

Optimal protocols and optimal transport in stochastic thermodynamics

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Thermodynamics of small systems has become an important field of statistical physics. They are driven out of equilibrium by a control, and the question is naturally posed how such a control can be optimized. We show that optimization problems in small system thermodynamics are solved by (deterministic) optimal transport, for which very efficient numerical methods have been developed, and of which there are applications in Cosmology, fluid mechanics, logistics, and many other fields. We show, in particular, that minimizing expected heat released or work done during a non-equilibrium transition in finite time is solved by Burgers equation of Cosmology and mass transport by the Burgers velocity field. Our contribution hence considerably extends the range of solvable optimization problems in small system thermodynamics.

PACS numbers: 05.40.-a,02.50.Ey,05.40.Jc,87.15.H-

The last two decades has seen a revolution in the understanding of thermodynamics of small systems driven out of equilibrium. Jarzynski's equality (JE) [1] relates an exponential average of the thermodynamic work W done on a system, driven from an initial equilibrium state to another final state, to the exponentiated free energy difference ΔF between these two states:

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F} . \quad (1)$$

Here and in the following $\beta = 1/k_B T$ is the inverse temperature, k_B the Boltzmann's constant and $\langle \cdot \rangle$ is an expectation over a non-equilibrium process, specified by a (time- and state-dependent) driving force or protocol. JE, and Crook's theorem [2], from which it follows, has been used to successfully determine binding free energies of *single* biomolecules through repeated pulling experiments [3], a feat which had previously been unimaginable. For stochastic thermodynamics (the setting of this paper), such transient non-equilibrium fluctuation relations are comprehensively reviewed in [4]. A counter-part of the transient fluctuation relations are equally important steady-state fluctuation relations [5–11], but these fall outside the scope of the present Letter where we consider only processes in a finite time interval.

The transient non-equilibrium fluctuation relations are identities; they hold irrespective of the protocol. Most quantities of interest however still depend on the protocol, and can then be varied and optimized. A first step in this direction was taken by Schmiedl & Seifert who showed that when pulling a small system by optical tweezers, (expected) heat released to the environment

and (expected) work done on the small system are minimized, not by naively smoothly pulling, but by protocols with discontinuities [12], a work which has generated considerable interest in the field [13–15]. For technical reasons, the analysis of Schmiedl & Seifert was limited to harmonic potentials.

In this Letter we show how such optimization problems in stochastic thermodynamics (minimizing heat, work, the variance of the JE estimate of free energy differences) can be mapped to problems of (deterministic) optimal transport. The optimal control (for any of these cases) is determined by the solution of an auxiliary problem. When optimizing heat or work, this auxiliary problem is none other than the Burgers equation of fluid dynamics and cosmology, and mass transport by the Burgers field. Very efficient numerical methods have been developed to solve such problems, and these methods can be directly applied. Our contribution hence extends considerably the range of solvable optimization problems in stochastic thermodynamics.

Stochastic thermodynamics and optimal protocols: We consider dynamics in the overdamped limit described by coupled Langevin equations:

$$\dot{\xi}_t = -\frac{1}{\tau} \partial_{\xi_t} V(\xi_t, t) + \sqrt{\frac{2}{\tau\beta}} \dot{w}_t , \quad (2)$$

with initial value $\xi_{t_0} = \mathbf{x}_o$, drift $-\partial_{\xi_t} V$ and \dot{w}_t a vector valued white noise with covariance $\langle \dot{w}_t \dot{w}_{t'} \rangle = \delta(t - t')$. The mobility is τ^{-1} and β the inverse temperature. For times $t < t_o$ the potential is $V(\mathbf{x}, t) = U_o(\mathbf{x})$, and for times $t > t_f$ is $V(\mathbf{x}, t) = U_f(\mathbf{x})$. In the control interval $[t_o, t_f]$ we allow the potential to be an explicit function of time $V(\mathbf{x}, t) = U(\mathbf{x}, t)$ eventually discontinuous at the boundaries $V(\mathbf{x}, t_o) = \varphi_o U_o(\mathbf{x}) + (1 - \varphi_o) U(\mathbf{x}, t_o)$ and $V(\mathbf{x}, t_f) = \varphi_f U(\mathbf{x}, t_f) + (1 - \varphi_f) U_f(\mathbf{x})$ with $0 \leq \varphi_i \leq 1$, $i = \{o, f\}$. For single stochastic trajectories we define δW , the Jarzynski work [1], and δQ , the heat released

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into the heat bath, in as [16]

$$\delta W = \int_{t_o}^{t_f} \partial_t V(\boldsymbol{\xi}_t, t) dt, \quad (3)$$

$$\delta Q = - \int_{t_o}^{t_f} \dot{\boldsymbol{\xi}}_t \cdot \partial_{\boldsymbol{\xi}_t} V(\boldsymbol{\xi}_t, t) dt. \quad (4)$$

The difference $\delta W - \delta Q$ satisfies 1st law, *i.e.* is the integral of an exact differential, if and only if the stochastic integral in δQ is defined in the sense of Stratonovich. The Stratonovich integral is the limit of Riemann sums where products $V(\boldsymbol{\xi}_t, t)dw_t$ are discretized according to the *mid-point* prescription *i.e.* $V((\boldsymbol{\xi}_{t_i} + \boldsymbol{\xi}_{t_{i+1}})/2, \bar{t}_i)(w_{t_{i+1}} - w_{t_i})$ for $t \in [t_i, t_{i+1}]$ and \bar{t}_i an arbitrary interpolation rule for t . Thus, the expression of the first law over $[t_o, t_f]$

$$\delta W - \delta Q = V(\boldsymbol{\xi}_{t_f}, t_f) - V(\boldsymbol{\xi}_{t_o}, t_o). \quad (5)$$

does not require $\varphi_f = \varphi_o = 1/2$ for discontinuities in the time argument although the choice may appear otherwise appealing.

The stochastic differential equations (2) lead to a (control-dependent) probability density $m(\mathbf{x}, t)$ evolving according the Fokker-Planck equation and the expectation value of a local quantity \mathcal{G} is

$$\langle \mathcal{G}(\boldsymbol{\xi}_t, t) \rangle = \int d\mathbf{x} m(\mathbf{x}, t) \mathcal{G}(\mathbf{x}, t). \quad (6)$$

Straightforward application of Itô lemma (see e.g.[17]) yields

$$\langle \delta Q \rangle = - \int_{t_o}^{t_f} dt \langle \mathfrak{L}_{\boldsymbol{\xi}_t}^{[-\partial_{\boldsymbol{\xi}_t} U]} U \rangle, \quad (7)$$

for $\mathfrak{L}_{\mathbf{x}}^{[\mathbf{b}]}$:= $\frac{\mathbf{b}}{\tau} \cdot \partial_{\mathbf{x}} + \frac{1}{\beta\tau} \partial_{\mathbf{x}}^2$ the generator of the diffusion process with drift \mathbf{b} . Given initial and final states, the minimal *variance* of the heat (or work) can be written as a Kullback-Leibler distance between a controlled and uncontrolled process, and this connection has been thoroughly explored in the literature [18, 19]. We will here be concerned with $\langle \delta Q \rangle$, $\langle \delta W \rangle$ and exponentially weighted functionals of the heat or the work.

Burgers equation in optimal stochastic control: We first focus on heat minimization. Following [20], we look for a function $A(\mathbf{x}, t)$ such that when evaluated along $\boldsymbol{\xi}_t$

$$0 = \int_{t_o}^{t_f} dt \langle \partial_t A + \mathfrak{L}_{\boldsymbol{\xi}_t}^{[-\partial_{\boldsymbol{\xi}_t} U]} (A + U) \rangle. \quad (8)$$

If such function can be found, the identity

$$\langle \delta Q \rangle = \langle A(\boldsymbol{\xi}_{t_o}, t_o) - A(\boldsymbol{\xi}_{t_f}, t_f) \rangle, \quad (9)$$

holds true as $\langle (\partial_t + \mathfrak{L}_{\boldsymbol{\xi}_t}^{[-\partial_{\boldsymbol{\xi}_t} U]}) A \rangle$ is the average of an exact stochastic differential. A sufficient condition for (8) to be satisfied is the so-called dynamic programming equation (DPE) $\partial_t A + \mathfrak{L}_{\mathbf{x}}^{[-\partial_{\mathbf{x}} U]} (A + U) = 0$ which for any given value of U yields a linear, backwards in time

evolution for A . The stationarity condition for DPE is obtained by taking the functional variation of (8) with respect to U . Introduce the (fictitious) potential $R(\mathbf{x}, t)$ corresponding to the state $m(\mathbf{x}, t)$ if it would have been in equilibrium *i.e.* $R = \frac{1}{\beta} \log m$. Then the variation of U yields the condition

$$\mathfrak{L}_{\mathbf{x}}^{[\partial_{\mathbf{x}} R]} (A - 2U - R) = 0, \quad (10)$$

which is satisfied independently of $\partial_{\mathbf{x}} R$ if the potential is

$$U_* = \frac{A - R}{2} + \phi, \quad (11)$$

where ϕ is an arbitrary function of time alone. The optimal control potential is therefore the solution of the coupled *backwards- forwards* equations

$$\partial_t A + \mathfrak{L}_{\mathbf{x}}^{[\partial_{\mathbf{x}} \frac{R-A}{2}]} \frac{A + R}{2} = 0, \quad (12)$$

$$\partial_t m + \partial_{\mathbf{x}} \cdot \left[\frac{\partial_{\mathbf{x}} (R - A)}{2\tau} m \right] = \frac{1}{\beta\tau} \partial_{\mathbf{x}}^2 m. \quad (13)$$

respectively obtained by plugging (11) into the DPE and Fokker-Planck equations. We note that the Fokker-Planck equation has the property that if we split the drift into an equilibrium piece $\partial_{\mathbf{x}} R$ and a remainder specified by the gradient of

$$\psi = -\frac{A + R}{2}, \quad (14)$$

then it becomes the deterministic transport equation in the gradient of the remainder:

$$\partial_t m + \frac{1}{\tau} \partial_{\mathbf{x}} \cdot [(\partial_{\mathbf{x}} \psi) m] = 0. \quad (15)$$

It is a perhaps surprising fact that using the definitions of R and ψ and the Fokker-Planck equation (13) reduces (12) to simply

$$\partial_t \psi + \frac{\|\partial_{\mathbf{x}} \psi\|^2}{2\tau} = 0. \quad (16)$$

Equation (16) is Burgers equation (for the velocity potential), and equation (15) is the equation of mass transport by the corresponding velocity field. These two equations are the first main result of this paper: we have reduced a complicated stochastic optimization problem to a classical problem of optimal deterministic transport. In addition, contrasting (8) with the expression of the work imposed by the first law, it is readily seen that *work* optimization brings about the same evolution equations (15), (16) now complemented by the *final* boundary condition

$$A(\mathbf{x}, t_f) = V(\mathbf{x}, t_f) = -[R(\mathbf{x}, t_f) + 2\psi(\mathbf{x}, t_f)]. \quad (17)$$

It is worthwhile remarking that the occurrence of final time constraints is a consequence of the backwards time evolution of the DPE and is a general feature of variational principles in the presence of boundary cost terms [20]. We now discuss how this transport problem can be

solved, first if the initial and final states are given, and then if the initial state and the final control are given.

Optimal heat between given initial and final states: The meaning of Burgers equation in (16) is somewhat peculiar in that it arises from a mixed forwards-backwards problem. In other words, it is not reasonable to regularize (possible) shocks (in the future or in the past) by either adding $+\nu\partial_{\mathbf{x}}^2\psi$ or $-\nu\partial_{\mathbf{x}}^2\psi$ on the right hand side; equation (16) should make sense in both directions. On the other hand, without shocks the solutions of Burgers equation are free-streaming motion, which we can specify by a *inverse Lagrangean map* $\mathbf{x}_o = \mathbf{x}_f - (t_f - t_o)\mathbf{v}(\mathbf{x}_f, t_f)$ where the velocity (constant along streamlines) is $\mathbf{v}(\mathbf{x}_f, t_f) = \frac{1}{\tau}\partial_{\mathbf{x}_f}\psi(\mathbf{x}_f, t_f)$. By mass conservation the inverse Lagrangean map must satisfy the Monge-Ampère equation

$$\|\det \frac{\partial \mathbf{x}_o}{\partial \mathbf{x}_f}\| = \frac{m_f(\mathbf{x}_f)}{m_o(\mathbf{x}_o)}, \quad (18)$$

where $m_o(\mathbf{x}) \equiv m(\mathbf{x}, t_o)$ is the initial state and $m_f(\mathbf{x}) \equiv m(\mathbf{x}, t_f)$ is the final state. In 1D this equation is immediately solved in terms of the cumulative mass functions $\frac{dM_f}{dx} = m_f$ and $\frac{dM_o}{dx} = m_o$. The inverse Lagrangean map is then determined by $M_o(\mathbf{x}_o) = M_f(\mathbf{x}_f)$. For higher dimensions we note that for free-streaming motion

$$\mathbf{x}_o = \partial_{\mathbf{x}} \left[\frac{\|\mathbf{x}_f\|^2}{2} - \frac{t_f - t_o}{\tau} \psi(\mathbf{x}_f, t_f) \right] := \Psi(\mathbf{x}_f; t_f, t_o) \quad (19)$$

and (18) becomes a partial differential equation in a scalar field Ψ :

$$\|\det \frac{\partial^2 \Psi}{\partial x_f^\alpha \partial x_f^\beta}\| = \frac{m_f(\mathbf{x}_f)}{m_o(\partial_{\mathbf{x}_f} \Psi)}. \quad (20)$$

Combining (9) with (14) the optimal released heat can be written as

$$\langle \delta Q \rangle = -\frac{1}{\beta} \Delta S + 2 \langle \psi(\boldsymbol{\xi}_{t_f}, t_f) - \psi(\boldsymbol{\xi}_{t_o}, t_o) \rangle \quad (21)$$

where $\Delta S = -\beta \langle \ln m_f(\boldsymbol{\xi}_{t_f}) - \ln m_o(\boldsymbol{\xi}_{t_o}) \rangle$ is the entropy change. Similarly, the minimal expected work is

$$\langle \delta W \rangle = \langle V(\boldsymbol{\xi}_{t_f}, t_f) - V(\boldsymbol{\xi}_{t_o}, t_o) \rangle + \langle \delta Q \rangle, \quad (22)$$

provided R and ψ satisfy (17). In both cases the difference $2 \langle \psi(\boldsymbol{\xi}_{t_f}, t_f) - \psi(\boldsymbol{\xi}_{t_o}, t_o) \rangle$ which represents dissipated work, can also be written

$$W_{diss} = \langle \frac{\|\boldsymbol{\xi}_{t_f} - \Psi(\boldsymbol{\xi}_{t_f}; t_f, t_o)\|^2 \tau}{t_f - t_o} \rangle. \quad (23)$$

Equation (23) means that the initial and final states can be specified by mass points $\{x_0^{(1)}, x_0^{(2)}, \dots, x_0^{(N)}\}$ and $\{x_f^{(1)}, x_f^{(2)}, \dots, x_f^{(N)}\}$, and a possible inverse Lagrangean map by a one-to-one assignment $x_f^{(i)} \rightarrow x_0^{(j)}$. The inverse Lagrangean map solving (20) is then given by the assignment which minimizes the quadratic cost function (23), an approach which has been used with great success to

reconstruct velocity fields in the early universe [21, 22]. The interpretation of this quadratic cost function as dissipated work in stochastic thermodynamics is, up to our knowledge, new.

Optimal heat with given final control: A setting which is closer to the problem of minimizing work discussed by Schmiedl and Seifert [12] is when the final control $V(\mathbf{x}, t_f)$ is specified, but not the final state. Let hence the initial potential be $U_o(\mathbf{x}) = \|\mathbf{x}\|^2/2 + \bar{U}_o$ and the initial state be $m_o(\mathbf{x}) \sim \exp\{-\beta U_o(\mathbf{x})\}$ and the final potential be $U_f(\mathbf{x}) = c \|\mathbf{x} - \mathbf{h}\|^2/2 + \bar{U}_f$ with $c > 0$ and \bar{U}_o, \bar{U}_f , arbitrary constants. By (11) and (14) U_* satisfies

$$U_*(\mathbf{x}, t) = -[\psi(\mathbf{x}, t) + R(\mathbf{x}, t)] + \phi(t). \quad (24)$$

The function ϕ can be, however, set to zero as the heat depends only upon the spatial gradient of U_* . Since for the heat there are no further conditions on ψ and R , we can set $U_*(\mathbf{x}, t_f) = U_f(\mathbf{x}) = V(\mathbf{x}, t_f)$. The problem can be then solved by a Gaussian Ansatz for the measure i.e.

$$R(\mathbf{x}, t) = -\frac{\|\mathbf{x} - \boldsymbol{\mu}_t\|^2}{2\sigma_t^2} + \frac{d}{2\beta} \ln \frac{1}{\sigma_t^2}. \quad (25)$$

We can then use (24) to write $\psi(\mathbf{x}, t_f)$ in terms of (25) and U_f hence obtaining Ψ by (19). Then, plugging Ψ into (20) yields

$$\boldsymbol{\mu}_{t_f} = \frac{cT\mathbf{h}}{Tc + \tau} \quad \& \quad \sigma_{t_f} = \frac{2T}{\sqrt{4T(cT + \tau) + \tau^2} - \tau}, \quad (26)$$

for $T := t_f - t_o$ and after straightforward algebra

$$\boldsymbol{\mu}_t = \frac{t - t_o}{T} \boldsymbol{\mu}_{t_f} \quad \& \quad \sigma_t = 1 + \frac{t - t_o}{T} (\sigma_{t_f} - 1), \quad (27)$$

for any $t \in [t_o, t_f]$. Finally the optimal heat and drift are

$$\langle \delta Q \rangle = \frac{\tau \|\boldsymbol{\mu}_{t_f}\|^2}{T} + \frac{d}{\beta} \left[\ln \frac{1}{\sigma_{t_f}} + \frac{\tau(\sigma_{t_f} - 1)^2}{T} \right], \quad (28)$$

$$-\partial_{\mathbf{x}} U_* = \frac{\boldsymbol{\mu}_t - \mathbf{x}}{\sigma_t^2} + \frac{\tau[\mathbf{x}(\sigma_{t_f} - 1) + \boldsymbol{\mu}_{t_f}]}{T\sigma_t}. \quad (29)$$

As expected the results do not depend on \bar{U}_o, \bar{U}_f . Whilst the state density (25) is continuous for all $t \in [t_o, t_f]$, the optimal drift (29) exhibits a discontinuity at $t = t_o$ as discussed in [13].

Optimal work with given final control: Work optimization, as considered in [12], exhibits more subtle features. The final condition (17) together with (24) now yield

$$\psi(\mathbf{x}, t_f) = -\frac{(1 - \wp_f)[U_f(\mathbf{x}) + R(\mathbf{x}, t_f)]}{2 - \wp_f} + \phi(t_f). \quad (30)$$

Using the Gaussian Ansatz (25) and proceeding as for the heat we find that (27), (29) still hold true but the final mean and variance are now given by

$$\boldsymbol{\mu}_{t_f} = \frac{cT\mathbf{h}\tilde{\wp}_f}{\tilde{\wp}_f T c + 2\tau} \quad \& \quad \sigma_{t_f} = \frac{\tilde{\wp}_f T}{K}, \quad (31)$$

with $K = \sqrt{\tilde{\wp}_f T (\tilde{\wp}_f c T + 2\tau) + \tau^2} - \tau$, and $\tilde{\wp}_i := (1 - \wp_i)/(1 - \wp_i/2)$, $i = \{o, f\}$. As before, drift and density do

not depend upon ϕ nor \bar{U}_o, \bar{U}_f . They, however, depend upon the shape of the discontinuities of the control V at the boundary. Note that for any $c > 1$, σ_{t_f} is a decreasing function of T such that $1 \geq \sigma_{t_f} \geq 1/\sqrt{c}$. The corresponding expression of the optimal work is

$$\begin{aligned} \prec \delta \mathcal{W} \succ = & \frac{4 - 3\tilde{\varphi}_o}{4(2 - \tilde{\varphi}_o)} \left\{ \frac{d\tilde{\varphi}_f}{\beta} \ln \frac{1}{\sigma_{t_f}} + \frac{2\tau d(1 - \sigma_{t_f})}{\beta T} \right. \\ & \left. + \frac{2\tau \|\boldsymbol{\mu}_{t_f}\|^2}{T} \frac{T\tilde{\varphi}_f + 2\sigma_{t_f}\tau}{T\tilde{\varphi}_f + 2(1 - \sigma_{t_f})\sigma_{t_f}\tau} \right\} + \Delta\bar{U}, \quad (32) \end{aligned}$$

where $\Delta\bar{U} = (1 - \varphi_f)\bar{U}_f + \varphi_f\phi(t_f) - (1 - \varphi_o)\phi(t_o) - \varphi_o\bar{U}_o$ can always be set to zero exploiting the arbitrariness of the function $\phi(t)$. It is straightforward to verify that the examples considered in [12] are worked out for the case $(\varphi_o, \varphi_f) = (1, 0)$ and that as such they are a special case of the formulas given above.

Optimizing the variance of the Jarzynski estimator: We now turn our attention to a different expectation value. The Jarzynski Equality (JE) is an equality in expectation (1), but does not hold for a finite number of samples [23]. Let there be N independent measurements of the work; then the free energy difference is estimated as $\Delta F = -\beta^{-1} \ln(\frac{1}{N} \sum_{i=1}^N e^{-\beta W_i})$, with a statistical error determined by $\text{Var}[e^{-\beta W}]/N$. Moreover, expectation and variance of a finite sampling will depend upon the details of the drift. It therefore makes sense to study the expectation value $g_\lambda(\mathbf{x}, t) = \prec e^{-\lambda\beta W} \succ_{\mathbf{x}, t}$, where we understand that the noise in the stochastic differential equation (2) is at inverse temperature β , and that the initial state is in equilibrium at the same temperature. Using the approach of [9] g_λ can be shown to satisfy for any given U a controlled diffusion equation which we can write for $A_\lambda = -\frac{1}{\lambda\beta} \log g_\lambda$ (note that $g_0 = 1$ by definition) as

$$\mathfrak{L}_{\mathbf{x}}^{[(2\lambda-1)\partial_{\mathbf{x}}U]} A_\lambda = -\mathfrak{L}_{\mathbf{x}}^{[(\lambda-1)\partial_{\mathbf{x}}U]} U + \frac{\lambda}{\tau} \|\partial_{\mathbf{x}} A_\lambda\|^2. \quad (33)$$

The extremum condition for the drift gives

$$\partial_{\mathbf{x}} U_* = \partial_{\mathbf{x}} \frac{(1 - 2\lambda)A_\lambda - R}{2(1 - \lambda)}. \quad (34)$$

If we again, as in (14), split the drift into an equilibrium piece and a remainder

$$\partial_{\mathbf{x}} \psi_\lambda = -(1 - 2\lambda) \partial_{\mathbf{x}} \frac{A_\lambda + R}{2(1 - \lambda)}, \quad (35)$$

we obtain the generalized optimal transport equations

$$\partial_t m + \frac{1}{\tau} \partial_{\mathbf{x}} \cdot (m \partial_{\mathbf{x}} \psi_\lambda) = 0, \quad (36)$$

$$\partial_t \psi + \frac{\|\partial_{\mathbf{x}} \psi\|^2}{2\tau(1 - 2\lambda)} + \frac{\lambda(\partial_{\mathbf{x}}^2 \psi)}{\beta\tau(1 - \lambda)} = \frac{\lambda(\partial_{\mathbf{x}} \psi) \cdot (\partial_{\mathbf{x}} m)}{m\beta\tau(\lambda - 1)}. \quad (37)$$

These equations are not immediately solved, and deserve further study.

In summary, we have shown how stochastic optimization problems are solved by the methods of optimal control. The solution is built on an auxiliary problem of optimal transport. When minimizing heat or work of a small system this optimal transport is a classic of fluid mechanics and cosmology, namely Burgers equation. Between any prescribed initial and final states, these problems can be solved numerically with the Monge-Ampère-Kantorovich method, introduced to reconstruct velocity fields in the early Universe. Boundary cost contributions to the work, penalizing discontinuous controls and hence overcoming ambiguities in the definition of the free energy, can be easily handled in the formalism in the form of Lagrange multipliers, and solved by fast-Legendre transforms methods for, at least, any convex potential. The direct connection between optimal transport and optimal protocols in small system thermodynamics was wholly unexpected, and is promising, as it applies to a whole wide class of related optimization problems.

This work was supported by the Swedish Research Council (E.A) through Linnaeus Center ACCESS and Academy of Finland center of excellence ‘‘Analysis and Dynamics Research’’, and Academy of Finland as part of it Distinguished Professor program grant 129024. C. M.-M. acknowledges support from the European Research Council and the Academy of Finland.

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