Phase transitions and symmetry breaking in singular diffusion

Jochen Denzler* and Robert J. McCann†‡

*Department of Mathematics, University of Tennessee, Knoxville, TN 37996-1300; and †Department of Mathematics, University of Toronto, Toronto, ON, Canada M5S 3G3

Communicated by Paul H. Rabinowitz, University of Wisconsin, Madison, WI, April 1, 2003 (received for review October 28, 2002)

The long-time asymptotics are determined for fast nonlinear diffusion by linearizing Otto's gradient descent model at the Barenblatt profile. The spectrum of the entropy is explicitly determined. The dynamics are found to undergo a phase transition in which rotational symmetry is broken as the strength of the nonlinearity is varied.

This report outlines the results of a spectral calculation, the mathematical details of which will be published separately. The calculation is motivated by the nonlinear diffusion

$$\frac{\partial u}{\partial t} = \kappa\Delta(u^{\frac{p+n-2}{p+n}}) + \sigma\,\mathrm{div}[xu] \qquad [1]$$

of a density $u(t, x) \geq 0$ throughout $[0, \infty[\times \mathbf{R}^n$. For different values of p and suitable boundary conditions, this equation has been used to model groundwater flow (1–3), thermalization in plasmas (4), curvature-driven evolution (5, 6), and avalanches in sandpiles (7, 8). Although most of these models require slow diffusion $p < -n$ or fast diffusion with decay of mass $p \in]-n, 0]$, here we focus on the regime $p > 0$ corresponding to conservative fast or singular diffusion, in which the diffusivity $u^{-2/(p+n)}$ diverges at low densities. It is well known that solutions to Eq. **1** for any value $\sigma = \sigma_1$ are related to the solutions for any other value $\sigma = \sigma_2 \in \mathbf{R}$ by a time-dependent rescaling of space, so it costs no generality to choose units of time and distance that make the constants $\sigma := p + n$ and $\kappa = \sigma/(p + n - 2)$. The scaling solution

$$u(t, x) = \rho(x) := \frac{1}{(1 + |x|^2)^{\frac{p+n}{2}}}, \quad p > 0 \qquad [2]$$

then becomes a fixed point of the dynamics (Eq. **1**), usually referred to as the Barenblatt self-similar (9) or source-type (10) profile. For $p \notin [-n, 0]$, the dynamics preserve the integral of $u(t, x)$ (11), and Friedman and Kamin (12) have shown that the scaling solution attracts all solutions that share its mass.

Recently, much effort has been devoted to quantifying the rate of convergence of solutions to the scaling solution for $n \geq 2$ (13).§ Various bounds on the nonlinear rate of convergence for $p < -n$ have been provided by Carrillo and Toscani (14), Dolbeault and del Pino (15), and Otto (16), and for $n \leq p \neq 2$ also (15, 16). All of them are sharp for convergence of translations $u_0(x) := \rho(x - x_0)$ to the centered scaling profile. For $0 < p < n$, different nonlinear bounds were derived by Carrillo and Vázquez (17) based on an earlier analysis of the linearized dynamics around the fixed point due to Carrillo *et al.* (18). These bounds are not sharp except for radially symmetric initial data u_0, where they correspond to the rate of convergence of dilations $u_0(x) = r_0^{-n}\rho(x/r_0)$ to the normalized scaling profile (Eq. **2**).

In most cases, the starting point for deriving these bounds has been the Lyapunov functional introduced by Newman (19, 20), akin to Rényi entropy (21), or its renormalization due to Lederman and Markowich (22),

$$E(u) := \int_{\mathbf{R}^n} \{e(u(x)) - e(\rho(x)) - e'(\rho(x))[u(x) - \rho(x)]\}\,dx \qquad [3]$$

$$= c_{p,n} - \frac{\kappa\sigma}{2}\int_{\mathbf{R}^n} [u(x)^{-\frac{2}{p+n}} - 1]\,u(x)\,dx + \frac{\sigma}{2}\int_{\mathbf{R}^n} x^2 u(x)\,dx, \qquad [4]$$

with convex density $e(\varrho) := -(\kappa\sigma/2)(\varrho^{1/\kappa} - \varrho)$. The second equality (Eq. **4**) must be omitted if $p \in]0, 2]$, because then $c_{p,n} = +\infty$, but Eq. **3** continues to define a nonnegative entropy $E(u) \geq 0$, which vanishes only at the scaling profile $u = \rho$.

Conceptually, Otto's work goes further to heuristically identify the dynamics (Eq. **1**) as the steepest descent or gradient flow of the entropy $E(u)$ on an infinite-dimensional Riemannian manifold $\mathcal{M}$ (16). Here $\mathcal{M}$ consists of all integrable densities $u(x) \geq 0$ with finite second moments and the mass $m_{p,n}$ of the scaling solution. The geodesic distance between two such densities u and v is given by the Wasserstein metric (23)

$$d_2(u, v)^2 := \inf_{\gamma\in\Gamma(u,v)} \int_{\mathbf{R}^n\times\mathbf{R}^n} |x - y|^2 d\gamma(x, y), \qquad [5]$$

the infimum being taken over the space $\Gamma(u, v)$ of joint measures $\gamma \geq 0$ on $\mathbf{R}^n \times \mathbf{R}^n$ with u and v for marginals. Thus $d_2(u, v)/\sqrt{m_{p,n}}$ represents the minimum root mean square distance required to pair the particles of u with those of v.

For a gradient flow $\dot{v}(t) = -\mathrm{grad}_{v(t)}E$ on any manifold, the dynamics near a fixed point ρ are determined by the Hessian $\mathrm{Hess}_\rho E$ of the entropy, viewed as a self-adjoint operator on the tangent space $\mathcal{T}_\rho\mathcal{M}$. This is the operator that we shall diagonalize.

A literal interpretation of Otto (16) asserts that the tangent space $\mathcal{T}_u\mathcal{M}$ to the manifold at u is the Hilbert-space completion of the smooth functions $\Psi : \mathbf{R}^n \to \mathbf{R}$ with compact support using the inner product

$$\langle\Psi;\,\Phi\rangle_u := \int_{\mathbf{R}^n} u(x)\nabla\Psi(x)\cdot\nabla\Phi(x)\,dx. \qquad [6]$$

Notice that two functions that differ by a constant will represent the same vector in this Hilbert space. Local coordinates $\exp_u : \mathcal{T}_u\mathcal{M} \to \mathcal{M}$ on the manifold are defined by the exponential map $v = \exp_u s\Psi$, where

$$v(x + s\nabla\Psi(x)) := u(x)/\det[I + sD^2\Psi(x)]. \qquad [7]$$

‡To whom correspondence should be addressed. E-mail: mccann@math.toronto.edu.

§The rate-of-convergence question for very fast diffusion was raised in a lecture by Peter Markowich at the 2000 Summer School "Mass Transportation Methods in Kinetic Theory and Hydrodynamics," organized in Azores by Maria Carvalho and the European Kinetic Theory Training and Mobility Research Network, September 4–9, 2000.

 www.pnas.org/cgi/doi/10.1073/pnas.1231896100

Taking two derivatives $d^2E(v_s)/ds^2$ along the geodesic curve Eq. **7**, we compute the formal Hessian of E at the scaling solution ρ to coincide with the quadratic form

$$Q_\rho(\Psi) := \int_{\mathbf{R}^n} \left(\operatorname{div} \frac{\nabla\Psi(\boldsymbol{x})}{(\sqrt{1+|\boldsymbol{x}|^2})^{p+n}} \right)^2 (\sqrt{1+|\boldsymbol{x}|^2})^{p+n+2} d\boldsymbol{x}. \quad [8]$$

Our first theorem computes the spectral gap of the dynamics as its Rayleigh–Ritz quotient on the Hilbert space $\mathcal{H} := T_\rho\mathcal{M}$. We call it a Sobolev inequality, because it implies the gradient $\nabla\Psi$ in Eq. **6** is controlled by $D^2\Psi$ in Eq. **8**; the weights are arranged such that two extra powers of $\sqrt{1+|\boldsymbol{x}|^2}$ in Eq. **8** compensate for the new derivatives of Ψ.

Theorem 1 (Sobolev Inequality with Phase Transition and Symmetry Breaking). *For $n \geq 2$, the infimum*

$$\Lambda_0 := \inf_{0\neq\Psi\in\mathcal{H}} \frac{Q_\rho(\Psi)}{\langle\Psi;\Psi\rangle_\rho} = \begin{cases} \left(\frac{p}{2}+1\right)^2 & p \in]0,2] \\ 2p & p \in]2,n] \\ p+n & p \geq n \end{cases} \quad [9]$$

is attained only if $p > 2$ and only by polynomials of degree ≤ 2 on $\mathbf{R}^n$. More precisely, there are no minimizers but $\Psi(\boldsymbol{x}) = \mathbf{a}\cdot\boldsymbol{x} + b$ if $p \geq n$, or $\Psi(\boldsymbol{x}) = c|\boldsymbol{x}|^2 + b$ if $2 < p \leq n$, with $\mathbf{a} \in \mathbf{R}^n$ and $b, c \in \mathbf{R}$ arbitrary.

A nondifferentiability of the spectral gap (Eq. **9**) occurs at $p = n$ due to a level crossing of eigenvalues. This crossing represents a phase transition from a regime in which the rate of convergence is governed by translations of ρ to one in which it is governed by dilations, and was discovered simultaneously and independently by Carrillo and Vázquez (17). This is also the precise exponent at which the dynamics cease to be a contraction in Wasserstein distance, because for $p < n$ the entropy $E(u)$ fails to satisfy McCann's notion of displacement convexity (24). Rotational symmetry is broken when $p > n$, and each minimizer becomes associated with a direction $\mathbf{a} \neq \mathbf{0}$ in $\mathbf{R}^n$. A second phase transition occurs at $p = 2$ due to the fact that the scaling solution no longer has finite variance; Wasserstein distance becomes too restrictive to measure rates of convergence effectively when $p \in]0,2]$, and we are no longer posing the problem in the correct Hilbert space.

To complete the picture, we give the spectral gap in one dimension as well, where there are no phase transitions.

Theorem 2 (Absence of Phase Transitions in One Dimension). *For $n = 1$ and all $p > 0$, the infimum (Eq. **10**) is attained only by $\Psi(x) = ax + b$, with $a, b \in \mathbf{R}$ arbitrary:*

$$\inf_{0\neq\Psi\in\mathcal{H}} \frac{Q_\rho(\Psi)}{\langle\Psi;\Psi\rangle_\rho} = p+1. \quad [10]$$

Both theorems are proved by finding the spectrum of the operator $\mathbf{H}$ defined on $\mathcal{H}$ by $\mathbf{H}\Psi := -(1+|\boldsymbol{x}|^2)\Delta\Psi + \sigma\boldsymbol{x}\cdot\nabla\Psi$, or more precisely its Friedrichs extension from the smooth functions with compact support. Note that $Q_\rho(\Psi) = \langle\Psi;\mathbf{H}\Psi\rangle_\rho$. Moreover, $[\mathbf{H}, \boldsymbol{L}^2] = 0$, where $\boldsymbol{L}^2 := -\Delta_{\mathbf{S}^{n-1}}$ is the total angular momentum operator, so both operators can be diagonalized simultaneously. Thus the eigenvalue problem $\mathbf{H}\Psi = \lambda\Psi$ separates in spherical coordinates, with the angular part being solved by spherical harmonics $Y_{l\mu}$ and the radial part reducing to a hypergeometric equation. This permits the spectrum to be understood completely; the eigenfunctions Ψ turn out to be polynomials of degree $2k + l < 1 + p/2$, thus growing slowly enough so that $\Psi \in \mathcal{H}$. Because the scaling solution (Eq. **2**) possesses only a finite number p of moments, this integrability restriction leads to continuous spectrum instead of larger eigenvalues.

Theorem 3 (Exact Spectrum). *Fix $p > 0$. For $l = 0, 1, 2, \ldots$, let $\mathbf{H}_l$ denote the restriction of $\mathbf{H}$ to the eigenspace of $\boldsymbol{L}^2 := -\Delta_{\mathbf{S}^{n-1}}$ corresponding to eigenvalue $L^2 = l(l+n-2)$. The eigenfunctions $\mathbf{H}_l\ \Psi_{lk\mu} = \lambda_{lk}\Psi_{lk\mu}$ in $\mathcal{H}$ are given by*

$$\Psi_{lk\mu}(\boldsymbol{x}) = \psi_{lk}(|\boldsymbol{x}|) Y_{l\mu}\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right) \quad \begin{matrix} k = 0, 1, 2, \ldots \\ 0 < l + 2k < 1 + p/2 \end{matrix}$$

where $Y_{l\mu}$ is a spherical harmonic $-\Delta_{\mathbf{S}^{n-1}} Y_{l\mu} = l(l+n-2)Y_{l\mu}$ and

$$\psi_{lk}(r) = \sum_{j=0}^{k} \frac{(-k)_j (k+l-1-p/2)_j}{(1)_j (l+n/2)_j} (-1)^j r^{2j+l} \quad [11]$$

with $(a)_j := a(a+1)\ldots(a+j-1)$. Apart from the corresponding eigenvalues $\lambda_{lk} = L^2 + [(p/2)+1]^2 - [(p/2)+1-l-2k]^2$, the spectrum of $\mathbf{H}_l$ is purely continuous, and consists of the interval $[\lambda_l^{\text{cont}}, +\infty[$ above the threshold $\lambda_l^{\text{cont}} := L^2 + [(p/2)+1]^2$.

The complete spectrum for dimension $n = 5$ is displayed in Fig. 1. Colors indicate the different spherical harmonics, whereas continuum thresholds are depicted as shaded parabolas. As discussed in our subsequent work, comparison of the evolving density to an appropriate translation or dilation of the Barenblatt solution should speed convergence by replacing the spectral gap associated with the ground state (Eq. **9**) by the next higher energy level:

$$\Lambda_1 = \begin{cases} \lambda_0^{\text{cont}} = \left(\frac{p}{2}+1\right)^2 & & p \in]0, \sqrt{n-1}] \\ \lambda_{10} = p+n & \text{(translation)} & p \in [\sqrt{n-1}, n] \\ \lambda_{01} = 2p & \text{(dilation)} & p \in [n, \infty], \end{cases}$$

or, if the Barenblatt is both translating and dilating,

$$\Lambda_2 = \begin{cases} \lambda_0^{\text{cont}} & & p \in]0,6] \\ \lambda_{02} = 4(p-2) & & p \in [6, n+4] \\ \lambda_{20} = 2(p+n) & \text{(affine)} & p \in [n+4, \infty]. \end{cases} \quad [12]$$

The last value λ_{20} corresponds to the rate of convergence in Wasserstein distance of an affine image to the Barenblatt. Note that the continuum threshold diverges $\lambda_l^{\text{cont}} \to +\infty$ as $p \to \infty$, whereas the spectrum of $p^{-1}\mathbf{H}$ collapses onto the positive integers. This follows from a hidden conjugacy between the heat equation (Eq. **1**) and the quantum harmonic oscillator. The same limit takes the middle contribution in Eq. **4** to Boltzmann's entropy, whereas the scaling solution, normalized to unit mass and variance, converges to a standard Gaussian.

To develop the analogy with thermodynamic phase transitions, we remark that the spectral gap computed in Eq. **9** predicts the asymptotic rate of convergence

$$\lim_{t\to\infty} \frac{\log d_2(u,\rho)}{t} = -\Lambda_0(p).$$

Here the distance $d_2(u(t),\rho)$ to equilibrium plays the role of the statistical mechanical partition function $Z_N^{-1}(\beta)$, with the degree of nonlinearity p in place of the inverse temperature β. Elapsed time t plays the role of system size N, so $t \to \infty$ is like a thermodynamic limit. A phase transition is said to occur where this limit depends nonsmoothly on parameters, as at $p = 2$ or $p = n$; an associated symmetry is broken at "low temperatures" $p >$

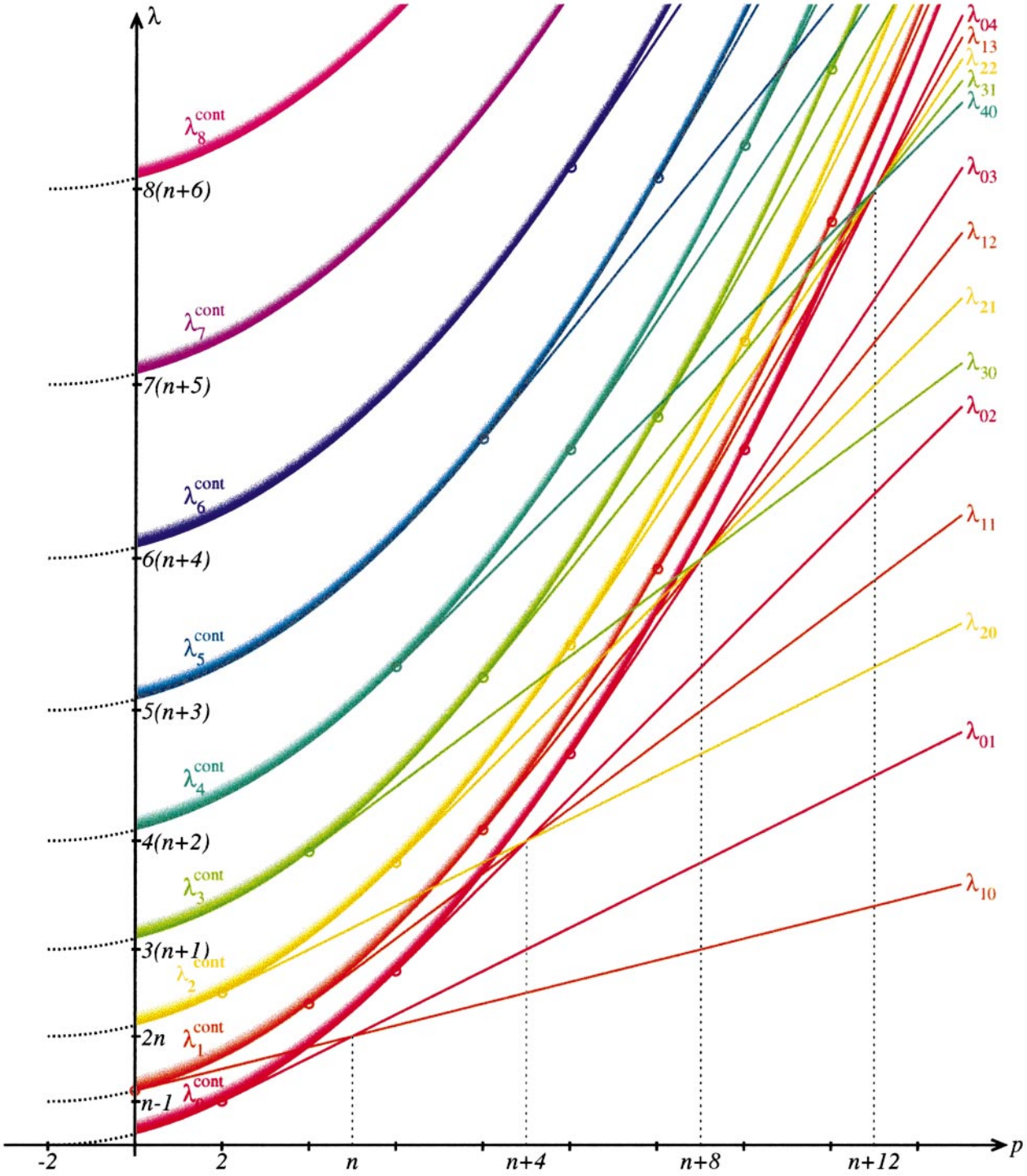

Fig. 1. Eigenvalues λ_{jk} and thresholds of continuous spectrum in dimension $n = 5$.

n. Level crossings at $p = n + 4$ in Fig. 1 represent phase transitions in the finer asymptotics of $d_2(u(t), \rho)$.

For the porous medium regime $p < -1$ in one dimension $n = 1$, Zel'dovich and Barenblatt (25) found a complete basis of eigenfunctions for the spectrum at the fixed point long ago. This was rediscovered by Angenent (26), who also derived the correct long-time asymptotics for the nonlinear equation (Eq. **1**). It is interesting to highlight the reasons for our success in producing the higher dimensional spectrum that Zel'dovich and Barenblatt claimed to be unable to resolve. One reason is technical, and the other is conceptual. The technical advantage to working in the singular-diffusion range $p > 0$ rather than the porous-medium regime $p < -n$ is that long-tailed distributions may be easier to deal with than compactly supported solutions, the evolving boundaries of which involve nontrivial geometry. However, we expect to surmount this difficulty with further study; we have not concentrated on $p < 0$, because our original motivation was to understand the $p \geq n$ restriction (15, 16, 24), which hinted at the presence of a phase transition. The conceptual reason for our success is that the Riemannian formulation of Otto puts the

problem in a Hilbert-space setting, where the Hessian **H** is self-adjoint, and angular momentum is conserved due to rotational symmetry. Thus the separation into radial and angular variables becomes as natural as it is inevitable. Without the Riemannian structure, one tries to analyze an operator on a Banach space, and the separation of angular variables remains as difficult to find as it is to solve.

We thank Eric Carlen, Dario Cordero-Erausquin, Wilfrid Gangbo, Anastasia Ruzmaikina, and Michael Sigal for providing fruitful discussions. We are grateful to José Carrillo and Juan Luis Vázquez for sharing their work with us in preprint form. R.J.M. was supported by National Science Foundation Grant DMS 0074037, Natural Sciences and Engineering Research Council of Canada Grant 217006-99 RGPIN, and an Ontario Premier's Research Award of Excellence.

1. Boussinesq, J. (1904) *J. Math. Pures Appl.* **10,** 5–78.
2. Muskat, M. (1937) *The Flow of Homogeneous Fluids Through Porous Media* (McGraw–Hill, New York).
3. Barenblatt, G. I., Entov, V. M. & Ryzhil, V. M. (1990) *Flow of Fluids Through Natural Rocks* (Kluwer, Dordrecht, The Netherlands).
4. Zel'dovich, Y. B. & Kompaneets, A. S. (1950) in *Collection in Honour of the 70th Birthday of Academician A. F. Ioffe* (Izv. Akad. Nauk SSSR, Moscow), pp. 61–71.
5. Vázquez, J. L., Esteban, J. R. & Rodríguez, A. (1996) *Adv. Differ. Equ.* **1,** 21–50.
6. del Pino, M. & Saez, M. (2001) *Indiana Univ. Math. J.* **50,** 612–628.
7. Carlson, J. M., Chayes, J. T., Grannan, E. R. & Swindle, G. H. (1990) *Phys. Rev. Lett.* **65,** 2547–2550.
8. Chayes, J. T., Osher, S. J. & Ralston, J. V. (1993) *Commun. Pure Appl. Math.* **46,** 1363–1377.
9. Barenblatt, G. I. (1952) *Akad. Nauk. SSSR Prikl. Mat. Mekh.* **16,** 67–78.
10. Pattle, R. E. (1959) *Q. J. Mech. Appl. Math.* **12,** 407–409.
11. Benilan, P. & Crandall, M. G. (1981) *Indiana Univ. Math. J.* **30,** 161–177.
12. Friedman, A. & Kamin, S. (1980) *Trans. Am. Math. Soc.* **262,** 551–563.
13. Vázquez, J. L. (2003) *J. Evol. Equ.* **3,** 67–118.
14. Carrillo, J. A. & Toscani, G. (2000) *Indiana Univ. Math. J.* **49,** 113–141.
15. Dolbeault, J. & del Pino, M. (2002) *J. Math. Pures Appl.* **81,** 847–875.
16. Otto, F. (2001) *Commun. Partial Differ. Equations* **26,** 101–174.
17. Carrillo, J. A. & Vázquez, J. L. (2003) in *Commun. Partial Differ. Equations*, in press.
18. Carrillo, J. A., Lederman, C., Markowich, P. A. & Toscani, G. (2002) *Nonlinearity* **15,** 565–580.
19. Newman, W. (1984) *J. Math. Phys.* **25,** 3120–3123.
20. Ralston, J. (1984) *J. Math. Phys.* **25,** 3124–3127.
21. Rényi, A. (1961) in *Proceedings of the 4th Berkeley Symposium on Mathematical Statistics and Probability* (Univ. of California Press, Berkeley), Vol. 1, pp. 547–561.
22. Lederman, C. & Markowich, P. A. (2003) *Commun. Partial Differ. Equations* **28,** 363–401.
23. Givens, C. R. & Shortt, R. M. (1984) *Michigan Math. J.* **31,** 231–240.
24. McCann, R. J. (1997) *Adv. Math.* **128,** 153–179.
25. Zel'dovich, Y. B. & Barenblatt, G. I. (1958) *Sov. Phys. Dokl.* **3,** 44–47.
26. Angenent, S. B. (1988) in *Nonlinear Diffusion Equations and Their Equilibrium States I (Mathematical Sciences Research Institute Publications, Vol. 13)* (Springer, New York), Vol. 12, pp. 21–34.