggested in Section 2, this can be done by defining from Q_M the conditional probability of S-time histories:

$$\begin{aligned} H_M{}^S(c_{1-S},\ldots, c_0|c_1,\ldots, c_M) \\ = \int Q_{M+S-1}(x|c_{2-S},\ldots, c_M)H_M^{S-1}(c_{2-S},\ldots, c_0|c_1,\ldots, c_M) \\ \times \prod_{\alpha,l} \delta\Big(c_{\alpha,l,1-S} - c_{\alpha,l,2-S} - \sum_f \sigma x_{\alpha f}\Big)\, dx \end{aligned} \tag{9}$$

where the induction begins with $H_M{}^0 \equiv 1$. This gives the exact distribution of S-time outcomes of experiments on systems with certain M-time initial measurements, which is the ultimate objective of the theory.

This paper is mostly concerned with the ordinary (nonturbulent) hydrodynamic case in which fluctuations can be ignored, i.e., probability distributions for all variables are narrow and only mean values are important. Then instead of Q_M, I require only

$$[x]_c \equiv \int xQ_M(x|c)\, dx \tag{10}$$

the conditional (on $c_{\alpha lm}$) mean values of the transfers $x_{\alpha f}$. The error involved in neglecting fluctuations can be estimated from the cumulant[6] correlation

$$[x_{\alpha f}x_{\alpha' f'}]_c \equiv \int x_{\alpha f}x_{\alpha' f'}Q_M(x|c)\, dx - [x_{\alpha f}]_c[x_{\alpha' f'}]_c \tag{11}$$

(this is a mean square fluctuation if $\alpha f = \alpha' f'$). The algorithm for determining the evolution of the system then involves iterating the "equation of change":

$$c_{\alpha l0} \cong c_{\alpha l1} + \sum_f \sigma(f, l)[x_{\alpha f}]_c \tag{12}$$

which gives the $t = 0$ contents in terms of the $t = -\tau$ (and implicitly through $[x]_c$, all earlier) contents. In the proper limit (Section 8) this becomes a discretized Navier–Stokes equation.

4. PARAMETRIZATION

I now have a formally exact theory of hydrodynamics, expressed in terms of a joint probability $P_M(x; c)$ of transfers and contents for many cells and times. This is of no use unless I can find a parametrization, a way of approximating P_M by an analytic expression involving a few parameters. Ideally, I would prefer a *convergent* parametrization, that is, a sequence of parametrizations $P_M{}^i$ ($i = 1,\ldots$) which converges to the exact P_M, in the distribution sense.[7]

Begin by combining the arguments of P_M into a single variable:

$$u = \begin{pmatrix} x \\ c \end{pmatrix} \tag{13}$$

The number, energy, and momentum conservation laws impose linear constraints on the contents $c_{\alpha lm}$, defining a linear manifold in the space of vectors u (the "conservation manifold," or CM). Clearly, $P_M(u)$ vanishes off the CM. Thus (denoting total contents by $c_{\alpha m}^{\text{tot}}$) a factor

$$\delta(\text{CM}) \equiv \prod_{\alpha} \prod_{m=1}^{M-1} \delta(c_{\alpha m}^{\text{tot}} - c_{\alpha M}^{\text{tot}}) \tag{14}$$

can be extracted from $P_M(u)$:

$$P_M(u) = \delta(\text{CM}) S_M(u) \tag{15}$$

My problem is now to parametrize $S_M(u)$, which is less singular than P_M but still contains all nonequilibrium behavior of the system, under physical conditions ranging from a dilute gas to a close-packed solid. No few-parameter approximation to S_M can be valid for all these cases, so I look for a parametrization valid when the variables u are near their equilibrium values $\langle u \rangle$ for some temperature T and chemical potential μ. As usual,(8) these values are singled out by weighting the probability distribution by a factor $\exp[-(E^{\text{tot}} + \mu N^{\text{tot}})/kT]$. This gives a distribution

$$S_M^{\lambda}(u) \equiv S_M(u) \exp\Big(-\sum_{\alpha} c_{\alpha M}^{\text{tot}} \lambda_{\alpha}\Big) \tag{16}$$

where I have defined $\lambda_N \equiv \mu/kT$, $\lambda_E \equiv 1/kT$, and $\lambda_P \equiv 0$. This peaks for u near the equilibrium means $\langle u \rangle$, and there is reason to believe it is nearly Gaussian: In equilibrium statistical mechanics the probability distribution for the hydrodynamic contents of fairly large cells is known(8) to be nearly Gaussian, and it can be shown(9) by cluster-expansion techniques that this is true of the equilibrium joint distribution of hydrodynamic contents of large cells (at a single time) in a gas. Thus it is reasonable to hope that this is true for contents at *different* times and for transfers, so that $S_M(u)$ resembles a Gaussian centered at $\langle u \rangle$, i.e., an exponential of a quadratic function of u. Clearly this can be turned into a completely general expansion of S_M by developing the exponent in a Taylor series about $\langle u \rangle$. Defining the deviation from the mean

$$v \equiv u - \langle u \rangle \tag{17}$$

and defining a distribution P_M^{λ} from S_M^{λ} analogously to Eq. (15), this gives a parametrization

$$P_M^{\lambda} \equiv \delta(\text{CM}) \exp(-A^0 - A_j^1 v_j - A_{jk}^2 v_j v_k - A_{jkl}^3 v_j v_k v_l - \cdots) \tag{18}$$

Here the index j labels the components of u [Eq. (13)] [so $j = (\alpha f)$ or (αlm)] and the Einstein summation convention is used. Because Eq. (18) is relevant only on the CM, we may assume that for v orthogonal to the CM,

$$\sum_j A^i_{jk\ldots} v_j = 0 \tag{19}$$

With the assumption of symmetry under permutation of subscripts, this determines the parameters $A^i_{jk\ldots}$ uniquely.

It is important to understand the role of the thermodynamic fields (temperature and chemical potential) in this theory. It is well known that temperature is well defined only in thermal equilibrium, and yet I am trying to compute the evolution of a nonequilibrium system with a theory in which the parameters $A^i_{jk\ldots}$ and $\langle u_j \rangle$ depend on λ. This paradox exists also in continuum hydrodynamics, where it is a fundamental problem. In cell hydrodynamics, however, the paradox can be resolved: Although λ appears in the theory, it may be chosen arbitrarily. Each choice of λ produces different means $\langle u_j \rangle$ (hence a different definition of the deviation v_j), different Taylor-series coefficients $A^i_{jk\ldots}$, but the *same* distribution P_M. In essence, when I change λ, I merely expand the same function in a Taylor series about a different point. [It is instructive to work out a one-dimensional analog $S(u) = u$, where the logarithm of $S^\lambda(u) = ue^{-\lambda u}$ can be expanded about its maximum for each "temperature" λ; this exhibits many of the features of the general problem.]

Of course, even though λ is irrelevant in principle, in practice it is important to make a reasonably good guess (i.e., pick T, μ so that the corresponding thermal-equilibrium mean density and energy density are close to those of my actual system; if necessary, the evolution of each cell may be computed using a different λ, which may also change with time). If I make a poor choice of λ, the theory still converges exactly, but since the v's [Eq. (17)] are then not small, I will need many more terms in Eq. (18) to achieve adequate convergence.

5. HYDRODYNAMIC EQUATIONS OF CHANGE

I now have a parametrization of the basic function P_M of the hydrodynamic theory described in Section 3. It determines parametrizations of the other quantities defined there, the conditional probability Q_M [Eq. (7)] and the conditional mean transfers $[x]_c$ [Eq. (10)], which are required for actual hydrodynamic calculations. Rather than discuss Q_M, I will combine Eqs. (7), (10), and (16) to define[9] $[x]_c$ directly in terms of $P_M{}^\lambda$:

$$[x]_c = \int x P_M{}^\lambda(x; c)\, dx \Big/ \int P_M{}^\lambda\, dx \tag{20}$$

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[9] Mathematically, $[x]_c$ is a distribution over test functions $f(c)$ and should be defined more carefully, but I will just manipulate it formally here.

In order to use the parametrization (18) for $P_M{}^\lambda$, I rewrite this in terms of the deviations

$$\tilde{x} \equiv x - \langle x \rangle, \qquad \tilde{c} \equiv c - \langle c \rangle \tag{21}$$

which are the components of v [by Eqs. (18) and (17)]

$$v = \begin{pmatrix} \tilde{x} \\ \tilde{c} \end{pmatrix} \tag{22}$$

This gives

$$\begin{aligned} [\tilde{x}]_c = [x]_c - \langle x \rangle &= \int \tilde{x} P_M{}^\lambda(x, c)\, d\tilde{x} \Big/ \int P_M{}^\lambda\, d\tilde{x} \\ &= \int \tilde{x} \exp(-A_j{}^1 v_j - A_{jk}^2 v_j v_k \cdots)\, d\tilde{x} \Big/ \int \exp(-A_j{}^1 v_j \cdots)\, d\tilde{x} \end{aligned} \tag{23}$$

[using Eq. (18), and noting that A^0 and $\delta(\text{CM})$ cancel]. In trying to do the integrals in Eq. (23), one must remember that some of them are really sums, which I write as integrals only for convenience. If my cells are fairly large, however, the mean values of the integer variables (number contents and number transfers, C_{Nlm} and x_{Nf}) are fairly large, the distributions are smooth, and the sum is well approximated by an integral. This can be made precise, for any size cell, by use of the Poisson sum formula,⁽¹⁰⁾ which replaces the sum by a rapidly converging series of integrals, the first of which is the one I would get by naively taking the integral signs in Eq. (23) at face value. In this paper I will do just that, noting that the corrections are small and can be taken into account if necessary (in fact, by the same techniques described below; the only change is that $A_j{}^1$ acquires an imaginary part). Then the integrals are easy to cope with mathematically up to the quadratic terms; all Gaussians can be integrated in closed form by algebraic techniques. The rest of the terms are small, and can be dealt with by expanding part of the exponential in powers of the v_j:

$$\exp(-A_{jkl}^3 v_j v_k v_l - \cdots) = 1 - A_{jkl}^3 v_j v_k v_l - \cdots \tag{24}$$

This leaves me with an integral of a Gaussian times a polynomial, which can also be done in closed form; the problem again becomes an algebraic one. I shall not carry the terms beyond quadratic through the algebra, in order to arrive at useful results as simply as possible. But it seems certain they can be included in a consistent way; a similar expansion (restricted to variables at a single time) has been used by Wilson in deriving the renormalization-group recursion relations.⁽¹¹⁾ By including higher order terms, the present theory might be made useful even when the distribution is not nearly Gaussian, for example, for very small cells or for critical phenomena.

Dropping therefore the third and higher order terms in Eq. (23), I may simplify the notation by omitting the superscript from A^2 and denoting A^1 by B:

$$[x]_c = \int x \exp(-B_j v_j - A_{jk} v_j v_k)\, dx \Big/ \int \exp(-B_j v_j - A_{jk} v_j v_k)\, dx \tag{25}$$

Since the integral is over only some of the variables v_j (namely the $x_{\alpha f}$) and not over the $c_{\alpha l m}$, it is useful to decompose the matrix A into four submatrices in the manner suggested by Eq. (13),

$$A = \begin{pmatrix} A^{xx} & A^{xc} \\ A^{cx} & A^{cc} \end{pmatrix} \tag{26}$$

(so that A^{xc} has elements $A^{xc}_{jj'} = A_{(\alpha f)(\alpha' l' m')}$, etc.). Similarly,

$$B = \begin{pmatrix} B^{x} \\ B^{c} \end{pmatrix} \tag{27}$$

(with elements $B_j^{x} = B_{\alpha f}$, $B_j^{c} = B_{\alpha l m}$). Then the exponent in Eq. (18) can be similarly decomposed: If we denote by v^t the transpose of v and use Eq. (22),

$$A_{jk} v_j v_k = v^t A v = (\tilde{x}^t \tilde{c}^t) \begin{pmatrix} A^{xx} & A^{xc} \\ A^{cx} & A^{cc} \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{c} \end{pmatrix} = \tilde{x}^t A^{xx} \tilde{x} + \tilde{c}^t A^{cx} \tilde{x} + \tilde{x}^t A^{xc} \tilde{c} + \tilde{c}^t A^{cc} \tilde{c} \tag{28}$$

Treating $B^t v$ similarly, the integrand is just a multivariate Gaussian in $\tilde{x}$, which can be straightforwardly integrated$^{(12)}$ by diagonalizing A^{xx} (which is symmetric), giving eventually

$$[\tilde{x}]_c = -(A^{xx})^{-1}(A^{xc}\tilde{c} + \tfrac{1}{2}B^{x}) \tag{29}$$

The fluctuations about these conditional means can also be computed [Eq. (11)]:

$$[xx]_c = [\tilde{x}\tilde{x}]_c = \tfrac{1}{2}(A^{xx})^{-1} \tag{30}$$

If I define a matrix

$$g \equiv -(A^{xx})^{-1} A^{xc} \tag{31}$$

and observe (see Section 6) that in my Gaussian approximation B vanishes identically, I can rewrite (29) as

$$[\tilde{x}]_c = g\tilde{c} \tag{32}$$

which determines the hydrodynamic evolution of the system.

Computation of the evolution matrix g from (31) cannot be done by standard matrix techniques (even for the tiny system of Fig. 1, A^{xx} is 10×10

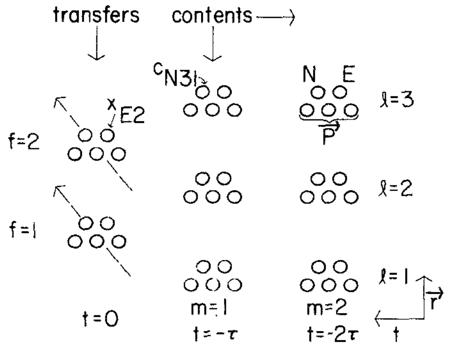

Fig. 1. Schematic diagram showing variables u_j for system with three cells $l = 1, 2, 3$ (stacked linearly so they are connected by two faces $f = 1, 2$), for $M = 2$. Each point (i.e., open circle) corresponds to one variable. Two are labeled, with indices $j = (\alpha, f) = (E, 2)$ [$u_j = x_{E2}$ = energy transfer across face 2, from cell 2 to cell 3, during $(-\tau, 0)$] and $j = (\alpha, l, m) = (N, 3, 1)$ ($u_j = c_{N31}$ = number content of cell 3 at time $-\tau$). Dashed arrows indicate direction of transfers.

and A^{xc} and g are 10×30). But the intuitive considerations of Section 2 suggest the A's are short-ranged in space and time.[10] If $(A_{xx})^{-1}$ is also short-ranged, one should be able to compute g using only nearby A's. It turns out there is a simple algorithm for doing this, which is best described geometrically. First, rewrite Eq. (31) as

$$\sum_{j'=(\alpha f)} A^{xx}_{jj'} g_{j'k} = -A^{xc}_{jk} \tag{33}$$

Note that each entry $A_{jj'}$ in A corresponds to a pair of points in Fig. 1; associate $A_{jj'}$ with a line connecting these two points, as in Fig. 2. Then A^{xx} connects pairs of points that are both on the left (i.e., transfers); A^{xc} and g connect points on the left to points on the right. Note that the $g_{j'k}$ with a fixed k can be computed independently of other g's [in other words, the matrix equation (33) can be solved independently for each column of g and A^{xc}]. So I begin the algorithm by fixing k (which I call the base point). The g_{jk} I want to calculate may be depicted as vectors with base point k and various end points j. I must decide on a set S_k of end points j for which I will calculate g_{jk} (these will be near k in space and time; S_k could be just the set

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[10] Meaning a component A_{jk} is small unless j is close to k in space and time. Note, however (Section 6), that A^{cc} is not short-ranged in space; fortunately it does not appear in Eq. (29) or Eq. (30). In fact these long-range problems cancel out of the theory completely (not just in the special case treated here); it is not hard to see that all coefficients $A^{\vdots}_{jk}\ldots$ with $j, k, \ldots$ all content variables (this is the long-ranged part of A) cancel out of Q_M exactly. This confirms (and makes precise) the intuitive expectation of Section 2 that Q is "short-ranged," even though P_M is not.

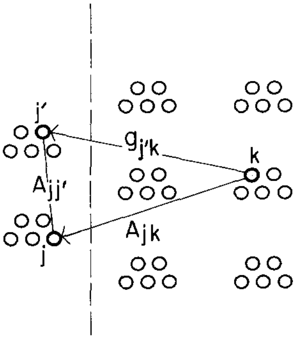

Fig. 2. Illustration (based on Fig. 1) of algorithm for determining evolution matrix g. Dashed line separates transfers from contents.

for which I know A_{jk}). Then for $j \in S_k$, Eq. (33) (with the sum restricted to $j' \in S_k$) is a linear relation among the $g_{j'k}$ with various end points j' (in which presumably g_{jk} has the largest coefficient A_{jj}; all coefficients $A_{jj'}$ may not be known, but I presume the large ones are, and the rest may be assumed to vanish). Repeating this for all $j \in S_k$ gives a system of linear equations, which can be solved, for example, by Gaussian elimination, taking j's in the order of increasing A_{jk}. As the set S_k becomes larger, the accuracy improves; when it includes all j's in the system, the algorithm is exact. Repeating the algorithm for each k eventually gives the entire matrix g.

The evolution matrix g computed by this procedure determines the hydrodynamic evolution of the system through Eq. (32) and the equations of change (12).

6. PARAMETER DETERMINATION

In order to compute the evolution matrix g by the technique of Section 5, I must know the parameters $A^i_{jk\ldots}$ and $\langle u_j \rangle$ of the distribution $P_M{}^\lambda$ [Eqs. (18) and (24)]. In a practical calculation on a macroscopic system, I want to use cells which are smaller than the scale on which the bulk hydrodynamic variables are expected to change, but which are still macroscopic and contain very many particles. Clearly there is no point trying to calculate the distribution P_M directly for macroscopic cells. That is essentially the same many-body problem I started with, merely rephrased. But as we shall see below, it *is* practical to determine the parameters of P_M for small cells. And clearly these contain *more* information than does P_M for large cells. In fact, there is a well-defined scaling[11] procedure for calculating a large-cell distribution from a smaller cell one. Suppose I know the parameters A and $\langle u \rangle$, which determine the distribution $P_M(x; c)$ of transfers x and contents c for cells of

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[11] The idea of scaling has been much discussed in the context of equilibrium critical phenomena (see Ref. 13).

length L at times separated by τ. Then if I want $P_M'(x'; c')$, the probability of finding transfers x' and contents c' for larger cells of length $2L$, I can compute it by enumerating all choices of x and c that give the desired x' and c' (clearly each x, c determines a unique x', c'; I need only add up a few small-cell contents or transfers to get each large-cell one) and summing the corresponding probabilities $P_M(x; c)$. This procedure can be turned into a scaling algorithm for computing the parameters A' and $\langle u' \rangle$ (which determine P_M') from the smaller scale parameters A and $\langle u \rangle$. It is also necessary to be able to do time-scaling. However, a detailed discussion of scaling will be deferred to a later paper$^{(14)}$ because it turns out that a limiting case of the theory which is already of some practical interest (giving the Navier–Stokes equation and the transport coefficients) can be worked out without it.

Assuming that the results can be properly scaled up, I address the problem of determining the parameters of the probability distribution for microscopic cells having a relatively small number of particles. Ideally, one would like to do this directly from the microscopic equations of motion. However, that approach may require considerable work, so I concentrate here on an alternative method which makes use of the already well-developed technique of molecular dynamics,$^{(15)}$ i.e. computer simulation of the behavior of equilibrium systems. The idea is to use equilibrium time-correlations calculated by molecular dynamics to determine the parameters $A^{i}_{jk\ldots}$ and $\langle u_j \rangle$ of my theory. The distribution $P_M{}^{\lambda}$ parametrized by A and $\langle u \rangle$ is exactly a thermal-equilibrium distribution for variables $x_{\alpha f}$ and $c_{\alpha l m}$ at different times, so the equilibrium correlations of these variables can certainly be obtained in terms of A and $\langle u \rangle$. By setting these equal to the correlations determined by molecular dynamics, I should be able to solve for the A's (and of course molecular dynamics gives $\langle u \rangle$ directly).

An observation is necessary about the general relationship between time-correlation functions (TCF) and hydrodynamic equations of motion. Clearly, the equations of motion (hence the transport coefficients) determine the fluid motions which are reflected in the TCF. Therefore the TCF, though they are much more complicated than the transport coefficients, contain no more information (at least not on a coarse scale); they therefore contain this information in a highly redundant way. There ought thus to be many ways to extract it; one is the Green–Kubo$^{(16)}$ approach, expressing the transport coefficient as a time integral of a TCF. This is somewhat hard to apply because the "long-time tail"$^{(17)}$ of the TCF makes it necessary to use a very large molecular-dynamics system which can be followed for a long time. It would be preferable to extract the transport coefficients from only the short-time, short-distance behavior of the TCF. That will be achieved by the present approach if the A's are short-ranged in time.

The time correlations obtainable from molecular dynamics are of the form

$$\langle u_j u_k \cdots \rangle \equiv \int u_j u_k \cdots P_M{}^\lambda(u)\, du \Big/ \int P_M{}^\lambda\, du \tag{34}$$

These can be specified more economically by giving the cumulant correlations $W^i_{jk\dots}$, defined inductively by

$$\langle u_j u_k \cdots \rangle = \sum W^i_{a,b,\dots} W^{i'}_{a',b',\dots} \cdots \tag{35}$$

where the sum is over all distinct partitions of the set $\{j, k, \dots\}$ into subsets $\{a, b, \dots\}$, $\{a', b', \dots\}, \dots$ with $i, i', \dots$ elements, respectively.[12] The first of these are

$$W_j{}^1 = \langle u_j \rangle, \qquad W^2_{jk} = \langle u_j u_k \rangle - \langle u_j \rangle \langle u_k \rangle \tag{36}$$

It is not hard to show that the cumulants obtained by using v (the deviation of u from equilibrium) instead of u in Eq. (35) or Eqs. (36) are the same except for the first; obviously

$$\langle v_j \rangle = 0 \neq W_j{}^1 \tag{37}$$

Below, I shall use v to compute W^i $(i > 1)$. Thus I need to calculate means like

$$\langle v_j v_k \cdots \rangle \equiv \int P_M{}^\lambda v_j v_k \cdots dv \Big/ \int P_M{}^\lambda\, dv \tag{38}$$

Using the parametrization (25) for $P_M{}^\lambda$ gives integrals of the form

$$\int \delta(\mathrm{CM})\, [\exp(-A^0 - A^1_{j'} v_{j'} - \cdots)] v_j v_k \cdots dv \tag{39}$$

Treating these analogously to the integrals of Section 5, I evaluate the sums over discrete v_j by the Poisson sum formula, and retain only the leading term. This is equivalent to treating the sums as integrals, and the Kronecker delta functions as Dirac ones. The delta function on the conservation manifold can be handled by decomposing v into components in CM and its orthogonal complement OC:

$$v = v_{\mathrm{CM}} + v_{\mathrm{OC}} \tag{40}$$

It is intuitively clear that $\delta(\mathrm{CM})$ is essentially $\delta(v_{\mathrm{OC}})$ since $v_{\mathrm{OC}} = 0$ defines the CM. This can be made precise by defining orthonormal bases for the CM and the OC, and transforming to an integral with respect to these coordinates; $dv = dv_{\mathrm{CM}}\, dv_{\mathrm{OC}}$. Then $\delta(\mathrm{CM})$ is $\delta(v_{\mathrm{OC}})$ except for a constant

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[12] If any of the indices $j, k, \dots$ are to be taken to be equal, it is important to enumerate the distinct partitions *before* substituting values for $j, k, \dots$. The definition (35) can be shown to be equivalent to the standard definition.(6) The form (35), which seems to be useful in physical problems, I have not seen written except in Ref. 19.

factor, a Jacobian determinant which cancels out of the ratio (38). So the integral over $v_{\rm OC}$ is trivial, and expression (39) becomes

$$\int [\exp(-A^0 - A^1_{j'}v_{j'} - \cdots)]v_jv_k \cdots dv_{\rm CM} \tag{41}$$

where the integrand is evaluated at $v_{\rm OC} = 0$. As in Section 5, I can expand the part of the exponential beyond A^2, getting a series of integrals having the form (41) with only a quadratic exponent, which can be evaluated in closed form. In this paper, however, I drop the terms beyond quadratic, leaving

$$\int [\exp(-A^0 - A^1_{j'}v_{j'} - A^2_{j'k'}v_{j'}v_{k'})]v_jv_k \cdots dv_{\rm CM} \tag{42}$$

I can now evaluate Eq. (38) by performing the simplifications (39)–(42) on both numerator and denominator. Since the cumulants of a Gaussian distribution vanish beyond second order,$^{(18)}$ I need only

$$\begin{aligned}\langle v_jv_k\rangle = &\left\{\int [\exp(-A^0 - A^1_{j'}v_{j'} - A^2_{j'k'}v_{j'}v_{k'})]v_jv_k\, dv_{\rm CM}\right\}\\ &\div \left[\int \exp(-A^0 - A^1_{j'}v_{j'} - A^2_{j'k'}v_{j'}v_{k'})\, dv_{\rm CM}\right]^{-1}\end{aligned} \tag{43}$$

Dropping the superscript on A^2, writing A^1 as B, cancelling A^0, and using the matrix notation of Section 5, this is the j, k component of the matrix

$$\langle vv^t\rangle = \int [\exp(-v^tAv - B^tv)]vv^t\, dv_{\rm CM}\Big/\int \exp(-v^tAv - B^tv)\, dv_{\rm CM} \tag{44}$$

All these matrices may be written either in terms of my original components of v (i.e., $\tilde{x}_{\alpha f}$, $\tilde{c}_{\alpha lm}$) or in terms of the new orthonormal bases of CM and OC. Clearly the latter is more appropriate for doing the integral over $v_{\rm CM}$, which is defined in these bases. It can be done by the same method as in the last section, involving diagonalizing A. Note that A maps CM into CM and vanishes on OC by Eq. (26), so I can find eigenvectors which are all either in CM or in OC; those in OC have eigenvalue zero. Then I can do the integrals in (44) regarding A as a matrix on CM only [note that Eq. (19) gives $B \in$ CM]; the standard technique$^{(12)}$ gives

$$\langle vv^t\rangle = \tfrac{1}{2}A^{-1} \tag{45}$$

[Note this is the cumulant W^2 [Eq. (36)] because $\langle v\rangle = 0$.] Computing $\langle v\rangle$ from an analog of Eq. (44) gives

$$\langle v\rangle = -\tfrac{1}{2}A^{-1}B \tag{46}$$

whose vanishing determines B:

$$B = 0 \quad (=A_j{}^1) \tag{47}$$

Equation (45), which determines A, may be rewritten

$$\langle vv^t \rangle A = \tfrac{1}{2} I^{\mathrm{CM}} \tag{48}$$

where I^{CM} is the identity matrix on CM. The linear operator equation (48) (which is so far defined only on CM) may be extended to all of u-space by noting that both matrices on the left side vanish on OC (obviously equilibrium averages satisfy the conservation laws) and arbitrarily defining I^{CM} on the right to vanish on OC. Thus I^{CM} becomes a projection operator onto CM; if I can express this in terms of my original basis, I may write Eq. (48) in this basis as

$$\sum_{j'} W_{jj'} A_{j'k} = \tfrac{1}{2} I_{jk}^{\mathrm{CM}} \tag{49}$$

(I have replaced $\langle vv^t \rangle$ by W^2 and dropped the superscript.)

It is not hard to define an explicit orthonormal basis for CM (for example, by Fourier transform), say $\{e^q\}$. Then the projection operator can be written

$$I_{jk}^{\mathrm{CM}} = \sum_q e_j{}^q e_k{}^q \tag{50}$$

In principle Eq. (49) can then be solved for $A_{j'k}$. In practice, I must find an algorithm like that of Section 5 which determines $A_{j'k}$ from "nearby" $W_{jj'}$ and I_{jk}^{CM} and depends on all these being short-ranged in space and time. It is not obvious from Eq. (50) that I_{jk}^{CM} is short-ranged, and in fact it is not; this is a consequence of the conservation laws, which couple contents of cells over large distances. But they do not restrict the transfers, so one might hope that the components I_{jk}^{CM} where j or k refers to a transfer variable [i.e., has the form (αf)] are short-ranged. In fact, they are not only short-ranged, they are trivial:

$$I^{\mathrm{CM}}_{(\alpha f)(\alpha l m)'} = I^{\mathrm{CM}}_{(\alpha l m)'(\alpha f)} = 0, \qquad I^{\mathrm{CM}}_{(\alpha f)(\alpha f)'} = \delta_{\alpha\alpha'}\, \delta_{ff'} \tag{51}$$

That is, I^{CM} acts as the identity matrix on vectors v whose content components vanish; to see this, note that such a v trivially satisfies the conservation laws, so $v \in \mathrm{CM}$ and the projection I^{CM} leaves it unchanged.

Fortunately, this partial knowledge of I^{CM} is enough to attack Eq. (49), because it can be solved column by column in I^{CM} and A. That is, a column of I^{CM} (I_{jk}^{CM} for all j, fixed k) determines the same column of A. So I can obtain A_{jk} only when k is a transfer variable; in the notation of Section 5, I get A^{xx} and A^{cx} (and A^{xc} since A is symmetric) but not A^{cc}. Fortunately, as observed in Section 5, this is all I need.

The algorithm for solving Eq. (49) is exactly analogous to that of Section 5, and may be described geometrically in terms of Fig. 3. After fixing a base

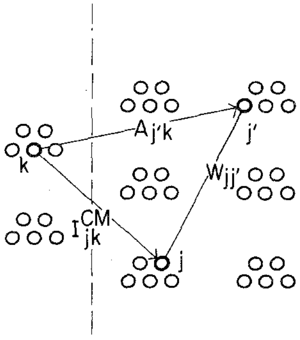

Fig. 3. Illustration (based on Fig. 1) of algorithm for determining parameters A.

point k (which must be on the left, i.e., a transfer) I decide what set S_k of end points j to compute A_{jk} for (perhaps those for which W_{jk} is known; note that j is allowed to be anywhere, not just on the right as shown in Fig. 3). For each $j \in S_k$, Eq. (49) (summed over $j' \in S_k$) is a linear relation among the $A_{j'k}$. Using Eq. (51) for the inhomogeneous terms I^{CM}, this system of linear equations can be solved for $A_{j'k}$. Doing this for all $k = (\alpha f)$ yields all components of A needed to determine the hydrodynamic equations of change of Section 5.

The net result of this section has been to give an algorithm for determining from the molecular dynamics data W^i (the cumulant equilibrium time-correlations, used here only for $i \leqslant 2$) the parameters A and $\langle u \rangle$ needed for computing (by the method of Section 5) the hydrodynamic evolution of a system.

7. INFINITE-SYSTEM LIMIT; SYMMETRY

The theory developed in the previous sections describes a system with periodic boundary conditions. It is physically relevant only in the infinite-system limit, which possesses complete rotational and translational symmetry. Clearly this simplifies the specification of the parameters A_{jk} and the cumulants W_{jk}; these depend only on the *relative* positions of the cells referred to by the indices j and k.

To make this precise, consider the rotational and translational invariances of the system. Since these must preserve the cell structure, the invariance group G is that of a simple cubic lattice: the product of the octahedral group (O_h in Schoenflies notation) and the group of translations whose components are multiples of L. The action of a transformation $R \in G$ on an index j (either α, l, m or α, f) can be defined in an obvious way: R takes l into some other cell and f into some other face, and takes α into itself if α is N or E. If α is P_x, P_y, or P_z, then R (whose rotational part determines a unique permutation of the x, y, and z axes) performs this same permutation on P_x, P_y, and P_z.

Clearly, transforming both indices of A_{jk} should not change its numerical value, except perhaps its sign. The sign changes, for example, if α is P_x, and R takes the x axis into the *negative* y axis. A sign change can also arise in rotating a face, if the conventional direction of positive flow is thereby reversed. If I denote the product of these signs by $\rho(R, j)$ ($= \pm 1$), the transformation law for the parameters $A^i_{jk\ldots}$ can then be shown to be

$$A^i_{jk\ldots} = A^i_{Rj,Rk,\ldots}\rho(R, j)\rho(R, k)\cdots \tag{52}$$

To exploit the fact that A is also symmetric under subscript permutation, define a group G_i which is the product of the rotation–translation group G and the permutation group of i indices. This group acts on index lists $(j, k, \ldots)$ and determines equivalence classes of such lists. Label the classes by $n = 1, 2, 3, \ldots$ and choose from the nth class (whose lists have length $i[n]$, say) an arbitrary (but fixed) representative $(j, k, \ldots)[n]$. Then the number

$$A[n] \equiv A^{i[n]}_{(j,k,\ldots)[n]} \tag{53}$$

determines [via Eq. (52)] A for all other index lists $(j'k'\cdots)$ in the nth class:

$$A^i_{(j'k'\ldots)} = \rho(j'k'\cdots)A[n] \tag{54}$$

Here $\rho(j'k'\cdots)$ is defined to be the product of the ρ's in Eq. (52) for the R taking $(j'k'\cdots)$ into $(jk\cdots)[n]$. Thus the entire array $A^i_{jk\ldots}$ can be represented in terms of a much smaller collection of numbers $A[n]$, one for each equiv-

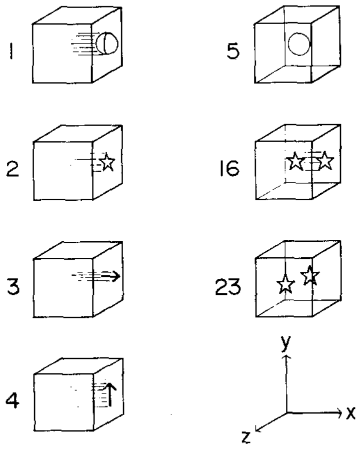

Fig. 4. Pictorial representation of some equivalence classes of index lists, numbered as in Table IB. Number, energy, and momentum variables are represented by open circles, stars, and appropriately directed arrows. Light lines indicate direction of transfers (across right-hand face).

alence class of index lists. Some of these equivalence classes are listed in Tables IA and IB; a few are depicted pictorially in Fig. 4. It is very useful to visualize an equivalence class as a cluster of i objects, bound rigidly to each other but capable of being relocated on the cell lattice by rotations and translations. Then the standard representative of the class corresponds to a particular unique position and orientation in the lattice, and all other positions and orientations correspond to other members of the class.

The other quantities in the theory are similarly simplified by symmetry; the cumulant correlations $W^i_{jk\ldots}$ can be represented by a smaller set of numbers $W[n]$, and the evolution matrix g_{jk} by $g[n]$ (note that $i[n]$ must be 2 here).

I now want to incorporate symmetry into the algorithms of Sections 5 and 6. Some reflection on the effect of symmetry on the algorithm (Section 5) for computing the evolution matrix g from A shows that we should proceed as follows: Pick an equivalence class n_0 for the base point (demanding $i[n_0] = 1$ and that the representative index $k \equiv j[n_0]$ be a content variable). Decide on a set $S(n_0)$ of equivalence classes n_2 for which we wish to calculate $g[n_2]$. Thinking of n_2 as a relocatable cluster of two points, we require that one point be locatable at k and that the other (the end point) be a transfer variable. (The set of possible positions j for the end point is the set S_k of Section 5.) Then pick some $n_1 \in S(n_0)$, and choose a particular way of attaching it to the base point k, i.e., choose a particular (j, k) in class n_1. For each n_0 and n_1 we get a linear equation in the $g[n_2]$ $[n_2 \in S(n_0)]$. To get the coefficient of $g[n_2]$ for some particular n_2, find all possible ways of relocating the cluster n_2 so one point remains the base point k, i.e., all ways of pivoting n_2 about the base point, giving different end points j'. For each j', determine the equivalence class n of (j, j'), and include a term [derived from Eqs. (33) and (54)]

$$\rho(j, j')\rho(j', k)A[n]g[n_2] \tag{55}$$

in the linear equation. The inhomogeneous term on the other side is

$$-\rho(j, k)A[n_1] \tag{56}$$

Repeat this for every n_1 and solve the resulting equations for g. Then start over with a new base point n_0, eventually getting all components of g.

The algorithm for computing A from W (Section 6) is very similar. This time choose the base point n_0 so its representative k is a transfer variable. The classes $n_2 \in S(n_0)$ should have base point k, but any end point is allowed. Determine a linear equation for each $n_1 \in S(n_0)$ (located at j, k) by taking

Table IA. Cells and Faces Used in Calculation of Section 8

Cells		Faces	
Label l	Coordinates of center	Label f	Cells connected[a]
1	$(0, 0, 0)$	1	1, 2
2	$(L, 0, 0)$		

[a] Conventional direction of positive flow is from the first cell listed to the second.

Table IB. Equivalence Classes of Index Lists[a]

Label n	Length $i[n]$	Representative list $(jk\ldots)[n]$
1	1	$(N1)$
2	1	$(E1)$
3	1	(P_x1)
4	1	(P_y1)
5	1	$(N11)$
6	1	$(E11)$
7	1	(P_x11)
8	2	$(N1), (N1)$
9	2	$(E1), (E1)$
10	2	$(P_x1), (P_x1)$
11	2	$(P_y1), (P_y1)$
12	2	$(N1), (N11)$
13	2	$(N1), (E11)$
14	2	$(N1), (P_x11)$
15	2	$(E1), (N11)$
16	2	$(E1), (E11)$
17	2	$(E1), (P_x11)$
18	2	$(P_x1), (N11)$
19	2	$(P_x1), (E11)$
20	2	$(P_x1), (P_x11)$
21	2	$(P_y1), (P_y11)$
22	2	$(N11), (N11)$
23	2	$(E11), (E11)$
24	2	$(P_x11), (P_x11)$

[a] All classes of one-index lists are given, with those two-index lists meeting the criteria described in the text for $W[n]$ to be important. Seven are omitted because $W[n] = A[n] = 0$ by symmetry [Eq. (52) gives $A = -A$ for some R].

all $n_2 \in S(n_0)$ and pivoting each in all possible ways about the base point; for each position (j', k), determine the class n of (j, j') and add

$$\rho(j, j')\rho(j', k)W[n]A[n_2] \tag{57}$$

to the equation, which has an inhomogeneous term 1/2 on the other side only if $j = k$ (i.e., n_1 has the same index twice).

The end result of these two algorithms is $g[n]$. To calculate the evolution of a system, one must compute the conditional mean transfers, which are expressed [Eq. (32)] in terms of g_{jk}. The procedure for determining a mean transfer $[\tilde{x}_j]_c$ from $g[n]$ is as follows: Determine the class n_0 of the base point j. Define the set $S(n_0)$ of equivalence classes n for which $g[n]$ is important (these should have $i[n] = 2$ and be locatable on the base point j, with the end point k being a content variable). For each $n \in S(n_0)$, and each way of pivoting n about j (i.e., each end point k) there is a term

$$\rho(j, k)g[n]\tilde{c}_k \tag{58}$$

in $[\tilde{x}_j]_c$.

All these algorithms will be carried out for a simple case in the next section.

8. APPLICATIONS: NAVIER–STOKES AND ENERGY FLOW EQUATIONS

The theory described in the previous sections is best suited for machine calculation,[13] especially if small cells are used so correlations extend over several cells. However, it turns out that simple approximations can be worked out by hand, so in this section I work out the theory for the simplest reasonably nontrivial approximation. It turns out that the circumstances (described below) under which this approximation is good are exactly those under which one intuitively expects the phenomenological linearized equations of continuum hydrodynamics (in a discretized form) to be valid. Since the resulting equations are, in fact, such discretized continuum equations (the continuity, Navier–Stokes, and energy-flow equations), in some sense this constitutes an a priori derivation of the continuum equations. Discussion of the exact sense in which they can be proved (or are true) must await analysis of their scaling properties.

Consider then the infinite-system limit described in Section 7 (i.e., consider fluid behavior far from boundaries in space and initial conditions in time). Assume the cells are large enough that the smoothing of the number variables and the restriction to Gaussian correlations ($i \leqslant 2$) of Sections 5 and 6 are valid ($i \leqslant 2$ also requires assuming deviations from equilibrium to

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[13] In fact a very similar algorithm, in a completely different context, has been programmed and used by the author (see Ref. 19).

be small). Assume also that fluctuations [Eq. (30)] are small enough (the system is not, for example, near a critical point) that only the mean values [Eq. (32)] need be computed, via the evolution matrix g [Eq. (31)]. (Clearly, if any of these assumptions were violated, one could not expect the linearized continuum equations to apply.) Under these circumstances, equilibrium statistical mechanics^(9) shows that the cumulant correlation $W_{\alpha l1,\alpha' l'1}$ is much smaller[14] for $l \neq l'$ than for $l = l'$, that is, that content variables in different cells are weakly correlated. It is likely that this is also true of transfers: $W_{\alpha f,\alpha' f'}$ is small unless $f = f'$. In this paper I make the further assumption[15] that $\alpha = \alpha'$ in the above W's. As for correlations between contents and transfers, the largest will clearly be between $c_{\alpha l1}$ and $x_{\alpha' f}$, where f is a face of cell l; I assume these may be important for all α and α'. These considerations determine which index pairs jk give significant W_{jk}; all equivalence classes of such pairs are listed in Table IB ($n = 8, \ldots, 24$). Since W determines A (Section 6) and g (Section 5), I assume A_{jk} and g_{jk} also are important only for these pairs. This uniquely determines the index-pair sets $S(n)$ of Section 7 (i.e., S_k of Sections 5 and 6), which determines my approximation uniquely via the algorithms of Section 7.

Application of the algorithms is now completely mechanical, and proceeds as follows. In calculating A from the equilibrium correlations W, the possible classes of base points are $n_0 = 1, 2, 3, 4$. Take $n_0 = 1$ first, so $k = (N1)$. Scanning Table IB for two-index lists containing k shows $S(n_0) = \{8, 12, 13, 14\}$. Obtain first the linear equation [Eq. (62a) below] for $n_1 = 8$; for this class the end point j is superimposed on the base point k as in Fig. 5a. To get the term corresponding to $n_2 = 8$, attach n_2 to the base point; there is only one way to do this, giving $j, j' = (N1)(N1)$, again in class 8 (so $n = 8$). The term (57) is then

$$W_8 A_8 \tag{59}$$

(In this section I write W_8 for $W[8]$, since the argument has no subscripts.) The sign factor is $+1$. For the next terms n_2 takes the next value in $S(n_0)$, $n_2 = 12$. Attaching n_2 at the base point k, its end point j' may pivot into two positions, $j' = (N11)$ or $(N21)$, as shown in Figs. 5b and 5c, respectively. The first gives $j, j' = (N1)(N11)$, which is the standard representative of class $n = 12$. The sign is $+1$, so our term is

$$W_{12} A_{12} \tag{60}$$

The second j' (Fig. 5c) gives $(j, j') = (N1)(N21)$, which is also in class $n = 12$ but requires a nontrivial rotation R (perhaps by π about an axis in the face f)

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[14] By one or more powers of the ratio, range of interparticle potential/L.

[15] Removing this assumption adds only two index pairs to Table IB (number-energy correlations for contents and transfers), somewhat increasing the algebraic labor.

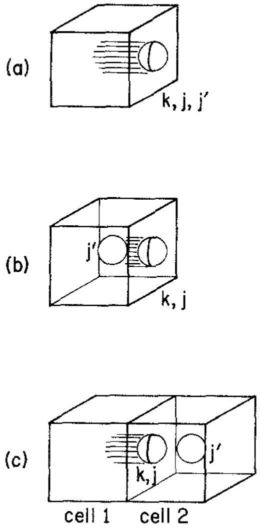

Fig. 5. Visual aids for deriving (a) Eq. (59), (b) Eq. (60), (c) Eq. (61). Symbols have meanings of Fig. 4.

to reach its standard position. This reverses the conventional direction of positive flow through the face, introducing a minus sign into $\rho(j, j')$ as discussed in Section 7. But since $\rho(j', k)$ is identical, the signs cancel and we have another term

$$+ W_{12}A_{12} \tag{61}$$

Proceeding in this manner through $n_2 = 13$ and 14, and including the inhomogeneous term 1/2 (since $j = k$ for $n_1 = 8$), we get the $n_1 = 8$ equation

$$W_8A_8 + 2W_{12}A_{12} + 2W_{13}A_{13} + 2W_{14}A_{14} = 1/2 \tag{62a}$$

Turning next to the equation for $n_1 = 12$, we find a term $W_{12}A_8$ for $n_2 = 8$. The next value $n_2 = 12$ gives a cluster which can be pivoted in two different ways, giving $(jj') = (N11, N11)$ and $(N11, N21)$. The former is in class $n = 22$, giving a term $W_{22}A_{12}$. The class of the latter is not listed in Table IB because it does not satisfy the importance criteria established at the beginning of this section. The $n_2 = 15$ and 18 terms vanish similarly, and the inhomogeneous term vanishes since the indices of n_1 are distinct, giving

$$W_{12}A_8 + W_{22}A_{12} = 0 \tag{62b}$$

Similarly $n_1 = 13$ and 14 give

$$W_{13}A_8 + W_{23}A_{13} = 0 \tag{62c}$$

$$W_{14}A_8 + W_{24}A_{14} = 0 \tag{62d}$$

We now have four equations in the four unknowns A_8, A_{12}, A_{13}, and A_{14}. These can be solved to give

$$A_8 = 1/2(W_8 - 2W_{12}^2/W_{22} - 2W_{13}^2/W_{23} - 2W_{14}^2/W_{24}) \tag{63}$$

and similar equations for the other variables. We now have the A's corresponding to $n_0 = 1$. Taking $n_0 = 2$ gives $S(2) = \{9, 15, 16, 17\}$, hence equations for A_9, A_{15}, A_{16}, and A_{17}. Then $S(3) = \{10, 18, 19, 20\}$ and $S(4) = \{11, 21\}$ give the remaining six variables. (As discussed in Section 6, A_{22}, A_{23}, and A_{24} are not computed.)

Next we must carry out the algorithm for computing g from A. This is quite simple, because most of the n's we get couple two different transfers, and such A_n have been presumed to vanish. Each equation is left with only one homogeneous term; the first (using $n_0 = 5$, $n_1 = 12$) is

$$A_8 g_{12} = -A_{12} \tag{64}$$

This gives immediately

$$g_{12} = -A_{12}/A_8 = +W_{12}/W_{22} \tag{65a}$$

[Using Eq. (62b); note it was unnecessary to solve for the A's, in this simple case.] It turns out that

$$g_{13} = W_{13}/W_{23} \tag{65b}$$

and the equations for $g_{14}, \ldots, g_{21}$ are similar; the subscripts in the denominator are 24, 22, 23, 24, 22, 23, 24, and 24, respectively.

We can now calculate the evolution of a system by determining the conditional mean transfers [Eq. (32)]. Equations for these are obtained from the last algorithm of Section 7. There are four nonequivalent transfers ($n_0 = 1, 2, 3, 4$). Taking $n_0 = 1$ (the class of number transfers), we compute the representative transfer $[\tilde{x}_j]_c$ (with $j = N1$) across face 1. (The equations for other faces will be obtainable by translation and rotation.) The relevant index pairs comprise $S(1) = \{12, 13, 14\}$. The first class $n = 12$ can be pivoted in two ways about j (corresponding to Figs. 5b and 5c except for labeling), giving $k = (N11)$ and $(N21)$. The corresponding terms (58) are

$$+g_{12}\tilde{c}_{N11} - g_{12}\tilde{c}_{N21} \tag{66}$$

[the minus sign arises from the same rotation discussed in connection with Eq. (61)]. The $n = 13$ and 14 terms are obtained similarly, giving the $n_0 = 1$ equation

$$[\tilde{x}_{N1}]_c = g_{12}(\tilde{c}_{N11} - \tilde{c}_{N21}) + g_{13}(\tilde{c}_{E11} - \tilde{c}_{E21}) + g_{14}(\tilde{c}_{P_x11} + \tilde{c}_{P_x21}) \tag{67a}$$

(The different sign in the third term arises because the rotation reverses the x momentum.) Letting $n_0 = 2$, 3, and 4 gives the equations

$$[\tilde{x}_{E1}]_c = g_{15}(\tilde{c}_{N11} - \tilde{c}_{N21}) + g_{16}(\tilde{c}_{E11} - \tilde{c}_{E21}) + g_{17}(\tilde{c}_{P_x11} + \tilde{c}_{P_x21}) \tag{67b}$$

$$[\tilde{x}_{P_x1}]_c = g_{18}(\tilde{c}_{N11} + \tilde{c}_{N21}) + g_{19}(\tilde{c}_{E11} + \tilde{c}_{E21}) + g_{20}(\tilde{c}_{P_x11} - \tilde{c}_{P_x21}) \tag{67c}$$

$$[\tilde{x}_{P_y1}]_c = g_{21}(\tilde{c}_{P_y11} - \tilde{c}_{P_y21}) \tag{67d}$$

These equations determine the evolution of the system via the equations of change (12).

The above equations are the main result of this paper, and constitute a solution to the problem posed in the introduction, namely the construction of a consistent, completely discrete theory of hydrodynamics, which becomes exact as more terms are included. However, it is interesting to look at continuum approximations to the theory to see whether the phenomenological continuum equations are obtained in the appropriate limit. Consider the linearized continuum equations for density $n(x, t)$, energy density $\epsilon(x, t)$, and monentum density $\mathbf{p}(x, t)$, in the following form[16]:

$$\frac{dn}{dt} = -\nabla\cdot\mathbf{j} \qquad \text{(continuity equation)} \tag{68a}$$

$$\frac{d\epsilon}{dt} = -\nabla\cdot\mathbf{q} \qquad \text{(energy-flow equation)} \tag{68b}$$

$$\frac{d\mathbf{p}}{dt} = -\nabla\cdot\Pi \qquad \text{(Navier–Stokes equation)} \tag{68c}$$

The particle flux $\mathbf{j}$, energy flux $\mathbf{q}$, and momentum flux tensor Π are given in terms of n, ϵ, and $\mathbf{p}$ by

$$\mathbf{j} = (1/m)\mathbf{p} \tag{69a}$$

$$\mathbf{q} = -\kappa\,\nabla T(n, \epsilon) + (\epsilon + \Pi_0)\mathbf{p}/nm \tag{69b}$$

$$\Pi = \Pi_0 1 - 2\eta\Lambda - (\zeta - \tfrac{2}{3}\eta)\,\mathrm{tr}\,\Lambda\, 1 \tag{69c}$$

Here, m is the particle mass, κ is the thermal conductivity, $T(n, \epsilon)$ is the temperature (equilibrium equation of state), Π_0 is the isotropic pressure, η is the shear viscosity, ζ is the bulk viscosity, and Λ is the symmetric part of the tensor $\nabla\mathbf{p}/nm$, with trace tr Λ. Note that $\mathbf{p}/nm$ is just the local fluid velocity.

To relate my discrete equations (67a)–(67d) to these continuum equations, I must express the content and transfer variables approximately in terms of

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[16] These are obtained from the full nonlinear equations(1) by expanding in the deviation from equilibrium and dropping nonlinear terms. The form used here has been given by Kadanoff and Martin (see Ref. 20).

the continuum functions $n(x, t)$, etc. Evidently the number contents at $t = -\tau$ of the two cells listed in Table IA are

$$c_{N11} \approx L^3 n(0, -\tau) \tag{70a}$$

$$c_{N21} \approx L^3 n(L\hat{x}, -\tau) \tag{70b}$$

Similar relations give the energy and momentum contents. The number transfer across the face separating these cells is

$$\tilde{x}_{N1} \approx L^2 \tau j_x(\tfrac{1}{2}L\hat{x}, -\tfrac{1}{2}\tau) \tag{71a}$$

and the other transfers are similarly (omitting space and time arguments)

$$\tilde{x}_{E1} \approx L^2 \tau q_x \tag{71b}$$

$$\tilde{x}_{P_x 1} \approx L^2 \tau \Pi_{xx} \tag{71c}$$

$$\tilde{x}_{P_y 1} \approx L^2 \tau \Pi_{xy} \tag{71d}$$

Similar equations for transfers across other faces involve other components of $\mathbf{q}$ and Π. Application of Eqs. (70)–(71) to the discrete equations of change (12) gives a finite-difference version of the continuum equations of change (68a)–(68c). Since this is quite straightforward, I will concentrate on the more interesting question of whether the transfer equations (67a)–(67d) reduce to the continuum flux equations (69a)–(69c). To rewrite Eqs. (67a)–(67d) in terms of continuum variables using Eqs. (70)–(71), it is necessary to relate $\tilde{x}$ and $\tilde{c}$ to x and c [Eq. (21)] using the means $\langle x \rangle$ and $\langle c \rangle$ (these are all functions of the chemical potential μ and the temperature T). Evidently all the $\langle x_j \rangle$ vanish by symmetry except for $j = P_x 1$. Denoting the mean isotropic pressure $\langle \Pi_{xx} \rangle$ by $\langle \Pi \rangle$, we see from Eq. (71c) that

$$\langle x_{P_x 1} \rangle = L^2 \tau \langle \Pi \rangle \tag{72a}$$

Similarly,

$$c_{N l 1} = L^3 \langle n \rangle \tag{72b}$$

$$c_{E l 1} = L^3 \langle \epsilon \rangle \tag{72c}$$

Note that $\langle c_{P_x l 1} \rangle = 0$ by symmetry. In Eq. (67a) the means cancel in the first term, which is a finite-difference approximation to $g_{12} L\, \partial(L^3 n)/\partial x$ (evaluated at the face center). The second term is similar. In the third term the means vanish, leaving $2(L^3 p_x)$ to lowest order in L. So Eq. (67a) becomes

$$j_x = -(g_{12} L^2/\tau)\, \partial n/\partial x - (g_{13} L^2/\tau)\, \partial \epsilon/\partial x + (2 g_{14} L/\tau) p_x$$

The rotated equations for the other components give

$$\mathbf{j} = -(g_{12} L^2/\tau)\, \nabla n - (g_{13} L^2/\tau)\, \nabla \epsilon + (2 g_{14} L/\tau) p \tag{73a}$$

Similarly Eq. (67b) becomes

$$\mathbf{q} = -(g_{15}L^2/\tau)\,\nabla n - (g_{16}L^2/\tau)\,\nabla\epsilon + (2g_{17}L/\tau)\mathbf{p} \tag{73b}$$

The equations for the momentum fluxes obtained from Eqs. (67c) and (67d) are

$$\Pi_{xx} = \langle\Pi\rangle + (2g_{18}L/\tau)(n - \langle n\rangle) + (2g_{19}L/\tau)(\epsilon - \langle\epsilon\rangle) - (g_{20}L^2/\tau)\,\partial p_x/\partial x$$
$$\Pi_{xy} = -(g_{21}L^2/\tau)\,\partial p_y/\partial x$$

Writing rotated equations for equivalent components gives the tensor equation

$$\begin{aligned}\Pi_{ij} = {} & [\langle\Pi\rangle + (2g_{18}L/\tau)(n - \langle n\rangle) + (2g_{19}L/\tau)(\epsilon - \langle\epsilon\rangle)]\,\delta_{ij} \\ & - (g_{21}L^2/\tau)\,\nabla_i p_j - (g_{20} - g_{21})(L^2/\tau)\,\delta_{ij}\,\nabla_i p_i\end{aligned} \tag{73c}$$

In comparing Eqs. (73a)–(73c) to the phenomenological equations, it is useful to have order-of-magnitude estimates of the coefficients (in parentheses). These are hard to guess for large cells but easy for small cells with $L \sim$ mean free path $\sim$ interparticle distance, and $\tau \sim$ mean time between collisions (I assume a liquidlike density). Of course Eqs. (73a)–(73c) are not very accurate for such small cells, but the coefficients should have the correct order of magnitude. The contents are roughly $N \sim 1$, $E \sim mv_0^2$, $P \sim mv_0$, where v_0 is the mean thermal velocity (so $E \sim kT$), and the transfers are of the same order. Simply multiplying these estimates in pairs gives me estimates of all the correlations W. Letting $v_0\tau \sim L$, we see [using Eqs. (65a) and (65b)] that the coefficients in Eq. (73a) are of orders Lv_0, L/mv_0, and $1/m$, respectively. In a system in which the mean free path L is very much smaller than the scale of variation of n, ϵ, and $\mathbf{p}$ (the hydrodynamic limit) the factors of L make the first two terms negligible. Thus Eq. (73a) becomes exactly the continuum equation (69a) if

$$2g_{14}L/\tau = 1/m \tag{74a}$$

Some insight into the first two terms can be gained by considering a steady-state system with $\mathbf{p} = \mathbf{j} = 0$; then the linear combination of ∇n and $\nabla\epsilon$ in Eq. (73a) must vanish exactly. Also, the pressure should be constant:

$$0 = \nabla\langle\Pi\rangle = (\partial\langle\Pi\rangle/\partial n)\,\nabla n + (\partial\langle\Pi\rangle/\partial\epsilon)\,\nabla\epsilon$$

(Assume the equilibrium mean $\langle\Pi\rangle$ has been expressed as a function of n and ϵ.) This suggests that the two linear combinations are proportional, i.e.,

$$g_{12}L^2/\tau = \gamma\,\partial\langle\Pi\rangle/\partial n \tag{74b}$$

$$g_{13}L^2/\tau = \gamma\,\partial\langle\Pi\rangle/\partial\epsilon \tag{74c}$$

for some transport coefficient γ which is very small, but perhaps not always negligible in non-steady-state systems.

Next, comparing Eqs. (73b) and (69b), we see that they are identical if

$$g_{15}L^2/\tau = \kappa\, \partial T/\partial n \tag{74d}$$

$$g_{16}L^2/\tau = \kappa\, \partial T/\partial \epsilon \tag{74e}$$

$$2g_{12}L/\tau = (\langle \epsilon \rangle + \langle \Pi \rangle)/\langle n \rangle m \tag{74f}$$

Again the first two terms are much smaller than the third, but this time they are observable because they need not cancel when the third term vanishes, as in a heat conduction experiment. The coefficient κ may be obtained from either of the equations in terms of molecular-dynamics data [see Eq. (75a) below].

Turning to the last equations (73c) and (69c), we see the first terms agree if

$$2g_{18}L/\tau = \partial\langle \Pi \rangle/\partial n \tag{74g}$$

$$2g_{19}L/\tau = \partial\langle \Pi \rangle/\partial \epsilon \tag{74h}$$

This illustrates the observation of Section 4 that if we use inappropriate equilibrium parameters μ and T, thereby getting the wrong pressure $\langle \Pi \rangle$, the theory compensates automatically (in this approximation, to first order in $n - \langle n \rangle$ and $\epsilon - \langle \epsilon \rangle$). The second terms require

$$g_{21}L^2/\tau = 2\eta/\langle n \rangle m \tag{74i}$$

which gives the shear viscosity in terms of molecular-dynamics data [Eq. (75b)]. The third terms show that g_{20} is related to the bulk viscosity. However, the terms are not identical. In fact, even the second terms are not identical if the flow is rotational (so $\nabla \mathbf{p}$ is not a symmetric tensor). These problems can be traced to the fact that some terms in the finite-difference form of Eq. (69c) require index pairs not included in the present very limited set (Table IB). A proper treatment of rotational flow and bulk viscosity probably requires additional index pairs.

An essential result of this section has been the emergence of the two most important transport coefficients κ and η in terms of molecular-dynamics correlations. Explicit formulas may be obtained from Eqs. (65), (74e), and (74i):

$$\kappa = (L^2/\tau)(\partial T/\partial \epsilon)^{-1}(W_{16}/W_{23}) \tag{75a}$$

$$\eta = (L^2/\tau)(\tfrac{1}{2}\langle n \rangle m)(W_{21}/W_{24}) \tag{75b}$$

In Eq. (75a), W_{16} is the cross-correlation between the energy content of a cell and the energy transfer out of it in time τ, and W_{23} is the mean square fluctuation of the content; these are depicted in Fig. 4. Of course the form (75) cannot be exact unless $L, \tau \to \infty$; its significance for finite L and τ is that it is the first of a sequence of approximations which can describe the evolution exactly.

9. CONCLUSION

It has been shown that cell hydrodynamics is both more natural theoretically and more useful computationally than continuum theories for describing the behavior of a classical fluid system. It appears very likely that this is true of macroscopic physical systems in general, and that cell theories will prove useful for describing quantum systems, charged systems (which require a cellular treatment of electromagnetic theory), etc.

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