Hamiltonian formulation for the diffusion equation

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A Hamiltonian formulation is presented for the diffusion equation. Going beyond the conservation of property in diffusive transport, conservation is shown to apply in the sense of classical Hamiltonian dynamics, provided the equation is transformed with Hermitian wavelets. The characteristic equations, obtained previously for the wavelet-transformed diffusion equation, are the canonical equations corresponding to a time-independent Hamiltonian. The configuration variables are defined by the canonical structure and its invariants, while the momenta determine the evolution of the system. Irreversibility results from the finite-time escape of trajectories, initiating from the smallest scales and eroding increasingly larger scales. However, this scale-dependent erosion of initial conditions does not necessarily imply memory loss. [S1063-651X(97)02902-4]

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I. INTRODUCTION

Formulations of diffusive problems come in several categories. The variational approach introduces adjoint fields, as in [1–3], and is suitable for computational purposes [4]. The physical meaning of these formulations is more limited than in the canonical theories, which can be divided into a classical treatment of inviscid flows [3] and a bracket formalism [5,6] that includes dissipative dynamics.

The approach developed here represents an alternative option. To quote Salmon [3] ''Just as any non-Euclidean manifold can be made Euclidean by embedding it in a higher dimensional space, any non-Hamiltonian dynamics can be made Hamiltonian . . . . '' He was referring to the addition of the adjunct field, but his remark could preface the introduction of the higher-dimensional wavelet space used here.

Several previous results by the present author were pointing in the general direction of conservative systems, with continuous Hermitian wavelet transforms [7,8] of the diffusion equation as the critical first step. A brief summary of relevant equations is presented in Appendix A. In [9], it was shown that the transformed equation admits characteristics, implying that information propagates in the field in a recognizable way. The existence of characteristics is specific of Hermitian wavelet transforms and goes beyond the classical integral representation [10] or the use of Green's functions [11]. In [12] (see Appendix D), rescaled Hermitian wavelets were actually shown to be the Green's propagators for source fields and initial and boundary conditions. In [13], the variance of the diffusing property was also shown to be conserved (in the sense that the energy loss occurs by viscous transport rather than by dissipation) if the first-order Hermitian wavelet is used.

Thus, it was apparent that Hermitian wavelets capture the dynamics of diffusion in a privileged manner, and this paper adds to the evidence. Starting with one-dimensional (1D) diffusion, the Hamiltonian is constructed in Sec. II, and the canonical equations are solved. Section III is devoted to the invariants of the process. In Sec. IV, the Legendre transform is used to construct a Lagrangian and the Hamilton-Jacobi equation is spelled out. The results are generalized to N-dimensional diffusion in Sec. V. A discussion and an interpretation follow in Sec. VI, including a reference to strongly nonlinear systems.

II. HAMILTONIAN FOR 1D DIFFUSION

Let us denote by u' the field of interest and by u its wavelet transform (see Appendix A for definitions and notations). In [9], the diffusion equation

$$\frac{\partial u'}{\partial t}=\nu\frac{\partial^2 u'}{\partial x^2} \tag{1}$$

was transformed into the first-order wave equation

$$\frac{\partial u}{\partial t}+\nu\kappa^3\frac{\partial u}{\partial\kappa}+\nu\kappa^2\left(n+\frac{1}{2}\right)u=0. \tag{2}$$

The wavelet number κ is a measure of inverse length scale, analogous to the wave number of Fourier analysis and equal to the inverse dilation factor a used in the wavelet literature. Following Courant and Hilbert [14], three of the corresponding characteristic equations (with a timelike parameter s) take the form

$$\frac{dt}{ds}=1, \tag{3}$$

$$\frac{d\kappa}{ds}=\nu\kappa^3, \tag{4}$$

and

$$\frac{du}{ds}=-\nu\kappa^2\left(n+\frac{1}{2}\right)u. \tag{5}$$

The propagation of initial conditions along characteristic lines implies a form of conservation that is consistent with non-dissipative mechanics. [If we imagine the relaxation of an initial bump, the bump retains its identity as it spreads and flattens out with constant area under the curve. The charac-

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teristic equations (4) and (5) track the spreading and the flattening. The conservative nature of the diffusive transport of velocity, vorticity, and other concentration, contrasted with the dissipation of energy, enstrophy, or variance of concentration, is emphasized in many textbooks.] From this perspective, a Hamiltonian can be sought. The construction procedure (see Appendix B and [15]) applicable to first-order partial differential equations relies on the interpretation of certain variables as being configuration variables or their associated momenta. This is invalidated by the eventual observation that the Hamiltonian cannot be a bilinear function of the momenta and that consequently κ and u must be the momenta. To that extent, the discovery of the Hamiltonian

$$H(K,U,\kappa,u)=\nu\kappa^3K-(n+\tfrac{1}{2})\nu\kappa^2uU \tag{6}$$

is serendipitous and is justified only by the consistency of the analytical structure built on it. We note that the Hamiltonian is constant in time and is homogeneous of degree 3 in the momenta and of degree 1 (in fact bilinear) in the configuration variables.

A. Momenta

Two of the canonical equations

$$\frac{d\kappa}{dt}=\frac{\partial H}{\partial K}=\nu\kappa^3 \tag{7}$$

and

$$\frac{du}{dt}=\frac{\partial H}{\partial U}=-\nu\left(n+\frac{1}{2}\right)\kappa^2u \tag{8}$$

are the characteristic equations (4) and (5). We denote $\kappa_0=\kappa(0)$ and $u_0=u(x,0)$. Integration as in [9] yields, respectively,

$$\kappa(t)=\frac{\kappa_0}{\sqrt{1-2\nu\kappa_0^2t}} \tag{9}$$

and

$$u(x,t)=u_0(1-2\nu\kappa_0^2t)^{n/2+1/4}=u_0\left(\frac{\kappa_0}{\kappa(t)}\right)^{(n+1/2)}. \tag{10}$$

The solutions are shown on Figs. 1 and 2. We see that for any given initial scale κ_0, $\kappa(t)$ becomes arbitrarily large in a finite time

$$t_c(\kappa_0)=1/(2\nu\kappa_0^2) \tag{11}$$

and that the corresponding u vanishes at that time. This occurs gradually for larger and larger scale components of the initial conditions. Furthermore, the time dependence of u is entirely captured by the relation

$$u(x,t)=v(x,\kappa(t)), \tag{12}$$

in agreement with our initial point of view that u, the wavelet transform of a field $u'(x,t)$, is a function of κ and x. The slope of the evolution lines (Fig. 2) corresponds to the as-

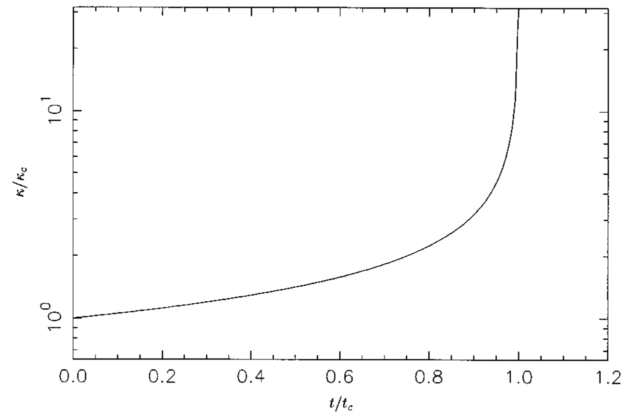

FIG. 1. Evolution of κ.

ymptotic slope for the Hermitian wavelet transform of any function, as illustrated by the g_2 (Mexican hat) transform of $v=e^{i\alpha x}$:

$$v(\kappa,x)=-\sqrt{2\pi}\kappa^{-5/2}\alpha^2e^{i\alpha x}e^{-\alpha^2/2\kappa^2}. \tag{13}$$

As the $\kappa^{-n-1/2}$ asymptote holds regardless of α, it also holds for any Fourier-expandable field. It should be noted that the evolutions shown on Figs. 2 and 3 are representative of the wavelet coefficients at each spatial location rather than of a mean power spectrum. The diffusion of a given field is now represented by the ''flow'' initiating from its continuous spectrum of wavelet coefficients at each x.

B. Irreversibility, selective memory, and reconstruction of the past

Further interpretation of Fig. 2 shows that, at time t_c, all initial spectral contributions at wavelet numbers $\kappa\geqslant\kappa_c=1/\sqrt{2\nu t_c}$ have vanished. The large-κ portion of the

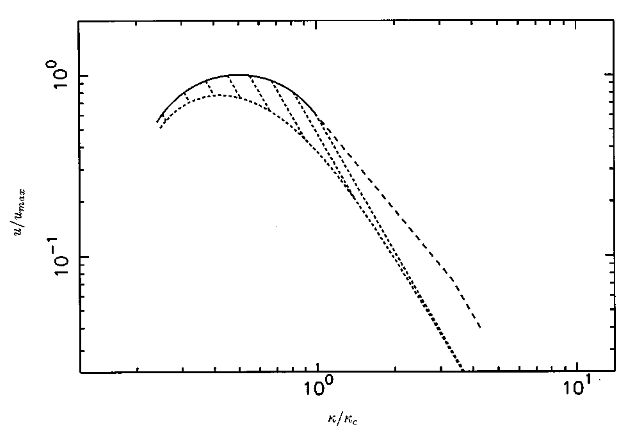

FIG. 2. Mapping (dotted lines) of initial momenta (solid line) to some future time t_c (dashed line); small scale (dashed line, large κ) initial conditions are forgotten after a finite time, but can be reconstructed by analytical continuation, as explained in the text.

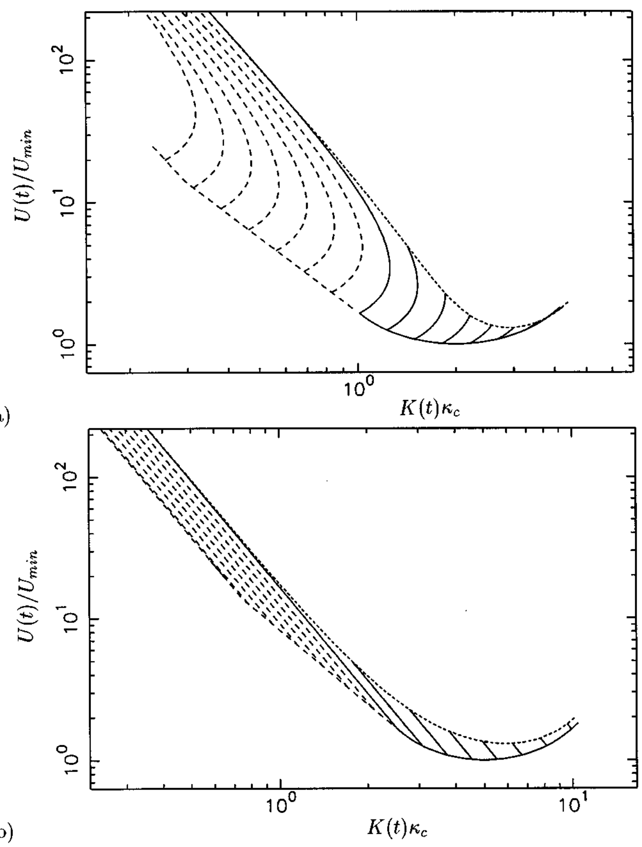

FIG. 3. Trajectories corresponding to the same initial conditions as in Fig. 2, based on $u_0U_0=1$ and (a) $\kappa_0K_0=1$ and (b) Eq. (19). The trajectories issuing from the dashed line (small scale, large κ_0) escape to infinity before time t_c; those issuing from the curved solid line generate the dotted time line.

spectrum has been repopulated by propagation of the smaller-κ initial conditions, with the values of κ initially just smaller than κ_c contributing to the asymptotic tail. At all times, we keep a continuous spectrum with $0<\kappa<\infty$. However, because of the scale-dependent attenuation described by Eq. (10), the dominant scale (e.g., corresponding to the top of the spectral curve at each spatial location) will gradually shift to smaller and smaller κ.

If we reverse the direction of time, only the ''initial'' values (solid line on Fig. 2) for $\kappa<\kappa_c$ are recovered spontaneously. We can interpret this as a form of irreversibility, by which one cycle of evolution and reverse evolution results in a truncation of the initial conditions. However, successive cycles of equal or shorter duration will not lead to further erosion of the initial field: irreversibility takes the form of a one-time escape for each initial scale, equivalent to the abrupt truncation of the initial conditions surviving beyond a given time.

In spite of this intrinsic irreversibility, the actual memory of the small-scale initial conditions (dashed line) is not lost. A reasonable extrapolation seems possible graphically; indeed, the extrapolation to larger κ's can be carried out by analytic continuation if all differentiability and convergence criteria are met in the following. Let us use the transform of the Fourier mode [Eq. (13)]. A Taylor series of $u(\kappa,x)$ around $\kappa_1<\kappa_c$ in terms of $\zeta-\zeta_1=\ln\kappa-\ln\kappa_1$ gives

$$\begin{aligned}\ln[u(\zeta,x)]&=\sum_{j=0}^{\infty}\frac{1}{j!}(\zeta-\zeta_1)^j\frac{\partial^j\ln u}{\partial\zeta_1^j}\\&=\ln[u(\zeta_1,x)]+\sum_{j=1}^{\infty}\frac{1}{j!}(\zeta-\zeta_1)^j\\&\quad\times\frac{\partial^{j-1}}{\partial\zeta_1^{j-1}}\left(\alpha^2e^{-2\zeta_1}-\frac{5}{2}\right)\\&=\ln[u(\zeta_1,x)]-\frac{5}{2}(\zeta-\zeta_1)\\&\quad+\sum_{j=1}^{\infty}\frac{1}{j!}(-2)^{j-1}(\zeta-\zeta_1)^j\alpha^2e^{-2\zeta_1}\\&=\ln[u(\zeta_1,x)]-\frac{5}{2}(\zeta-\zeta_1)\\&\quad-\frac{\alpha^2}{2}e^{-2\zeta_1}\sum_{j=1}^{\infty}\frac{1}{j!}(-2)^{j-1}(\zeta-\zeta_1)^j\\&=\ln[u(\zeta_1,x)]-\frac{5}{2}\ln\left(\frac{\kappa}{\kappa_1}\right)-\frac{\alpha^2}{2}(e^{-2\zeta_1}-e^{-2\zeta})\\&=\ln[u(\zeta_1,x)]-\frac{5}{2}\ln\left(\frac{\kappa}{\kappa_1}\right)+\frac{\alpha^2}{2}\left(\frac{1}{\kappa_1^2}-\frac{1}{\kappa^2}\right),\end{aligned}\tag{14}$$

which restores all truncated scales. By superposition of Fourier components, this algorithm can be implemented on any given field. This is consistent with the classical Fourier analysis of the diffusion equation, in which the scale-dependent exponential attenuation can be reversed.

C. Trajectories

The second pair of canonical equations

$$\frac{dK}{dt}=-\frac{\partial H}{\partial\kappa}=-3\nu\kappa^2K+2\left(n+\frac{1}{2}\right)\nu\kappa uU \tag{15}$$

and

$$\frac{dU}{dt}=-\frac{\partial H}{\partial u}=\left(n+\frac{1}{2}\right)\nu\kappa^2U \tag{16}$$

are the equations for the trajectories. Substitution of Eqs. (9) and (10) and integration make a simple excercise. We get first

$$U=U_0\frac{u_0}{u}. \tag{17}$$

This shows that the product Uu is constant, implying that as u relaxes toward zero in a finite time t_c according to Eq. (10), U becomes ever larger. Furthermore, Eq. (15) yields

$$K=K_0\left\{\left[1-\left(n+\frac{1}{2}\right)\frac{u_0U_0}{\kappa_0K_0}\right]\left(\frac{\kappa_0}{\kappa(t)}\right)^3+\left(n+\frac{1}{2}\right)\frac{u_0U_0}{\kappa_0K_0}\frac{\kappa_0}{\kappa(t)}\right\}, \tag{18}$$

so that K collapses to the origin after time t_c. Accordingly, the trajectories for the diffusion problem escape to infinity in

U at vanishing K's, while the momenta escape to larger and larger κ's at vanishing u's, all in finite time.

The selection of any (nonsingular) origin (K_0U_0) of trajectories should not affect the solution of the diffusion problem as presented in Sec. II.A. With regard to Eq. (17), there is therefore no loss of generality to assume that the same value of u_0U_0 is used for all trajectories. For Eq. (18), two simplifying options impose themselves: we can assume that the same κ_0K_0 applies to all trajectories, yielding Fig. 3(a), or that the particular value

$$K_0=\left(n+\frac{1}{2}\right)\frac{u_0U_0}{\kappa_0} \tag{19}$$

is adopted as for Fig. 3(b). In this latter instance, $K(t)$ becomes inversely proportional to $\kappa(t)$ and the Hamiltonian [Eq. (6)] vanishes (up to an arbitrary constant). Clearly, the mapping of the trajectories is quantitatively affected by these choices, but without any effect on their topology or on the diffusion itself.

III. INVARIANTS

Several invariants can be noted. First, it is clear that

$$I_1=H \tag{20}$$

remains constant during the process. Specifically, the choice of the configuration variables discussed at the end of the preceding subsection will fix the value of H for each trajectory. In general, this constant can vary from trajectory to trajectory, i.e., be κ dependent; the particular case of Eq. (19) leads to a uniform H for all trajectories. A second invariant is found from the balance between the increase in κ and the decrease in u, in the form

$$I_2=u(t)\kappa(t)^{n+1/2}. \tag{21}$$

A third invariant is

$$I_3=u(t)U(t). \tag{22}$$

The interpretation of I_2 is easiest: it expresses the balance between the spreading and the magnitude of a ''bump'' under diffusion and can be read as an expression of ''mass'' conservation. I_3 makes u and U reciprocals of each other, up to a proportionality constant, and we will see in Sec. VI that it can be interpreted as a definition of U. It can be noted that Eq. (18) can be obtained directly from Eq. (6) as well as by integration of Eq. (15) and will not yield an independent invariant. A fuller discussion of the invariants will benefit from the N-dimensional results (Sec. V) and is delayed until Sec. VI.

IV. VARIATIONAL FORMULATION

The variational formulation associated with the canonical equations (7), (8), (15), and (16) follows from the construction of an associated Lagrangian L. Let us define

$$L(K,U,\dot{K},\dot{U})=\kappa\frac{\partial H}{\partial\kappa}+u\frac{\partial H}{\partial u}-H, \tag{23}$$

in which the original momenta κ and u are expressed in terms of K, $\dot{K}$, U, and $\dot{U}$. The Jacobian of the transformation,

$$J=\det\left(\frac{\partial^2 H}{\partial\pi_i\partial\pi_j}\right)=-4\left(n+\frac{1}{2}\right)\nu^2\kappa^2U^2, \tag{24}$$

does not vanish by virtue of Eqs. (17) and (9) until each trajectory escapes at its own t_c.

From Eqs. (15) and (16), it is easy to show that

$$\kappa(K,U,\dot{K},\dot{U})=\left(\frac{1}{\nu(n+\frac{1}{2})}\frac{\dot{U}}{U}\right)^{1/2} \tag{25}$$

and

$$u(K,U,\dot{K},\dot{U})=\frac{\dot{K}+\frac{3}{(n+\frac{1}{2})}\frac{K\dot{U}}{U}}{2\sqrt{(n+\frac{1}{2})\nu U\dot{U}}}. \tag{26}$$

Substitution into Eq. (23) shows that the Lagrangian takes the form

$$\begin{aligned}L(K,U,\dot{K},\dot{U})&=-\frac{\dot{U}^2K+(n+\frac{1}{2})U\dot{U}\dot{K}}{\sqrt{\nu}[(n+\frac{1}{2})U]^{3/2}\sqrt{\dot{U}}}\\&=2H(K,U,\kappa(K,U,\dot{K},\dot{U}),u(K,U,\dot{K},\dot{U})).\end{aligned} \tag{27}$$

The Lagrangian L is homogeneous of degree $-\frac{1}{2}$ in the configuration variables and of degree $\frac{3}{2}$ in their derivatives. When this Lagrangian is associated with the variational problem

$$\delta\int L\,dt=0, \tag{28}$$

it is staighforward to show that the Euler-Lagrange equations are identical to the characteristic equations (4) and (5) and to the canonical equations (7) and (8).

Finally, the diffusion equation can be cast in the form of a Hamilton-Jacobi equation, following well-known procedures [15]. From Eq. (6), we obtain

$$\begin{aligned}&\frac{\partial S}{\partial t}+H\left(K,U,\frac{\partial S}{\partial K},\frac{\partial S}{\partial U}\right)\\&\quad=\frac{\partial S}{\partial t}+\nu K\left(\frac{\partial S}{\partial K}\right)^3-\left(n+\frac{1}{2}\right)\nu U\left(\frac{\partial S}{\partial K}\right)^2\frac{\partial S}{\partial U}=0.\end{aligned} \tag{29}$$

It is well known [15] that $\int_{t_1}^{t_2}L\,dt$ is the geodesic distance between surfaces of constant $S=\Sigma_1$ and Σ_2.

V. THE N-DIMENSIONAL DIFFUSION EQUATION

Because the scaling factors κ_j are not endowed with vector transformation properties, the summation convention is suspended in the remainder of this paper. The wavelet-transformed N-dimensional diffusion equation of an M-component field u_i takes the form

$$\frac{\partial u_i}{\partial t}+\nu\sum_j \kappa_j^3\frac{\partial u_i}{\partial \kappa_j}+\nu\sum_j \kappa_j^2\left(n+\frac{1}{2}\right)u_i=0, \tag{30}$$

analogous to Eq. (2). The present author knows of no systematic procedure to generate the N-dimensional Hamiltonian. However, with the requirement that the characteristic equations corresponding to Eq. (30) (see [9]) should be obtained among the canonical equations, the generalization is easy. We propose

$$H(K_k,U_i,\kappa_k,u_i)=\sum_k \left[\nu\kappa_k^3K_k-\left(n+\frac{1}{2}\right)\nu\kappa_k^2\sum_i u_iU_i\right]$$

$$=\sum_k H_k. \tag{31}$$

H is a Hamiltonian in the sense that the canonical equations

$$\frac{du_i}{dt}=\frac{\partial H}{\partial U_i}=-\nu\left(n+\frac{1}{2}\right)u_i\sum_k \kappa_k^2 \tag{32}$$

and

$$\frac{d\kappa_j}{dt}=\frac{\partial H}{\partial K_j}=\nu\kappa_j^3 \tag{33}$$

are the characteristic equations for N-dimensional diffusion. The definition of the ''configuration variables'' U_i and K_j is found in the other pair of canonical equations

$$\frac{dK_j}{dt}=-\frac{\partial H}{\partial \kappa_j}=-3\nu\kappa_j^2K_j+2\left(n+\frac{1}{2}\right)\nu\kappa_j\sum_i u_iU_i \tag{34}$$

and

$$\frac{dU_i}{dt}=-\frac{\partial H}{\partial u_i}=\left(n+\frac{1}{2}\right)\nu U_i\sum_k \kappa_k^2. \tag{35}$$

Again the trajectories can be obtained by integration. We have

$$\kappa_j(t)=\kappa_{j0}(1-2\nu\kappa_{j0}^2t)^{-1/2}, \tag{36}$$

$$u_i=u_{i0}\prod_j (1-2\nu\kappa_{j0}^2t)^{n/2+1/4}=u_{i0}\prod_j \left(\frac{\kappa_{j0}}{\kappa_j(t)}\right)^{n+1/2}, \tag{37}$$

$$U_i=U_{i0}\frac{u_{i0}}{u_i}, \tag{38}$$

and

$$K_j=\left[K_{j0}-\left(n+\frac{1}{2}\right)\frac{\Sigma_iu_{i0}U_{i0}}{\kappa_{j0}}\right]\left(\frac{\kappa_{j0}}{\kappa_j(t)}\right)^3+\left(n+\frac{1}{2}\right)\frac{\Sigma_iu_{i0}U_{i0}}{\kappa_j(t)}. \tag{39}$$

The invariants generalize those listed in Sec. III. Obviously, H is an invariant, but in fact each of the H_k's is conserved independently. Indeed,

$$\frac{\partial H}{\partial K_m}=\delta_{mk}\frac{\partial H_k}{\partial K_m}, \tag{40}$$

with similar expressions for κ_m derivatives, so that the Poisson bracket of H and H_k vanishes,

$$\begin{aligned}[H,H_k]&=\sum_m \frac{\partial H}{\partial K_m}\frac{\partial H_k}{\partial \kappa_m}+\sum_i \frac{\partial H}{\partial U_i}\frac{\partial H_k}{\partial u_i}-\sum_m \frac{\partial H}{\partial \kappa_m}\frac{\partial H_k}{\partial K_m}\\
&\quad-\sum_i \frac{\partial H}{\partial u_i}\frac{\partial H_k}{\partial U_i}\\
&=\sum_m \frac{d\kappa_m}{dt}\delta_{mk}\left(-\frac{dK_m}{dt}\right)+\sum_i \frac{du_i}{dt}\\
&\quad\times[-\nu(n+1/2)\kappa_k^2U_i]-\sum_m \left(-\frac{dK_m}{dt}\right)\delta_{mk}\frac{d\kappa_m}{dt}\\
&\quad-\sum_i \left(-\frac{dU_i}{dt}\right)[-\nu(n+1/2)\kappa_k^2u_i]\\
&=0,\end{aligned} \tag{41}$$

when the odd symmetry of Eqs. (32) and (34) is taken into account. This yields N invariants of the type

$$I_{1k}=H_k. \tag{42}$$

The ''conservation equation'' corresponding to I_2,

$$I_{2i}=u_i(t)\prod_j \kappa_j(t)^{n+1/2} \tag{43}$$

holds for each component i, but combines all spatial directions, consistently with our interpretation. Finally,

$$I_{3i}=u_i(t)U_i(t) \tag{44}$$

also holds for each component separately. A straightforward extension of Eq. (23), the N-dimensional Lagrangian is defined as

$$\begin{aligned}&L(K's,U_i,\dot K's,\dot U_i)\\
&\quad=\sum_k \kappa_k\frac{\partial H}{\partial \kappa_k}+\sum_i u_i\frac{\partial H}{\partial u_i}-H\\
&\quad=2H(K's,U_i,\kappa's(K's,U_j,\dot K's,\dot U_j),\\
&\qquad u_i(K's,U_j,\dot K's,\dot U_j))\end{aligned} \tag{45}$$

and a matching Hamilton-Jacobi equation, not spelled out here, follows naturally.

VI. DISCUSSION

In this paper, the diffusion equation is reformulated with the combination of purely classical techniques: canonical formalism, theory of first-order partial differential equations, method of characteristics, variational formulations, harmonic analysis, and its latest addition, wavelet transform. The key to the canonical formulation of the diffusion problem lies in the continuous Hermitian wavelet transform, which captures the phenomenon in a different (arguably simpler) way.

The combined spatial and spectral discrimination performed by the wavelet transform in Eq. (A2) rearranges the physics of diffusion in such a way that the scale-dependent local dynamics become conservative and correspond to a strict variational problem. The conservative nature of the system can be traced to the existence of characteristics, itself a consequence of the compatibility relation [Eq. (A3)], and is conceptually related to the Green's function propagation of initial conditions: both artifacts of the wavelet transformation. The space variable x, although part of the wavelet space and implied in all wavelet-transformed equations, plays only the role of a parameter in the absence of convective effects.

Elementary dimensional considerations are in order. Since the diffusion equation is linear, u' can stand for any of the temperature, velocity, or concentration fields encountered in many problems; let us denote its dimensions by D. Then it follows from Eq. (A2) that u has dimensions $DL^{-1/2}$. Regardless of the particular field at hand, the diffusion coefficient ν has dimensions L^2T^{-1}. Then, in order to have a dimensionally consistent Hamiltonian H in Eq. (6), K must have dimensions L inverse of those of κ, and U have dimensions $L^{1/2}D^{-1}$ inverse of those of u, except for an arbitrary dimensional factor common to both K and U. Taking everything into account, assuming this common factor to be dimensionless, H has the same dimensions as the group $\nu\kappa^2$, i.e., T^{-1}. This is consistent with the Hamilton-Jacobi equation (29) when the Jacobi function S is dimensionless. Therefore, H emerges as the evolution operator familiar from classical and quantum mechanics.

The physical meaning of the Hamiltonian can be determined in conjunction with the invariants of the process. For clarity, one can emphasize first that the Hamiltonian defined by Eq. (31) is not of ''energy'' type and is unrelated to Salmon's cases of diffusive motion [3], the dissipative bracket formalism [5,6], or the conservation of energy under g_1 transform [13]. Among the invariants, the M I_{2i}'s can be interpreted as the conservation of ''mass'' under diffusive transport, a well-established idea. The other invariants offer the following pattern: we have N I_{1k}'s, from which the K's can be obtained (as well as from their respective differential equations) and the M I_{3i}'s are simple algebraic relation between the configuration variables (the U's) and the momenta (the u's) appearing in relation to the original problem. Thus, in numbers and analytical content, the I_{1k} and I_{3i} invariants can be interpreted as *definition* relations for the configuration variables, just as Eqs. (35) and (36), from which they were derived, were regarded as definition equations for the same variables. One can note that the definitions themselves are part of the Hamiltonian structure, so that the configuration variables U and K are fundamentally different from the adjoint variables in the restricted variational approaches of [2,1,16,17] and others mentioned in [3]. This explains why only the equations for the momenta are needed to solve the diffusion equation: the configuration variables play no dynamical role other than completing the canonical structure.

Within the Hamiltonian structure, a peculiar form of irreversibility was discoverd in Sec. II. The decomposition of the field by continuous Hermitian wavelets corresponds to a scale-dependent escape time. As noted in Sec. II, the gradual scale-dependent erosion of the initial conditions does not imply a memory loss, as long as the field is sufficiently smooth.

For the diffusion equation studied in this paper, the advantages of a Hamiltonian formulation are conceptual rather than computational. Many effective methods exist to solve the diffusion problem, and the doubling of independent variables associated with the wavelet transform hardly goes in the direction of increased economy of calculation. However, at the conceptual level, a number of surprises are noteworthy: the definition of a configuration space K-U in which the canonical formulation is valid, the formal manipulations associated with a simplectic structure, and the emergence of the Hamiltonian as an evolution operator for diffusion, both in the deterministic sense (Hamilton-Jacobi) and in the statistical sense (see, e.g., [18]), all enrich our knowledge of a classical problem.

Finally, the strong focus on linear diffusion adopted in this paper should not be perceived as an exclusion of strong nonlinearities. Hamiltonians for the Burgers equation and the Navier-Stokes equations are discussed in Appendix C and are the object of continuing work. The hope there is that the organization of turbulent flows around coherent structures might emerge in the newly defined phase space. Obviously, the complexities of the convolutions in wavelet space present difficulties of their own, but the existence of tools (e.g. renormalization applied to critical pheonmena) making use of Hamiltonians for complex systems offers some hope of success. In conclusion, we have derived a consistent framework in which to study diffusive processes.

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APPENDIX A: HERMITIAN WAVELET TRANSFORMS

It was shown by Meneveau [19] that the wavelet transformation (see [7,8]) can be applied to the Navier-Stokes equations. Then, the present author [9] made further progress by using Hermitian wavelets, i.e., wavelets obtained recursively as derivatives of the Gaussian bell curve g_0:

$$g_n(\zeta) = -\frac{d}{d\zeta} g_{n-1}(\zeta) \quad \text{where} \quad g_0(\zeta) = e^{-\zeta^2/2}. \tag{A1}$$

For $n>0$, the Hermitian wavelet transform at scale κ of a velocity $u(x)$ follows from the general definition and reads

$$u(\kappa,x) = \kappa^{1/2} \int_{-\infty}^{\infty} u'(y) g_n(\kappa(y-x)) dy. \tag{A2}$$

(κ,x) will be referred to as wavelet space and κ (>0) as the wavelet number. Integration by parts and the Hermite recursion relations yield the compatibility equation

$$\kappa^3 \frac{\partial u}{\partial \kappa} + \frac{\partial^2 u}{\partial x^2} + \left(n + \frac{1}{2}\right) \kappa^2 u = 0, \tag{A3}$$

which removes some of the redundancy associated with doubling the number of independent variables.

The properties of the transform used in the previous sections can be generalized to N dimensions if the transform is carried out in each Cartesian direction independently and if the same wavelet index n applies in each direction. Accordingly, the N-dimensional wavelet transform of the velocity field $u_i(\mathbf{x})$ is

$$u_i(\kappa' s,\mathbf{x},t)=\int \cdots \int_{-\infty}^{\infty} u_i'(\mathbf{y},t) \times\prod_{j=1}^{N} [\kappa_j^{1/2} g_n(\kappa_j(y_j-x_j))dy_j]. \quad \text{(A4)}$$

It can be noted that κ_j is a set of positive scaling coefficients and is not a vector. This fact is reflected in the notation, where $\boldsymbol{\kappa}$ will be avoided, and where the summation convention does not apply to κ_j. The N-dimensional compatibility equation assumes the form

$$\sum_j \kappa_j^3 \frac{\partial u_i}{\partial \kappa}+\sum_j \frac{\partial^2 u_i}{\partial x_j^2}+\left(n+\frac{1}{2}\right)\sum_j \kappa_j^2 u_i=0. \quad \text{(A5)}$$

APPENDIX B: CONSTRUCTION OF THE HAMILTONIAN

The construction of a Hamiltonian for diffusion follows the general presentation of Rund (see [15], pp. 60–63). Assume that the solution is implicitly given by a relation of the form

$$z(t,\kappa,u(t,\kappa))=0. \quad \text{(B1)}$$

Then define the variables

$$T=\frac{\partial z}{\partial t}, \quad \text{(B2)}$$

$$K=\frac{\partial z}{\partial \kappa}, \quad \text{(B3)}$$

and

$$U=\frac{\partial z}{\partial u}. \quad \text{(B4)}$$

Let

$$H(K,U,T,\kappa,u,t)=-UF\left(t,\kappa,u,-\frac{T}{U},-\frac{K}{U}\right). \quad \text{(B5)}$$

Rund shows that H is a Hamiltonian for some timelike parameter τ. In the case of Eq. (2), we obtain

$$H(K,U,T,\kappa,u,t)=T+\nu\kappa^3 K-\left(n+\frac{1}{2}\right)\nu\kappa^2 uU. \quad \text{(B6)}$$

Two of the canonical equations, namely,

$$\frac{dt}{d\tau}=\frac{\partial H}{\partial T}=1 \quad \text{(B7)}$$

and

$$\frac{dT}{d\tau}=-\frac{\partial H}{\partial t}=0, \quad \text{(B8)}$$

make it clear that t can be adopted as the independent parameter. Then, the Hamiltonian reduces to Eq. (6)

APPENDIX C: EXTENSION TO NONLINEAR PROBLEMS

Whatever simplifications wavelets can bring to linear problems do not extend to nonlinearities. The convolution of quadratic terms has been studied in [19,9] and presents definite disadvantages relative to the Fourier decomposition, particularly in the treatment of pressure in incompressible flows. These disadvantages may be offset by the existence of a canonical structure, and this appendix shows that a Hamiltonian formulation of nonlinear dissipative systems is possible.

As in [9], the Burgers equation

$$\frac{\partial u'}{\partial t}+u'\frac{\partial u'}{\partial x}=\nu\frac{\partial^2 u'}{\partial x^2} \quad \text{(C1)}$$

provides a good stepping stone toward the Navier-Stokes equations if the nonlinear terms are treated as source terms. The convolution is greatly simplified if the Hermitian wavelet is of even order, in which case the simplifying expression holds for the inverse transform:

$$u'(x,t)=\gamma\int_0^{\infty}\kappa^{-1/2}u(\kappa,x,t)d\kappa, \quad \text{(C2)}$$

where

$$\gamma=\left(-\frac{1}{2}\right)^{n/2}\frac{1}{\sqrt{2\pi}}\frac{1}{\Gamma(n)}. \quad \text{(C3)}$$

Then we can write

$$u'^2(x,t)=\gamma^2\int_0^{\infty}\int_0^{\infty}(\kappa_1\kappa_2)^{-1/2}u(\kappa_1,x,t)u(\kappa_2,x,t)d\kappa_1 d\kappa_2 =C(x,t), \quad \text{(C4)}$$

so that the convolution C combines contributions from all scales at each location. Upon wavelet transformation, the characteristic equation (7) remains unchanged and the wavelet-transformed nonlinear terms must be added to the right-hand side of Eq. (8), which is replaced by

$$\frac{du}{dt}=\frac{\partial H}{\partial U}=-\nu\left(n+\frac{1}{2}\right)\kappa^2 u -\frac{1}{2}\frac{\partial}{\partial x}\left(\int_0^{\infty}d\kappa C(x,t)\kappa^{1/2}g_n(\kappa(y-x))\right). \quad \text{(C5)}$$

Therefore, when we write the Hamiltonian as

$$H(K,U,\kappa,u)=\nu\kappa^3 K-U\left(n+\frac{1}{2}\right)\nu\kappa^2\widetilde{u} -\frac{U}{2}\frac{\partial}{\partial x}\left(\int_0^{\infty}d\kappa C(x,t)\kappa^{1/2}g_n(\kappa(y-x))\right), \quad \text{(C6)}$$

the first pair of canonical equations gives Eqs. (7) and (C5), so that the Burgers equation is derived from H. For the associated configuration variables K and U, defined by the other pair of canonical equations, it is not clear how the κ and u derivatives should be carried out. This issue will be examined elsewhere. Regardless of how it is resolved, the Hamiltonian now includes nonlocal contributions, spanning all κ's and a corresponding window of nearby x's, which makes a variational formulation unlikely.

No new complications are introduced by considering the incompressible Navier-Stokes equations. Let us define

$$C'_{ij}(\mathbf{x},t)=u'_i(\mathbf{x},t)u'_j(\mathbf{x},t)$$
$$=\gamma^6\int_0^\infty\cdots\int_0^\infty\prod_k\,[d\kappa_{1k}d\kappa_{2k}(\kappa_{1k}\kappa_{2k})^{-1/2}]$$
$$\times u_i(\kappa'_1 s,\mathbf{x},t)u_j(\kappa'_2 s,\mathbf{x},t) \qquad \text{(C7)}$$

and its wavelet transform

$$C_{ij}(\kappa' s,\mathbf{x},t)=\int_{-\infty}^\infty\cdots\int_{-\infty}^\infty C'_{ij}$$
$$\times\prod_k\,[dy_k\kappa_k^{1/2}g_n(\kappa_k(y_k-x_k))]. \qquad \text{(C8)}$$

With these notations, the wavelet-transformed pressure field [9] associated with the velocity derivatives can be rewritten as

$$\frac{p}{\rho}=-\sum_j\,\sum_m\,\frac{\partial}{\partial x_m}\,\frac{\partial}{\partial x_j}\int_{-\infty}^0 ds C_{jm}(\kappa_k(s),\mathbf{x},t)$$
$$\times\prod_k\,(1-2s\kappa_k^2)^{n/2+1/4} \qquad \text{(C9)}$$

and the characteristic equation for velocity u_i becomes

$$\frac{du_i}{ds}=-\nu\left(n+\frac{1}{2}\right)u_i\sum_k\,\kappa_k^2-\frac{1}{\rho}\,\frac{\partial p}{\partial x_i}-\sum_j\,\frac{\partial}{\partial x_j}C_{ij}. \qquad \text{(C10)}$$

With these expressions, the Hamiltonian governing Newtonian incompressible flows is

$$H(K's,U_i,\kappa's,u_i)$$
$$=\nu\sum_k\,\kappa_k^3K_k-\left(n+\frac{1}{2}\right)\nu\sum_i\,U_iu_i\sum_k\,\kappa_k^2$$
$$-\sum_i\,\sum_j\,U_i\frac{\partial}{\partial x_j}C_{ij}-\sum_i\,\sum_j\,\sum_m\,U_i\frac{\partial}{\partial x_i}\,\frac{\partial}{\partial x_m}\,\frac{\partial}{\partial x_j}$$
$$\times\int_{-\infty}^0 ds C_{jm}(\kappa_k(s),\mathbf{x},t)\prod_k\,(1-2s\kappa_k^2)^{n/2+1/4}. \qquad \text{(C11)}$$

Starting from Eq. (C11), the charactersitic form of the Navier-Stokes equations can be derived as one pair of canonical equations. As in the case of the Burgers equation, the definition of the configuration variables remains to be elucidated.

APPENDIX D: HERMITIAN WAVELETS AS GREEN'S FUNCTIONS

Another profound relation between Hermitian wavelets and the diffusion equation is illustrated here (This material was presented as part of [12].) In the presence of a source field, the diffusion equation takes the form

$$\frac{\partial f}{\partial t}-\nu\frac{\partial^2 f}{\partial x_i^2}=\Phi_{\mathrm{rhs}}. \qquad \text{(D1)}$$

The field $f(\mathbf{x},t)$ is determined by a combination of the source field Φ_{rhs} and suitable boundary and initial conditions. The Green's-function formalism [11] captures concisely this dependence:

$$f(\mathbf{x},t)=\int_{t_0}^{t+}dt_0\int dV_0G^d(\mathbf{x},t|\mathbf{x}_0,t_0)\Phi_{\mathrm{rhs}}(\mathbf{x}_0,t_0)$$
$$+\int dV_0G^d(\mathbf{x},t|\mathbf{x}_0,0)f^0(\mathbf{x}_0,0)+\nu\int_{t_0}^{t+}dt_0$$
$$\times\oint d\mathbf{A}_0\cdot[G^d\nabla_0 f(\mathbf{x}_0,t_0)-f(\mathbf{x}_0,t_0)\nabla_0G^d]$$
$$=\int G^d(\mathbf{x},t|\mathbf{x}_0,t_0)\psi(x_0,t_0)=G^d\circ\psi, \qquad \text{(D2)}$$

where ψ stands indifferently for sources or initial or boundary conditions, and G^d is used as the integration kernel or the integral operator.

Let us focus on one-dimensional diffusion first. In an infinite domain, the function G^d is

$$G^d(x,t|x_0,t_0)$$
$$=H(t-t_0)\frac{1}{\sqrt{4\pi\nu(t-t_0)}}\exp\left[-\left(\frac{(x-x_0)^2}{4\nu(t-t_0)}\right)\right]$$
$$=H(t-t_0)\frac{\kappa_\nu}{\sqrt{2\pi}}\exp\left[-\left(\frac{\kappa_\nu^2(x-x_0)^2}{2}\right)\right] \qquad \text{(D3)}$$

when we define a time-dependent inverse length scale κ_ν as

$$\kappa_\nu=[2\nu(t-t_0)]^{-1/2}. \qquad \text{(D4)}$$

The Green's function is thus identical (for $t>t_0$) to the "basic solution" as presented in Widder [10]. Furthermore, Widder's presentation of differentiation, integration and convolution of the basic solution established the link between the Gaussian bell curve and the Hermite functions, and the diffusion equation.

This appendix goes one step further, by showing that for a (multiscale) resolution of the field in terms of Hermitian wavelets, the same family of wavelets serves as functional basis, as convolution kernel, *and* as Green's function. The wavelet transformation is defined for real wavelets such as g_n by the equation [9]

$$f_n(\kappa,x,t)=W_n(\kappa)\circ f(x,t)=\int_{-\infty}^\infty f(y,t)\kappa^{1/2}g_n(\kappa(y-x))dy. \qquad \text{(D5)}$$

Because of the existence of an inverse transform (see [7]), the f_n's can be interpreted as a local spectral decomposition of the field f. The wavelet transform is now applied to the solution given by Eq. (D2). It is straightforward to verify that

$$\begin{aligned} W_n(\kappa)\circ f(x,t) &= W_n(\kappa)\circ \int G^d(x,t|x_0,t_0)\psi(x_0,t_0) \\ &= \int [W_n(\kappa)\circ G^d(x,t|x_0,t_0)]\psi(x_0,t_0) \\ &= [W_n(\kappa)\circ G^d]\circ\psi = G_n^d(\kappa)\circ\psi. \end{aligned} \tag{D6}$$

The propagator G_n^d in the transformed space is defined by Eq.(D6), and is calculated to be

$$G_n^d(\kappa)=W_n(\kappa)\circ G^d = H(t-t_0)\left(\frac{\kappa_\nu^*}{\kappa}\right)^{n+1/2} W_n(\kappa_\nu^*), \tag{D7}$$

with

$$\kappa_\nu^* = \frac{\kappa\kappa_\nu}{\sqrt{\kappa^2+\kappa_\nu^2}} = \frac{\kappa}{\sqrt{1+2\nu\kappa^2(t-t_0)}}. \tag{D8}$$

Therefore, we see that the solution of the diffusion problem is a rescaled wavelet transform of the source field and of the initial and boundary conditions.

The N-dimensional result can be obtained also by a different method. We use the nonisotropic wavelet transform [9]:

$$f_n(\kappa_k,\mathbf{x},t)=\int\int\int_{-\infty}^{\infty} f(\mathbf{y},t)\prod_{j=1}^{3}[\kappa_j^{1/2} g_n(\kappa_j(y_j-x_j))dy_j]. \tag{D9}$$

Making use of the compatibility relation for Hermitian wavelet transforms [9], the equation governing the wavelet transform of the Green's function is

$$\begin{aligned} &\frac{\partial G_n^d}{\partial t}+\nu\sum_i \kappa_i^3\frac{\partial G_n^d}{\partial\kappa_i}+(n+1/2)\nu\sum_i \kappa_i^2 G_n^d \\ &= \delta(t-t_0)W_n(\kappa_k)\circ\delta(\underline{\mathbf{x}}-\underline{\mathbf{x}}_0) \\ &= \delta(t-t_0)\prod_i \kappa_i^{1/2} g_n(\kappa_i(x_{i0}-x_i)). \end{aligned} \tag{D10}$$

This equation can be integrated by the method of characteristics [9], yielding the solution

$$\begin{aligned} &G_n^d(\kappa_k,\mathbf{x},t|\mathbf{x}_0,t_0) \\ &= H(t-t_0)\prod_i\left[\left(\frac{\kappa_i}{\kappa_{\nu i}^*}\right)^{-n-1/2}\kappa_{\nu i}^{*\,1/2} g_n(\kappa_{\nu i}^*(x_i-x_{i0}))\right], \end{aligned} \tag{D11}$$

equivalent to Eq.(D7) when $N=1$.

Therefore, the solution of Eq.(D1) in an infinite domain is

$$\begin{aligned} f_n(\kappa_i,\mathbf{x},t) &= \int_{t_0}^{t+} dt_0 \prod_j\left(\frac{\kappa_{\nu j}^*(t-t_0)}{\kappa_j}\right)^{n+1/2} \\ &\times W_n(\kappa_\nu^*)\circ\Phi_{\rm rhs}(\mathbf{x},t_0) \\ &+ \prod_j\left(\frac{\kappa_{\nu j}^*(t-t_0)}{\kappa_j}\right)^{n+1/2} W_n(\kappa_\nu^*)\circ f^0(\mathbf{x},0) \\ &+ \nu\int_{t_0}^{t+} dt_0 \oint d\mathbf{A}_0\cdot[G_n^d(\kappa,\mathbf{x},t|\mathbf{x}_0,t_0)\nabla_0 f(\mathbf{x}_0,t_0) \\ &- f(\mathbf{x}_0,t_0)\nabla_0 G_n^d(\kappa,\mathbf{x},t|\mathbf{x}_0,t_0)] \end{aligned} \tag{D12}$$

.

This reduces to the solution obtained by other methods [9] in the absence of boundaries.

In conclusion, a fundamental relation exists between the Hermitian wavelets and the diffusion equation. The rescaled wavelets, obtained previously [9] by the method of characteristics applied to source terms and initial conditions, are in fact Green's propagators in an infinite domain. By superposition of images [20], the result extends as well to simple finite geometries. The kinship between the diffusion Green's function and the Hermitian wavelets explains that diffusion processes appear so different when transformed with these wavelets. In the rapidly expanding wavelet literature, orthogonal wavelets have become the widely preferred tool, because of the economy of representation they offer; in contrast, this paper points to analytical benefits available from Hermitian continuous wavelets.

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