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Exact Fixed Points in Discrete Hydrodynamics

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Recently a discrete formulation of hydrodynamics was introduced, which was shown to be exactly renormalizable in a certain sense: a procedure was given for computing the equations of motion on a coarse space and time scale from those on a finer scale. In this paper we carry out this coarsening procedure explicitly, giving exact numerical results for a one-dimensional diffusive system. The coarsening transformation is found to have a one-parameter family of nontrivial fixed points, parameterized by a diffusion parameter D. This result gives a new way of understanding why so many systems obey Fick's law $j = -D' dn/dx$. Any of an extremely broad class of microscopic equations of motion, when viewed on a coarse enough scale, obey the fixed-point equations (which are equivalent to Fick's law). The methods used here are equally applicable to higher-dimensionality systems such as fluids.

KEY WORDS: Fixed points; renormalization group; transport equations.

A formal procedure for exactly coarsening[2] the equations of motion in discrete hydrodynamics was recently given.(1) In the present paper we show how this procedure may be carried out numerically, giving results for a particular case. A description of the coarsening procedure is given in the Appendix. In the paper itself we will sketch the formulation of discrete hydrodynamics and give the numerical results.

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[2]In the language of critical phenomena, what we call "space coarsening" might be referred to as "real-space dynamic renormalization." However, this expression refers to Hamiltonian (rather than equation-of-motion) renormalization, in theories in which time is continuous, so there is no analog of "time coarsening." For this reason, and because the word "renormalization" has undergone so many mutations that its ordinary meaning has no relation to its technical one, we prefer "coarsening" here.

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Discrete hydrodynamics was introduced[2] because it can be formulated more precisely than continuum theories, and because it is as complete a description of a system as possible on any particular distance and time scale (in a sense defined in Ref. 2). The general method is described in detail in Ref. 1; we are here concerned with the simplest application of the method, to a one-dimensional diffusive system (for example, to a solute diffusing in a capillary tube, or various well-known mathematical models: Markovian or non-Markovian random walks, discrete or continuous in space and time). Given a distance scale W and a time scale τ, we want to describe the system in terms of a set of variables related to discrete cells. In one dimension, the cells are line segments with centers at lW (l is a half-integer). The end points of the segments ("faces") are at fW (f is an integer). The analog of the continuum density variable is the cell content $c(l,m)$. This is the number of particles in cell l at time $m\tau$, where m is an integer. The intervals between these times are labeled by half-integers m (so $m\tau$ is the midpoint of a time interval). The quantity we wish to predict is the transfer $x(f,m)$, the net number of particles transferred to the right during the interval m, across the point fW separating two cells (f is an integer). The theory is based on a complete description of the joint probability distribution of transfers $x(f,1/2)$ in the ensemble of fixed discrete history [fixed $c(l,0)$ and $x(f,m)$ for $m<0$]. This description involves a power series expansion of the moments of the distribution, which we refer to as an "equation of motion." For any specific system, the equation-of-motion coefficients may in principle be computed from the microscopic dynamics (this has in fact been done for a fluid model[9,10]). Our interest in this paper, however, is not in specific systems but in looking for fixed points (in the manifold of all possible equations of motion, describing all possible one-dimensional diffusive systems) under a coarsening transformation. We expect this fixed-point equation of motion to be linear (since Fick's law is) so we consider here only linear terms in the power series. In addition, we will concern ourselves only with the first and second cumulant moments[1] of the transfer distribution (this leads to exact results if the distributions are multivariate Gaussians, and becomes increasingly accurate as we approach the coarse-cell limit). We denote these moments by $[x(f,1/2)]$ and $[x(f,1/2)x(f',1/2)]$. Each is a function of all history variables; expanding the former to lowest nonvanishing order gives

$$\left[x(f,1/2)\right] = \sum_{l} \left[x(f,1/2)\right]_{c(l,0)} c(l,0) + \sum_{f',m<0} \left[x(f,1/2)\right]_{x(f',m)} x(f',m) \tag{1}$$

where we have denoted the coefficient describing the influence of $c(l,0)$ on $x(f,1/2)$ by $[x(f,1/2)]_{c(l,0)}$ (this was called B in Refs. 1, 9, and 10). The

lowest-order term in the power series for the second moment is just the constant term, which we simply denote by $[x(f, 1/2)x(f', 1/2)]$.

The equation of motion of our system is thus uniquely determined by three sets of numbers, which are listed for a number of different equations of motion in Table I. The line labeled $[xx]$ contains the fluctuation moments $[x(f, 1/2)x(f', 1/2)]$ for $|f - f'| = 0, 1, 2, \ldots$, respectively. The

Table I. Various Stages of Coarsening Transformations. Spatial Separation Increases to the Right (1/2, 3/2, 5/2, ... for $[x]_c$, 0, 1, 2, ... for $[xx]$ or $[x]_x$)

$[xx]$	1.0000					
$[x]_c$	−0.2500					
$[x]_x$	0.0000					$D = 0.2500$
			T-coarsen			
$[xx]$	1.3750	0.2500	0.0625	0.0000		
$[x]_c$	−0.3125	−0.0625	0.0000			
$[x]_x$	0.0000	0.0000				$D = 0.5000$
			S-coarsen			
$[xx]$	1.5530	0.1538	0.0025	0.0002	−0.0000	0.0000
$[x]_c$	−0.1825	0.0045	−0.0004	0.0001	−0.0000	0.0000
$[x]_x$	−0.1406	−0.0667	0.0033	−0.0003	0.0000	−0.0000
$m = -3/2$	−0.0366	−0.0178	0.0003	−0.0001	0.0000	
$m = -5/2$	−0.0095	−0.0048	−0.0001	−0.0001	0.0000	
$m = -7/2$	−0.0025	−0.0013	−0.0000			
$m = -9/2$	−0.0006	−0.0003				
$m = -11/2$	−0.0002					$D = 0.1250$
			T-coarsen			
$[xx]$	2.0304	0.3939	0.0453	0.0026	0.0000	−0.0000
$[x]_c$	−0.2535	−0.0180	0.0011	0.0001	−0.0000	0.0000
$[x]_x$	−0.0747	−0.0435	−0.0056	0.0007	0.0001	−0.0000
$m = -3/2$	−0.0119	−0.0075	−0.0015	0.0002	0.0001	
$m = -5/2$	−0.0018	−0.0012	−0.0003	−0.0000		
$m = -7/2$	−0.0002	−0.0001	−0.0000			
$m = -9/2$	−0.0000	−0.0000				$D = 0.2501$[a]
			TST-coarsen again			
$[xx]$	3.8051	0.8300	0.1051	0.0058	0.0000	0.0000
$[x]_c$	−0.2532	−0.0174	0.0016	−0.0000	−0.0000	0.0000
$[x]_x$	−0.0744	−0.0409	−0.0032	0.0010	−0.0000	−0.0000
$m = -3/2$	−0.0115	−0.0067	−0.0007	0.0003	0.0000	
$m = -5/2$	−0.0017	−0.0010	−0.0002	0.0000		
$m = -7/2$	−0.0002	−0.0001	−0.0000			
$m = -9/2$	−0.0000	−0.0000				$D = 0.2503$[a]

[a] This upward drift of D is due to the truncation of the apparently exponential long-time tail of the space-coarsened equation of motion.

linear coefficients $[x(f,1/2)]_{c(l,0)}$ are given for $l-f=1/2, 3/2, 5/2, \ldots$, and then the non-Markovian coefficients $[x]_x$ for $m=-(1/2)(|f-f'|=0, 1, 2, \ldots$ on one line), $m=-3/2$ (next line), etc.

A particular model (say, a random walk) need not have equations of motion of this form (they could, for example, be non-Gaussian). But after a few coarsening transformations the non-Gaussian parts will become small (they are "irrelevant" in the Wilson sense).

A quantity which is important in one-dimensional diffusive systems is, of course, the diffusivity D'. This can be determined from the discrete equations of motion by applying them to a system with a uniform content gradient and uniform transfer.[12] The ratio of the corresponding flux j to the density gradient is

$$D' = D\frac{W^2}{\tau} \tag{2}$$

where D is a dimensionless diffusion parameter determined by

$$D = \sum_l (f-l)\left[x(f,1/2)\right]_{c(l,0)} + D\sum_{f',m}\left[x(f,1/2)\right]_{x(f',m)} \tag{3}$$

The first three lines of Table I describe the simplest possible nontrivial equation of motion, in which each transfer is influenced only by the cell on either side ($[x(0,1/2)]_{c(\pm 1/2,0)} = \mp 1/4$, which gives $D=1/4$; this value was chosen for no particular reason). The transfers are uncorrelated with each other ($[x(0,1/2)x(f,1/2)]=0$ if $f\neq 0$). Such an equation of motion for cells of width W exactly determines[1] the equation of motion of the same system for cells of width $2W$, by a space-coarsening transformation. The coarsened equation of motion gives moments of the transfers $x(f,1/2)$ in an ensemble in which we fix only coarse-cell contents, say, $C(L,0)$ [L is an odd integer; the coarse cell at WL contains two fine cells centered at $(L\pm 1/2)W$]. Evidently $C(L,0)$ is the sum $c(L-1/2,0)+c(L+1/2,0)$. We know (from the fine-cell equation of motion) how the transfer depends on the fine contents c; specifying these is equivalent to specifying their sum C and one other linear combination, which may as well be taken to be the content difference $c(L-1/2,0)-c(L+1/2,0)$. This fluctuates in the new coarse ensemble. We can still exactly calculate the moments of the transfer distribution if we know the moments of the distribution of this content difference. Its fluctuations are caused by previous transfers across the "internal face" at WL, the center of the coarse cell, which are in turn described by the fine-cell equations of motion. The calculation of the moments is straightforward but intricate, and is described in detail in the Appendix. Also described in the Appendix is the coarsening procedure which computes moments of X, a coarse transfer over a time interval from 0 to 2τ, which is the sum of two fine transfers over the intervals $(0,\tau)$ and $(\tau,2\tau)$.

We first try out the time-coarsening transformation; the result is given in lines 4–6 of Table I. Because of the special (Markovian) nature of these fine-scale equations, this can be done exactly, with no truncation error (all coefficients appearing are rational). It will be noted that $[x]_c$ is increasing in size and spatial range, and the associated diffusion parameter has doubled to 0.5000. To reverse these tendencies, we next coarsen the space scale. The resulting equations of motion (describing cells of width $2W$ instead of W) are given next in Table I. Now the dependence on the history becomes important ($[x(0, 1/2)]_{x(0,-1/2)} = -0.1406$, etc.), and $D = 0.1250$.

These changes in D are consistent with the notion that the diffusivity D' [Eq. (2)] should be an invariant of the coarsening transformation (so when W doubles, D decreases by $1/4$, etc.). This invariance is not expected for nonlinear equations of motion,[1,3,4] but seems to be true for the present linear ones. Thus the parameter D will be invariant under a triple-coarsening transformation we will refer to as TST (one space and two time coarsenings; their order is not critical, but TST is most convenient from the point of view of numerical convergence because it minimizes the variation of D from its initial value). Obviously, looking for a fixed point under T or S alone would be futile because even D is not fixed. It is possible that TST may have a fixed point, though, so we bring D back to $1/4$ by another T coarsening. This is seen (Table I) to shorten (halve, in some sense) the time range of the equation of motion. In fact, the output of this first TST is very similar to the input, except for a doubling of the fluctuations (i.e., an increase in root-mean-square fluctuation of $2^{1/2}$). However, the scale of the fluctuations is somewhat arbitrary; in any real system the average content would have doubled, so the *relative* rms fluctuation has decreased by $2^{-1/2}$. In the large-cell limit the relative fluctuations vanish. The important (linear) parts of the equation of motion seem to be near a fixed point of TST. Performing TST again (Table I) confirms this suspicion, in fact showing remarkably fast convergence to the fixed point, again with a doubling of the fluctuations. We may search for the fixed point without assuming anything about the overall scale of the fluctuations (but requiring their space dependence to remain fixed) by renormalizing them to $[x(0, 1/2)^2] = 1.0$ (that is, by dividing each by $[x(0, 1/2)^2]$) after each TST transformation. A practical iterative procedure for finding the fixed point also requires renormalizing $[x]_c$ to return D to its correct value (otherwise small truncation errors cause D to drift significantly over many iterations). The resulting fixed point[3] for $D = 1/4$ is given in Table II; the fixed points for

[3] Convergence to the fixed point is not as rapid as Table I might suggest. It is controlled by the largest eigenvalue of our transformation, which appears to be about 0.6 (we have effectively projected out eigenvectors with eigenvalues 2.0 and 1.0, by renormalizing $[x^2]$ and $[x]_c$, respectively). The slow eigenvector corresponds to changes in the amplitude of the tail $[x]_x$; four-figure accuracy requires about 15 iterations.

Table II. Equations of Motion at Fick's Points

			$D = 1/4$			
$[xx]$	1.0000	0.2365	0.0290	0.0016	0.0000	− 0.0000
$[x]_c$	− 0.2480	− 0.0143	0.0011	− 0.0001	− 0.0000	0.0000
$[x]_x$	− 0.0616	− 0.0321	− 0.0011	0.0007	− 0.0001	− 0.0000
$m = -3/2$	− 0.0078	− 0.0042	− 0.0001	0.0002	− 0.0000	
$m = -5/2$	− 0.0010	− 0.0005	− 0.0001	0.0000		
$m = -7/2$	− 0.0001	− 0.0001	− 0.0000			
$m = -9/2$	− 0.0000	− 0.0000				$D = 0.2501$[a]
						$f = 2.0006$[b]
			$D = 1/2$			
$[xx]$	1.0000	0.3697	0.0995	0.0187	0.0023	0.0002
$[x]_c$	− 0.3120	− 0.0685	− 0.0047	0.0004	− 0.0000	− 0.0000
$[x]_x$	− 0.0257	− 0.0179	− 0.0054	0.0000	0.0003	0.0000
$m = -3/2$	− 0.0018	− 0.0013	− 0.0004	0.0000	0.0000	
$m = -5/2$	− 0.0001	− 0.0001	− 0.0000	− 0.0000		
$m = -7/2$	− 0.0000	− 0.0000	− 0.0000			$D = 0.4996$[a]
$m = -9/2$	0.0000	0.0000				$f = 2.0005$[b]
			$D = 1/8$			
$[xx]$	1.0000	0.1287	0.0023	0.0001	− 0.0000	0.0000
$[x]_c$	− 0.1784	0.0084	− 0.0011	0.0002	− 0.0000	0.0000
$[x]_x$	− 0.1238	− 0.0473	0.0064	− 0.0009	0.0001	− 0.0000
$m = -3/2$	− 0.0274	− 0.0103	0.0025	− 0.0005	0.0001	
$m = -5/2$	− 0.0063	− 0.0021	0.0008	− 0.0002		
$m = -7/2$	− 0.0014	− 0.0004	0.0002			
$m = -9/2$	− 0.0003	− 0.0001				

[a] Diffusion parameter before renormalization to 1/4 or 1/2.
[b] $[x(0, 1/2)^2]$, before renormalizing to 1.0.

$D = 1/2$ and $D = 1/8$ (obtained as by-products) are also given. The $D = 1/2$ equation of motion so obtained is clearly a fixed point of TTS; we have checked that it is also a fixed point of TST, to within 10^{-3}. This provides a strong check on the computer program; it would be a remarkable coincidence if the result of an incorrect T were invariant under an incorrect TST. Evidently the fixed point for D equal to any power of 2 can be obtained by repeated coarsening. However, Table II shows that increasing D causes $[x]_c$ to spread out in space. Going beyond $D = 1/2$, retaining four-digit accuracy, would require including more terms than we have used (see Appendix); in fact the large (10^{-3}) error in applying TST to the $D = 1/2$ equation of motion occurs because the $D = 1$ equation extends significantly beyond $f - l = 5\frac{1}{2}$, our present limit. Similarly, decreasing D causes $[x]_x$ to spread out in time; the equation of motion becomes very non-Markovian.

For very large D, one expects the behavior to be nearly Markovian, so

the ensemble of fixed contents (say, $c = 1.0$ in cell $l = 0$ only) can be approximated by a continuum initial-value problem with density uniformly distributed in this cell. The transfers can then be obtained exactly in terms of the integral of the error function; to be precise,

$$[x(f, 1/2)]_{c(l,0)} = D^{1/2}\left[i^1 \operatorname{erfc}\left(\frac{f - l - 1/2}{2D^{1/2}} \right) - i^1 \operatorname{erfc}\left(\frac{f - l + 1/2}{2D^{1/2}} \right) \right] \tag{4}$$

using the notation of Ref. 5. This gives 0.315, 0.075, 0.0081, 0.0004 for $D = 1/2$ and 0.257, 0,0246, 0.0005 for $D = 1/4$. The first of these differs only by 1% from the value in Table II; evidently D does not have to be very large for Eq. (4) to be a good approximation.

We know of no comparable heuristic estimate of the lengthening of the time tail in $[x]_x$ for small D. Empirically, however, this tail appears to be exponential: to our numerical accuracy (rarely better than 5% in the tails) the ratio $[x(f, 1/2)]_{x(0,m)}/[x(f, 1/2)]_{x(0,m-1)}$ is constant, approximately 0.221, 0.126, and 0.0682 for $D = 1/8$, $1/4$, and $1/2$, respectively.

It is important to realize that the coarsening transformation used in this paper is *not* an approximate one, such as those which have been frequently used in the renormalization of critical systems (Migdal[6] or bond-decimation approximations, ϵ expansions,[7] second-order cumulant expansions,[8] etc.). If one of the equations of motion in Table I or Table II exactly describes a system (and we can certainly define a model system for which this is true) then the joint probability distribution of coarsened transfers is *exactly* described (except for truncation errors, which can be made arbitrarily small) by the coarsened equations given in the table. Among the methods mentioned above which have been used for critical systems some are formally successive-approximation schemes and therefore potentially exact; however, it has not proved practical to carry them to convergence. Of course the critical systems they describe are more complex than the system we treat here. Nevertheless, the exactness with which the discrete method obtains the diffusive fixed point suggests that it may be useful for critical systems. It would also be interesting to apply the coarsening transformation of the Appendix to the case of a three-dimensional fluid, for which discrete equations of motion on a small scale have already been calculated numerically.[9,10]

One may view the present results in the context of a fundamental principle of statistical mechanics[11]: large classes of microscopic equations of motion, differing greatly in detail, become similar ("obey Fick's law") on a sufficiently coarse space and time scale. This has in fact often been demonstrated explicitly for discrete microscopic models (e.g., random walks). What has apparently not been previously realized is that the

coarsening can be done in such a way that the coarsened equations have the *same form* as the fine-scale ones, and that to do this precisely requires the former to be discrete in space and time. One can then introduce the very powerful notion of a "fixed point," and instead of showing one-by-one that various specific microscopic models have a common large-scale behavior, one can demonstrate that very large classes of systems (excluding only pathological ones for which the equation-of-motion parameterization does not converge) have such common behavior, described by the fixed-point equation of motion. To develop this point of view completely would require a careful analysis of the domain of attraction of the fixed point, which has not yet been done.

It is interesting to ask what the role of the differential equations of continuum hydrodynamics (for example, Fick's law) would be in such a theory. It appears that Fick's law and the fixed-point discrete equations of motion should be regarded as the same thing, in some sense. Consider a continuum system with density $n(x,t)$ and current $j(x,t)$, in which n varies on a certain scale ξ (meaning $\xi|\partial n/\partial x| \lesssim n$). One may then identify the content $c(l,m)$ with $Wn(lW,m\tau)$ if $W \ll \xi$, and $x(f,m)$ with $\tau j(fW,m\tau)$ if $\tau \ll \xi^2/D'$. If one then examines the meaning of the statement "this system obeys Fick's law" (using the definition of the derivative), it is essentially equivalent to "given any desired accuracy for the equation of motion, W and τ may be made sufficiently small so the system behaves as though it were described by the simplest possible discrete equation of motion [like the first in Table I, with its single parameter $[x]_c$ chosen to satisfy Eqs. (2) and (3)]." Because of the properties of the fixed point this is in turn equivalent to "given any desired accuracy for the equations of motion, W_0 and τ_0 may be found such that the system obeys the fixed-point equations of motion [with D defined by Eq. (2)] for *any* $W > W_0$, $\tau > \tau_0$." From a fundamental point of view, the latter ("fixed-point") statement of Fick's law is more appealing than the former ("differential-equation") statement since the former requires conceptually applying a diffusionlike equation to the system on arbitrarily small scales, which is physically meaningless.

APPENDIX: DERIVATION OF COARSENING TRANSFORMATION

We have used for this calculation essentially the method derived for a general hydrodynamic system in Ref. 1. It turns out that the calculation is simpler if one uses a set of Fourier-transformed variables, so we will give here a derivation in terms of these variables.

When we begin a coarsening transformation, we are given the fine-scale equations of motion which describe the distribution of transfers $x(f,1/2)$ in an ensemble of fixed "history variables" $h(l,m)$, with $m \leqslant 0$.

Here $h(l,m)$ is the content $c(l,m)$ if m is an integer (and l a half-integer), or $x(l,m)$ if m is a half-integer (and l an integer). This distribution is described by a power series expansion of its moments.[1] A general moment can be denoted $[x]^F$ (where F indicates we are using an ensemble of fixed fine-scale history, as opposed to the coarse scale used below) if we use a concise notation in which x may denote a product of $x(f,1/2)$'s. If h denotes a product of history variables, the expansion may be written

$$[x]^F = \sum_h [x]_h^F h \tag{A1}$$

The sum is over ordered[4] sets of variables; h may denote either this set or the product of its variables. In the present numerical calculation we consider only coefficients $[x]_h^F$ with one x and one h, or two x's and no h's (i.e., $x = x_a x_b$ and $h = \emptyset$, the null set). However, we will describe the coarsening transformation for the general case.

We wish to calculate coefficients like $[x]_h^F$ for the coarsened system. In the case of space coarsening, this means computing moments in an ensemble in which only the coarse-cell contents and previous transfers are fixed. It turns out that the simplest way to relate the coarse and fine variables is by doing a sort of limited Fourier transform (over only one coarse cell) of the fine variables. That is, we define

$$C(k,L,m) = \sum_{l \subset L} (-1)^{k \cdot (l - \tilde{l})} c(l,m) \tag{A2}$$

For a d-dimensional system, k, L, l, and $\tilde{l}$ are d-vectors, and L labels coarse cells of width $2W$ (whose centers have position vectors WL). The components of L are odd integers; those of l, odd half-integers. Here $\tilde{l}$ is the "lower left" fine cell in the coarse cell L [i.e., has components $L_i - 1/2$, $i = 1, d$; its only function is to make Eq. (A2) real]. The components of the "wave vector" k take only the values 0 and 1. The advantage of this transformation is, of course, that $C(0,L,m)$ is exactly the coarse-cell content. The other $2^d - 1$ variables for this L describe internal fluctuations (in one dimension, the left–right content difference described previously) within cell L.

We label the faces of the coarse cells by the vector F (the face is centered at WF). Then we can define a Fourier-transformed transfer

$$X(k,F,m) = \sum_{f \subset F} (-1)^{k \cdot (f - \tilde{f})} x(f,m) \tag{A3}$$

Here k is a $(d-1)$-dimensional vector (in the plane of the face) and $\tilde{f}$ is the lower left fine face in F. However, there are only $2^{d-1} d$ fine faces on the d

[4] Unordered sets were used in Ref. 1; this only changes the coefficients by combinatorial factors.

exterior faces associated with each coarse cell. There are another $2^{d-1}d$ "interior" fine faces, which may be combined in groups of 2^{d-1} to form d "internal coarse faces" centered at the cell center. We may form linear combinations of these in any way we please; one convenient way is to use Eq. (A3) but allow F to refer to the cell center (position WF). There are then d internal coarse faces with this designation; we may distinguish them by setting the unused component of k (i.e., the component normal to the face) equal to an arbitrary flag, say, 2.

In one dimension, Eq. (A3) reduces to

$$X(k,F,m) = x(F,m) \tag{A4}$$

which is a transfer across an external "face" (i.e., a point at the end of a coarse cell) if F is even, and an internal "face" (at the center of a cell) if F is odd.

We may now Fourier-transform (FT) the equation-of-motion coefficients $[x]_h^F$. We denote the result [obtained below, Eqs. (A11–A14)] in general by $[X]_H^F$, where X is a product of FT transfers [Eq. (A3)] and H is a product of FT history variables [Eq. (A2) or (A3)]. Thus Eq. (A1) becomes

$$[X]^F = \sum_H [X]_H^F H \tag{A5}$$

Our ultimate objective, the coarse equation of motion, describes moments in a different (larger) ensemble, of fixed coarse history. If $X(k=0)$ denotes a product of FT transfers with $k=0$, i.e., coarse-cell transfers, we denote such a moment by $[X(k=0)]^{C0}$ (C for coarse, 0 because variables with $m \leqslant 0$ are fixed). It may be obtained by averaging Eq. (A5) over the coarse ensemble:

$$[X(k=0)]^{C0} = \sum_H [X]_H^F [H]^{C0} \tag{A6}$$

and the coefficient of a product H' (with $k=0$) of coarse-history variables is

$$[X(k=0)]_{H'}^{C0} = \sum_H [X]_H^F [H]_{H'}^{C0} \tag{A7}$$

It is now apparent that computing the coarse equations of motion (A7) requires knowing the distribution of fine-cell FT variables H, in the ensemble of fixed coarse-cell variables H' ($k=0$), as described by the coefficients $[H]_{H'(k=0)}^{C0}$. (Only the $k \neq 0$ H''s vary in this ensemble.) These may be computed by a relaxation procedure justified and described in detail in Section 4 of Ref. 1. Basically it involves assuming a form for $[H]_{H'}^{C0}$, the distribution of fluctuations at times $\leqslant 0$ in the ensemble "$C0$," and allowing the system to evolve (via the fine-scale equations of motion) to $m=1$. Coefficients $[H_1]_{H'}^{C1}$, which describe fluctuations in the ensemble

"$C1$" (coarse variables fixed for $m \leqslant 1$) may then be computed, and may be used as input ($[H]^{C0}_{H'}$) for the next iteration. The procedure converges very rapidly to self-consistency (giving four-figure accuracy in five or six iterations even with a very poor starting estimate).

To carry out this relaxation procedure, we need moments of variables at times $\leqslant 1$ in the $C0$ ensemble. We must first obtain such moments $[h_1]^F_h$ in the fine ensemble, from the equation of continuity[1]

$$c(l,1) = c(l,0) + \sum_f \sigma x(f,1/2) \tag{A8}$$

(σ is $+1$ if x is a transfer into cell l, -1 if out). This gives

$$\left[h_1 c(l,1)\right]^F_h = \left[h_1 c(l,0)\right]^F_h + \sum_f \sigma \left[h_1 x(f,1/2)\right]^F_h \tag{A9}$$

Here h_1 is any product of variables at times $\leqslant 1$, and h any product at times $\leqslant 0$. The first term on the right-hand side vanishes unless $h = c(l,0)h'$ for some h', in which case it is $[h_1]^F_{h'}$. The right-hand side of Eq. (A9) is initially known only when h_1 involves only times $\leqslant 1/2$, but by using Eq. (A9) recursively we can get any $[h_1]^F_h$. Let us denote its Fourier transform by $[H_1]^F_H$, satisfying

$$\left[H_1\right]^F = \sum_H \left[H_1\right]^F_H H \tag{A10}$$

We can obtain $[H_1]^F_H$ recursively from

$$\left[H_1 C(k,L,m) h_1\right]^F_h = \sum_{l \subset L} (-1)^{k\cdot(l-\tilde{l})} \left[H_1 c(l,m) h_1\right]^F_h \tag{A11}$$

$$\left[H_1 X(k,F,m) h_1\right]^F_h = \sum_{f \subset F} (-1)^{k\cdot(f-\tilde{f})} \left[H_1 x(f,m) h_1\right]^F_h \tag{A12}$$

$$\left[H_1\right]^F_{HC(k,L,m)h} = 2^{-d} \sum_{l \subset L} (-1)^{-k\cdot(l-\tilde{l})} \left[H_1\right]^F_{Hc(l,m)h} \tag{A13}$$

$$\left[H_1\right]^F_{HX(k,F,m)h} = 2^{1-d} \sum_{f \subset F} (-1)^{-k\cdot(f-\tilde{f})} \left[H_1\right]^F_{Hx(f,m)h} \tag{A14}$$

[obtained from Eqs. (A2) and (A3)]. Equations (A11) and (A12) are used first to compute moments with one coarse factor (so $H_1 = \emptyset$), then those with two factors, then three (two in H_1 and one C), etc.

The moments of H_1 in the ensemble ("$C0$") of fixed coarse variables are computed from a slight generalization of Eq. (A7):

$$\left[H_1\right]^{C0}_{H'(k=0)} = \sum_H \left[H_1\right]^F_H \left[H\right]^{C0}_{H'(k=0)} \tag{A15}$$

The form of Eq. (A15) is one which will arise twice more below. It relates moments in a large ensemble L (here $C0$) to those of a subensemble S (here

F) and may be written

$$[pf]_c^L = \sum_{f'c'} [pf]_{f'c'}^S [f'c']_c^L \tag{A16}$$

Variables constrained in the large ensemble L are denoted c [here, $H(k=0, m \leqslant 0)$], variables which fluctuate in the L ensemble but are fixed in the smaller ensemble S are denoted f [here, $H(k \neq 0, m \leqslant 0)$], and predicted variables (not constrained in either ensemble) are denoted p [here, $H(m > 0)$].

We need coefficients $[H_1]_{H_1'(k=0)}^{C1}$ describing the ensemble in which coarse variables at times $\leqslant 1$ are fixed (i.e., in addition to the variables fixed in the $C0$ ensemble, $X(0, F, 1/2)$ is fixed for all F). These satisfy

$$[H_1]^{C1} = \sum_{H''} [H_1]_{H''}^{C1} H'' \tag{A17}$$

where H'' is a product of variables $H(k=0, m \leqslant 1)$. Since $C1$ is a subensemble of $C0$, Eq. (A16) applies with $L = C0$, $S = C1$. The c's are $H(k=0, m \leqslant 0)$ as before, but f's are $X(k=0,\ m=1/2)$ and p's are $H(k \neq 0,\ m \leqslant 1)$. In this case, Eq. (A16) must be solved for the small-ensemble moments $[p]_{f'c}^S$, i.e., we must infer the effects of the fluctuations f on the predicted variables p by observing their correlations $[pf]^L$ in the larger ensemble. The solution $[\ ]^{C1}$, with time indices translated backwards by 1, is then to be used for $[\ ]^{C0}$ in Eq. (A15) to continue the relaxation process.

We now have a complete set of equations [(A9), (A11)–(A14), (A16) with $S = F$ or $C1$] for carrying out the coarsening transformation. In practice this must be done using cumulant moments, for reasons discussed in Section 5 of Ref. 1. These are defined by, e.g.,

$$[x]_h^F = \sum_{x1 \cdots h1 \cdots} [x1]_{h1}^{F,c} [x2]_{h2}^{F,c} \cdots \tag{A18}$$

where the sum is over all factorizations of the product x into smaller products $x1$, $x2$, etc., and over similar factorizations of h. We will omit the superscript c below; all moments will be cumulant moments. In terms of cumulants, Eqs. (A9) and (A11)–(A14) are unchanged. Equation (A16) has a cumulant form in which the right side is factorized in all possible ways, subject to a linkage condition (essentially Eq. 5.5 or 5.6 of Ref. 1). However, we have discovered a recursive form which is much more useful computationally because it involves multiplying only two factors at a time. This is accomplished by defining certain results of partial summation:

$$[pf]_{cf'}^L = [pf]_{cf'}^S + \sum_{f''} \sum_{\text{fact.}} [p_a f_a]_{c_a f'' f'}^L [p_b f_b f'']_{c_b}^L \tag{A19}$$

The outer sum is over all ordered sets of (one or more) fluctuation variables

f'', and the inner sum is over all possible factorizations $p = p_a p_b$, $f = f_a f_b$, and $c = c_a c_b$, such that p_a contains the first variable of p (this avoids double counting). Note that the cumulant $[pf]^S_{cf'}$ vanishes if $f \neq \emptyset$ (because f is fixed in this ensemble; we assume $p \neq \emptyset$).

Were it not for f', the left side of Eq. (A19) would be one of the cumulant power series coefficients describing the L ensemble. When $f' \neq \emptyset$, however, $[pf]^L_{cf'}$ has no direct interpretation as a power series coefficient, but is uniquely defined by Eq. (A19) in a recursive manner: a coefficient in which f' has $n \geqslant 1$ factors is expressed in terms of those in which it has more than n factors (coefficients with very large n must be assumed negligible).

The utility of these new coefficients lies in the fact that equations for the desired cumulant coefficients can be written in terms of them. In fact (A19) itself looks like such an equation, provided it is true for $f' = \emptyset$ (for $f' \neq \emptyset$ it is true by definition, but we are not free to redefine $[pf]^L_c$). It should be possible to prove Eq. (A19) for $f' = \emptyset$ by substituting it into a cumulant expansion [from Eq. (A18)] of Eq. (A16) and showing that both sides have the same terms. This can be easily verified for low-order cases (two or three factors; our numerical results require only two) but is not easy to see in general. We believe, however, that Eq. (A19) is the correct generalization.

Equation (A19) is used in two ways: once (with $L = C0$, $S = F$) to calculate $[\ ]^L$, and then (with $L = C0$, $S = C1$) to solve for $[\ ]^S$. In the first case, Eq. (A19) expresses $[pf]^L_{cf'}$ in terms of coefficients with a smaller p, or an equal p but larger f'. It can thus be calculated recursively using an outer loop over an increasing number of factors in p, and an inner loop over decreasing f'. We will write explicitly the cases of Eq. (A19) used in this paper: we may have one p and one f',

$$[p]^L_{f'} = [p]^S_{f'} \tag{A19a}$$

(there is no summation because $[p]^L_{f''f'}$ vanishes) or one p and one c,

$$[p]^L_c = [p]^S_c + \sum_{f''} [p]^L_{f''} [f'']^L_c \tag{A19b}$$

or one p and one f

$$[pf]^L_\emptyset = \sum_{f''} [p]^L_{f''} [ff'']^L_\emptyset \tag{A19c}$$

or two p's

$$[p_\alpha p_\beta]^L_\emptyset = [p_\alpha p_\beta]^S_\emptyset + \sum_{f''} [p_\alpha]^L_{f''} [p_\beta f'']^L_\emptyset \tag{A19d}$$

In calculating these for $L = C0$ and $S = F$, p is a product of $H(m > 0)$, c of $H(k = 0, m \leqslant 0)$, and f of $H(k \neq 0, m \leqslant 0)$.

The other context in which Eq. (A19) is used is in solving for $[\ ]^S$ (with $S = C1$). First we must calculate the new $[pf]^L_{cf'}$ (with $f' \neq \emptyset$), by a simple iterative procedure. Consider $[pf]^L_{c\tilde{f}\tilde{f}'}$ (we have replaced f' by $\tilde{f}\tilde{f}'$ where $\tilde{f}$ is a *single* variable, since f' had at least one factor; the new f' may be $\emptyset$). Then Eq. (A19) for $[pf\tilde{f}]^L_{cf'}$ has a term

$$[pf]^L_{c\tilde{f}\tilde{f}'}[\tilde{f}\tilde{f}]^L_{\emptyset}$$

on the right (using $f'' = \tilde{f}$). The second factor is intrinsically positive (and generally large), and we can easily solve for $[pf]^L_{c\tilde{f}\tilde{f}'}$ in terms of (previous estimates of) the other $[\ ]^L$'s. Once these have been calculated iteratively [this involves only Eq. (19c) in our case] the unused equations (19) are exactly those for which $f = \emptyset$, in which $[\ ]^S$ appears and can be calculated directly.

After Eq. (A19) has been thusly solved for $[H_1]^{C1}_{H(k=0)}$, these must be time translated and used for $[\ ]^{C0}$ in the next stage of relaxation. The coefficients $[H_1]^{C1}_{H'(k=0)}$ describe averages in the ensemble of fixed coarse history, specified by transfers with $m < 1$ and contents at $m = 0$. This is exactly the same ensemble as that obtained by fixing contents at $m = 1$ [since these are related to those at $m = 0$ by a continuity equation like (A8)]. The coefficients of a power series in this new set of variables will be denoted $[H_1]^N_{H'}$ (so here H' contains contents at $m = 1$). We may obtain these recursively from a series of "partly new" coefficients defined by expressing the first n variables of H'' in Eq. (A17) in terms of new variables via (A8). The coefficient of any $H'H''$ in this expression will be denoted $[H_1]^{N,n}_{H'H''}$. Here H' consists of the first n factors, if there are that many; these factors, if contents, are at $m = 1$. Let us write the $(n+1)$st factor explicitly, denoting the product by $H'C(0, L, 0)H''$ or $H'X(0, F, 1/2)H''$. If we express the $(n+1)$st variable in terms of new variables, and examine the coefficient of a product $H'C(0, 1, 1)H''$ we find

$$[H_1]^{N,n+1}_{H'C(0,L,1)H''} = [H_1]^{N,n}_{H'C(0,L,0)H''} \tag{A20}$$

Similarly,

$$[H_1]^{N,n+1}_{H'X(0,F,1/2)H''} = [H_1]^{N,n}_{H'X(0,F,1/2)H''} - \sum_L \sigma [H_1]^{N,n}_{H'C(0,L,0)H''} \tag{A21}$$

By using Eqs. (A20)–(A21) recursively for $n = 0, 1, \ldots$ (up to the number of factors in the subscript) we obtain $[H_1]^N_{H'}$, which is used as a new approximation to $[\ ]^{C0}$ (after a trivial backward time translation of all variables).

We have so far discussed only space coarsening. For time coarsening, we must Fourier-transform in time; instead of Eq. (A2) we use

$$X(\omega, f, M) = \sum_{m \subset M} (-1)^{\omega(m-\tilde{m})} x(f, m) \tag{A22}$$

where the sum is over the two fine intervals labeled by $m = M \pm 1/2$ contained in the coarse interval M (of length 2τ, centered at $M\tau$), $\tilde{m} \equiv M + 1/2$, and the "frequency" ω is 0 or 1. The contents have no FT, but for convenience we will define

$$C(0, l, M) = c(l, M) \tag{A23}$$

As in space coarsening, we must calculate fluctuations [of $X(1, F, M)$, an "ac transfer"] in the ensemble $C0$ of fixed contents $C(0, l, 0)$ and "dc transfers" $X(0, F, M)$. This is again done by a relaxation technique involving Eq. (A19); in fact the meanings of c, f, and p are almost unchanged (we must read ω for k). The moments $[H_1]_H^F$ in Eq. (15) involve times $< 2\tau$ and can be calculated by Fourier-transforming fine-scale averages $[h_2]_h^F$ where h_2 is a product of $x(f, m)$ for $m < 2$. This $[h_2]_h^F$ is calculated exactly as in Ref. 1: Eqs. (A8) and (A9) give $[h_1]_h^F$, to which we may apply time-translated equation-of-motion parameters $[x(m = 3/2)]^{F1}$ describing the ensemble of fixed $c(l, 1)$, $x(f, m < 1)$. This gives

$$[xh_1]_h^F = \sum_{h''} [x]_{h''}^{F1} [h'' h_1]_h^F \tag{A24}$$

This has exactly the form of Eq. (A16) with $L = F$, $S = F1$, $c = h(m \leqslant 0)$, $f = x(m = 1/2)$, $p = x(m = 3/2)$. Thus the required cumulants $[h_2]_h^F$ can be calculated recursively from Eq. (A19). We FT$[h_2]_h$ by recursive equations similar to Eqs. (A11)–(A14):

$$[H_1 X(\omega, f, M) h_2]_h = \sum_{m \subset M} (-1)^{\omega(m - \tilde{m})} [H_1 x(f, m) h_2]_h \tag{A25}$$

$$[H_1]_{HX(\omega, f, M)h} = \frac{1}{2} \sum_{m \subset M} (-1)^{-\omega(m - \tilde{m})} [H_1]_{Hx(f, m)h} \tag{A26}$$

Thus time coarsening can be done with Eqs. (A8)–(A9), (A24)–(A26), and (A19).

Carrying out the coarsening procedure numerically requires two types of coefficients: Those (denoted F) describing the ensemble of fixed fine history (involving both FT and non-FT variables) and those (denoted $C0$) describing the ensemble of fixed coarse history. We began with a list of "start-up" coefficients containing one member of each equivalence class under space and time translations (i.e., adding or subtracting an integer from any single coordinate L, l, F, f, or m). For space coarsening there are 37 such classes for the fine ensemble and 18 for $C0$. The latter may easily be enumerated as the left-hand sides of Eqs. (19a)–(19d), together with $[H_\alpha H_\beta]_\emptyset^{C0}$ and $[H]_{H'}^{C0}$. The next approximation (85 fine, 46 coarse) was obtained by including all "neighbors" (in which L, l, F, f, or m differs by 1) of the start-up coefficients. This process was repeated five times, giving finally 387 fine and 291 coarse coefficients. The equations (A15) used to

Table AI. Successive Approximations to the $D = 0.25$ Fixed Point

$[xx]$	1.0000					
$[x]_c$	− 0.2621					$D = 0.2407^a$
$[x]_x$	− 0.0483					$f = 1.6016^b$
$[xx]$	1.0000	0.1551				
$[x]_c$	− 0.2285	− 0.0135				$D = 0.2720$
$[x]_x$	− 0.0435	− 0.0160				$f = 2.0483$
$[xx]$	1.0000	0.2132	0.0208			
$[x]_c$	− 0.2407	− 0.0151	− 0.0006			
$[x]_x$	− 0.0654	− 0.0356	− 0.0048			$D = 0.2560$
$m = -3/2$	− 0.0053	− 0.0021				$f = 1.9663$
$[xx]$	1.0000	0.2372	0.0275	0.0016		
$[x]_c$	− 0.2503	− 0.0142	0.0015	0.0000		
$[x]_x$	− 0.0600	− 0.0317	− 0.0015	0.0011		
$m = -3/2$	− 0.0067	− 0.0037	− 0.0006			$D = 0.2488$
$m = -5/2$	− 0.0004	− 0.0002				$f = 2.0039$
$[xx]$	1.0000	0.2361	0.0287	0.0014	− 0.0002	
$[x]_c$	− 0.2482	− 0.0143	0.0011	− 0.0001	− 0.0000	
$[x]_x$	− 0.0616	− 0.0323	− 0.0012	0.0008	− 0.0001	
$m = -3/2$	− 0.0077	− 0.0042	− 0.0003	0.0002		
$m = -5/2$	− 0.0008	− 0.0005	− 0.0001			$D = 0.2499$
$m = -7/2$	− 0.0001	− 0.0000				$f = 1.9999$

(See Table II for best approximation)

[a] Diffusion parameter, before renormalizing to 0.25.
[b] $[x(0, 1/2)^2]$, before renormalizing to 1.0.

calculate the latter had a total of 3818 terms. The same process for time coarsening led to 309 fine and 165 coarse coefficients.

The convergence of this successive-approximation scheme is quite rapid. We list in Table AI the results obtained for the $D = 0.25$ fixed point in the first four approximations (the fifth is in Table II). All of the equation-of-motion coefficients have converged to four decimal places. It is not practical to tabulate all the fluctuation moments $[H]^{C0}_{H'}$; two numerically important ones for space coarsening are $[C(1, 1, 0)]^{C0}_{X(0,0,-1/2)} = 0.2710$ and $[C(1, 1, 0)]^{C0}_{C(0,3,0)} = -0.0953$.

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