Optimal Protocols and Optimal Transport in Stochastic Thermodynamics

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Thermodynamics of small systems has become an important field of statistical physics. Such systems 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 nonequilibrium transition in finite time is solved by the Burgers equation and mass transport by the Burgers velocity field. Our contribution hence considerably extends the range of solvable optimization problems in small system thermodynamics.

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The last two decades have 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:

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

Here and in the following $\beta = 1/k_B T$ is the inverse temperature, k_B the Boltzmann's constant that we set to 1, and $\langle\cdots\rangle$ is an expectation over a nonequilibrium process, specified by a (time- and state-dependent) driving force or protocol. JE, and Crook's theorem [2], from which it follows, have been used to successfully determine binding free energies of *single* biomolecules through repeated pulling experiments [3]. For stochastic thermodynamics (the setting of this Letter), such transient nonequilibrium fluctuation relations are comprehensively reviewed in [4]. Equally important steady-state fluctuation relations are a counterpart of the transient fluctuation relations [5–11].

The transient nonequilibrium 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 a small system, 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 considerably extends 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:

$$\dot{\boldsymbol{\xi}}_t = -\frac{1}{\tau}\partial_{\boldsymbol{\xi}_t} V(\boldsymbol{\xi}_t, t) + \sqrt{\frac{2}{\tau\beta}}\dot{\boldsymbol{\omega}}_t, \tag{2}$$

with initial value $\boldsymbol{\xi}_{t_0} = \boldsymbol{x}_0$, drift $-\partial_{\boldsymbol{\xi}_t} V$, and $\dot{\boldsymbol{\omega}}_t$, a vector valued white noise with covariance $\langle \dot{\boldsymbol{\omega}}_t \dot{\boldsymbol{\omega}}_{t'}\rangle = \delta(t - t')$, and mobility τ^{-1}. For times $t < t_0$ the potential is $V(\boldsymbol{x}, t) = U_0(\boldsymbol{x})$, and for times $t > t_f$ it is $V(\boldsymbol{x}, t) = U_f(\boldsymbol{x})$. In the control interval $[t_0, t_f]$ we allow the potential to be an explicit function of time $V(\boldsymbol{x}, t) = U(\boldsymbol{x}, t)$. For single stochastic trajectories we define δW, the Jarzynski work [1], and δQ, the heat released into the heat bath, as [16]

$$\delta W = \int_{t_0}^{t_f} \partial_t V(\boldsymbol{\xi}_t, t) dt, \tag{3}$$

$$\delta Q = -\int_{t_0}^{t_f} \dot{\boldsymbol{\xi}}_t \cdot \partial_{\boldsymbol{\xi}_t} V(\boldsymbol{\xi}_t, t) dt. \tag{4}$$

The definition of the work (3) follows after requiring that $\delta W - \delta Q$ is the integral of an exact differential, namely

$$\delta W - \delta Q = U_f(\boldsymbol{\xi}_{t_f}, t_f) - U_0(\boldsymbol{\xi}_{t_0}, t_0), \tag{5}$$

which expresses the 1st law over $[t_0, t_f]$. It holds if and only if the stochastic integral in δQ is defined in the sense of Stratonovich.

The stochastic differential Eqs. (2) lead to a (control-dependent) probability density $\rho(\boldsymbol{x}, t)$ defining the expectation value of local quantities as

$$\langle \mathcal{G}(\boldsymbol{\xi}_t, t) \rangle = \int_{\mathbb{R}^d} \mathbf{d}x \rho(\boldsymbol{x}, t) \mathcal{G}(\boldsymbol{x}, t).$$

Straightforward application of the Itô lemma (see, e.g., [17]) yields the average heat release

$$\langle \delta Q \rangle = \int_{t_0}^{t_f} \frac{dt}{\tau} \langle \| \partial_{\boldsymbol{\xi}_t} U \|^2 - \frac{1}{\beta} \partial^2_{\boldsymbol{\xi}_t} U \rangle, \tag{6}$$

where we switch from V to U to emphasize that the potential now has the meaning of a control. 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].

The Burgers equation in optimal stochastic control.—We first focus on heat minimization. Following [20] we look for a function $A(\boldsymbol{x}, t)$ such that

$$\left\langle \left[\partial_t - \frac{1}{\tau} \partial_{\boldsymbol{x}} U(\boldsymbol{x}, t) \cdot \partial_{\boldsymbol{x}} + \frac{1}{\beta \tau} \partial^2_{\boldsymbol{x}} \right] A(\boldsymbol{x}, t) \right\rangle = -\frac{1}{\tau} \left\langle \| \partial_{\boldsymbol{x}} U(\boldsymbol{x}, t) \|^2 - \frac{1}{\beta} \partial^2_{\boldsymbol{x}} U(\boldsymbol{x}, t) \right\rangle, \tag{7}$$

with ρ evolving according to the Fokker-Planck equation

$$\partial_t \rho - \frac{1}{\tau} \partial_{\boldsymbol{x}} \cdot (\rho \partial_{\boldsymbol{x}} U) = \frac{1}{\beta \tau} \partial^2_{\boldsymbol{x}} \rho. \tag{8}$$

If such function A can be found, the left-hand side of (7) becomes the average of a stochastic differential so that

$$\langle \delta Q \rangle = \langle A(\boldsymbol{\xi}_{t_0}, t_0) - A(\boldsymbol{\xi}_{t_f}, t_f) \rangle. \tag{9}$$

Introducing the (fictitious) potential $R(\boldsymbol{x}, t)$ as if it would have been in equilibrium, i.e., $R := \beta^{-1} \ln \rho$, the stationary condition is obtained by taking the functional variation of (7) with respect to U, yielding $(\partial_{\boldsymbol{x}} R \cdot \partial_{\boldsymbol{x}} + \beta^{-1} \partial^2_{\boldsymbol{x}})(A - 2U - R) = 0$. In the absence of constant flux solutions for ρ, the stationarity condition is

$$U_* = \frac{A - R}{2} + \phi, \tag{10}$$

where ϕ is an arbitrary function of time alone [21].

From (10) we obtain for A and R the following coupled *backwards-forwards* equations

$$\partial_t A - \frac{\| \partial_{\boldsymbol{x}} A \|^2 - \| \partial_{\boldsymbol{x}} R \|^2}{4\tau} = -\frac{\partial^2_{\boldsymbol{x}} (A + R)}{2\beta\tau}, \tag{11}$$

$$\partial_t \rho - \partial_{\boldsymbol{x}} \cdot \left[\frac{\partial_{\boldsymbol{x}} (A - R)}{2\tau} \rho \right] = \frac{1}{\beta\tau} \partial^2_{\boldsymbol{x}} \rho. \tag{12}$$

We note that these equations have the property that if we split the drift into an equilibrium piece $\partial_{\boldsymbol{x}} R$ and a remainder specified by the gradient of

$$\psi = -\frac{A + R}{2}, \tag{13}$$

the Eqs. (11) and (12) reduce to the deterministic transport equations

$$\partial_t \psi + \frac{\| \partial_{\boldsymbol{x}} \psi \|^2}{2\tau} = 0, \tag{14}$$

$$\partial_t \rho + \frac{1}{\tau} \partial_{\boldsymbol{x}} \cdot [(\partial_{\boldsymbol{x}} \psi) \rho] = 0. \tag{15}$$

Equation (14) is the Burgers equation (for the velocity potential), and (15) is the equation of mass transport by the corresponding velocity field. These two equations are the first main result of this Letter: we have reduced a complicated stochastic optimization problem to a classical problem of optimal deterministic transport.

Optimal heat between given initial and final states.—In the theory of deterministic optimal control it is well justified to construct unique solutions in viscosity sense [22]. The mixed forwards-backwards nature of the problem here considered renders the application to the Burgers equation (14) of viscosity solution theory a nontrivial extension. On the other hand, without shocks the solutions of the Burgers equation are free-streaming motion, which we can specify by an inverse Lagrangian map $\boldsymbol{x}_0 = \boldsymbol{x}_f - (t_f - t_0) \boldsymbol{v}(\boldsymbol{x}_f, t_f)$ where the velocity (constant along streamlines) is $\boldsymbol{v}(\boldsymbol{x}_f, t_f) = \frac{1}{\tau} \partial_{\boldsymbol{x}_f} \psi(\boldsymbol{x}_f, t_f)$. By mass conservation the inverse Lagrangian map must satisfy the Monge-Ampère equation

$$\det \frac{\partial x_0}{\partial x_f} = \frac{\rho_f(\boldsymbol{x}_f)}{\rho_0(\boldsymbol{x}_0)}, \tag{16}$$

where $\rho_0(\boldsymbol{x}) \equiv \rho(\boldsymbol{x}, t_0)$ is the initial state and $\rho_f(\boldsymbol{x}) \equiv \rho(\boldsymbol{x}, t_f)$ is the final state. In 1D this equation is immediately solved in terms of the cumulative mass functions $\frac{dM_f}{dx} = \rho_f$ and $\frac{dM_0}{dx} = \rho_0$. The inverse Lagrangian map is then determined by $M_0(\boldsymbol{x}_0) = M_f(\boldsymbol{x}_f)$. We note that in dimensions higher than one the free-streaming motion has the following potential representation:

$$\boldsymbol{x}_0 = \partial_{\boldsymbol{x}_f}\left[\frac{\| \boldsymbol{x}_f \|^2}{2} - \frac{t_f - t_0}{\tau}\psi(\boldsymbol{x}_f, t_f)\right] := \partial_{\boldsymbol{x}_f}\Psi, \quad (17)$$

and (16) becomes a partial differential equation in the gradient of the scalar field $\Psi \equiv \Psi(\boldsymbol{x}_f; t_f, t_0)$

$$\det\frac{\partial^2\Psi}{\partial x_f^\alpha \partial x_f^\beta} = \frac{\rho_f(\boldsymbol{x}_f)}{\rho_0(\partial_{\boldsymbol{x}_f}\Psi)}. \quad (18)$$

Combining (9) with (13) the optimal released heat can be written as

$$\langle \delta Q\rangle = -\beta^{-1}\Delta S + 2\langle \psi(\boldsymbol{\xi}_{t_f}, t_f) - \psi(\boldsymbol{\xi}_{t_0}, t_0)\rangle, \quad (19)$$

where $\Delta S = -\langle \ln\rho_f(\boldsymbol{\xi}_{t_f}) - \ln\rho_0(\boldsymbol{\xi}_{t_0})\rangle$ is the entropy change. Similarly, the minimal expected work is

$$\langle \delta W\rangle = \langle U_f(\boldsymbol{\xi}_{t_f}, t_f) - U_0(\boldsymbol{\xi}_{t_0}, t_0)\rangle + \langle \delta Q\rangle. \quad (20)$$

The last term in Eq. (19) represents the dissipated work W_{diss}. Noticing that in the shockless Burgers equation $2[\psi(\boldsymbol{x}_f, t_f) - \psi(\boldsymbol{x}_0, t_0)] = \tau \| \boldsymbol{x}_f - \boldsymbol{x}_0 \|^2/(t_f - t_0)$, and using $\boldsymbol{x}_0$ given by (17) and mass conservation, the dissipated work can be written as

$$W_{\mathrm{diss}} = \frac{\tau}{t_f - t_0}\langle \| \boldsymbol{\xi}_{t_f} - \partial_{\boldsymbol{\xi}_{t_f}}\Psi(\boldsymbol{\xi}_{t_f}; t_f, t_0) \|^2\rangle. \quad (21)$$

Equation (21) means that the initial and final states can be specified by mass points $\{x_0^{(1)}, x_0^{(2)}, \ldots, x_0^{(N)}\}$ and $\{x_f^{(1)}, x_f^{(2)}, \ldots, x_f^{(N)}\}$, and a possible inverse Lagrangian map by a one-to-one assignment $x_f^{(i)} \to x_0^{(j)}$. The inverse Lagrangian map solving (18) is then given by the assignment which minimizes the quadratic cost function (21), an approach which has been used with great success to reconstruct velocity fields in the early universe [23,24]. The interpretation of this quadratic cost function as dissipated work in stochastic thermodynamics is, up to now, to the best of our knowledge, new.

Optimal work with given final control.—Optimal work with given initial state and given final control can be seen as a variational problem over the (unknown) final state minimizing the functional (20). This is the second result of our Letter, and, as we will show below, for the examples previously introduced by Schmiedl & Seifert [12] the minimization can be done exactly. For general initial states and final controls the minimization can be carried out numerically using the Monge-Ampère-Kantorovich approach or the variational equation; this is, however, somewhat involved and will be left to a future contribution.

Optimal work in transitions in an optical trap.—We combine here the two examples discussed [12] moving the center and changing the stiffness of a harmonic potential. The initial potential is $U_0(\boldsymbol{x}) = \| \boldsymbol{x} \|^2/2$ and the initial state, in equilibrium with this potential, is $\rho_0(\boldsymbol{x}) \sim \exp\{-\beta U_0(\boldsymbol{x})\}$. The final control potential is $U_f(\boldsymbol{x}) = c \| \boldsymbol{x} - \boldsymbol{h} \|^2/2$ and thus characterized by the position $\boldsymbol{h}$ and stiffness c, which in the examples in [12] is ≥ 1. We now evoke that the transition is effectuated by changing the harmonic potential in some (time-dependent) manner. The stochastic process inside the control interval is then a generalized Ornstein-Uhlenbeck process, and it follows easily that the final state must also be Gaussian. We therefore make the ansatz

$$R(\boldsymbol{x}, t) = -r\frac{\| \boldsymbol{x} - \boldsymbol{\mu}_t \|^2}{2} + \frac{d}{2\beta}\ln\frac{r}{2\pi}. \quad (22)$$

All the terms in (20) are now determined by (22), and we are left with an optimization problem in the two parameters $\boldsymbol{\mu}$ and r which is

$$Q(\boldsymbol{\mu}, r) = \frac{1}{2\beta}\left(\frac{c}{r} - 1\right) + \frac{c}{2}|\boldsymbol{q} - \boldsymbol{\mu}|^2 + \frac{\log r}{2\beta} + \frac{1}{t_f - t_i}\left(|\boldsymbol{q}|^2 + \frac{(1 - \sqrt{r})^2}{r\beta}\right). \quad (23)$$

The last term above follows from similarity when mapping an initial Gaussian state to a final Gaussian state by a Lagrangian map which is a linear transformation. Variation of Q with respect to $\boldsymbol{\mu}$ and r gives

$$\boldsymbol{\mu}_{t_f} = \frac{c\Delta t\boldsymbol{h}}{\Delta t c + 2\tau} \quad \text{and} \quad r = \frac{K^2}{(\Delta t)^2} \quad (24)$$

with $K = \sqrt{\Delta t(c\Delta t + 2\tau) + \tau^2} - \tau$. For these examples, as found in [12], there are discontinuities in the control both at the initial and the final time.

Optimizing the variance of the Jarzynski estimator.—We now turn our attention to a different expectation value. The Jarzynski equality (1) is an equality in expectation, but does not hold for a finite number of samples [25]. Let there be N independent measurements of the work; then the free energy difference is estimated as $\Delta F = -\beta^{-1}\ln(\frac{1}{N}\times\sum_{i=1}^N e^{-\beta W_i})$, with a statistical error determined by $\mathrm{Var}[e^{-\beta W}]/N$. 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 $g_\lambda(\boldsymbol{x}, t) = \langle e^{-\lambda\beta W}\rangle_{\boldsymbol{x},t}$, with respect to the initial state that we assume in equilibrium at inverse temperature β. 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 $A_\lambda := -(\lambda\beta)^{-1}\ln g_\lambda$ as $\tau\partial_t A_\lambda + (2\lambda - 1)\partial_{\boldsymbol{x}}U\cdot\partial_{\boldsymbol{x}}A_\lambda + \beta^{-1}\partial_{\boldsymbol{x}}^2(A_\lambda - U) = (\lambda - 1)\| \partial_{\boldsymbol{x}}U \|^2 + \lambda \| \partial_{\boldsymbol{x}}A_\lambda \|^2$. Now the extremum condition for the drift gives $\partial_{\boldsymbol{x}}U_* = \partial_{\boldsymbol{x}}[(1 - 2\lambda)A_\lambda - R]/[2(1 - \lambda)]$, with $R = \beta^{-1}\ln\rho$. If we again split the drift into an equilibrium piece $\partial_x R$ and a remainder $\partial_{\boldsymbol{x}}\psi_\lambda = -(1 - 2\lambda)\partial_{\boldsymbol{x}}(A_\lambda + R)/(1 - \lambda)$, we obtain the generalized optimal transport equations

$$\partial_t\rho + \frac{1}{\tau}\partial_{\boldsymbol{x}}\cdot(\rho\partial_{\boldsymbol{x}}\psi_\lambda) = 0, \quad (25)$$

$$\partial_t \psi + \frac{\| \partial_x \psi \|^2}{2\tau(1-2\lambda)} + \frac{\lambda(\partial_x^2 \psi)}{\beta\tau(1-\lambda)} = \frac{\lambda(\partial_x \psi)\cdot(\partial_x \rho)}{\rho\beta\tau(\lambda-1)}. \quad (26)$$

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

A toy model of nucleation.—As an illustration of new physics which can be investigated by the methods introduced in this Letter, we consider the minimization of heat release in a toy model of nucleation in one dimension. We model nucleation as a transition between states specified by assigning $-R(x, t)$ at times t_0, t_f such that it has local minima at $x \approx \pm\bar{x}$, and such that at the initial time t_0 the well at $x \approx -\bar{x}$ has the lowest energy, while at the final time t_f the global minimum is at $x \approx +\bar{x}$. An example is $-R_i(x) = x^2(2 - x^2/\bar{x}^2) + (-1)^i \ell x + \beta^{-1} \ln Z_i(\beta)$, $i = 0$ denoting the initial state and $i = 1$ the final one while $\ell > 0$ governs the asymmetry of the wells. We expect a trade-off between dissipated work, which by (21) can be written as $\Delta t \langle [\partial_x \psi(x, t_0)]^2 \rangle / \tau$, for $\Delta t = t_f - t_0$, and not moving the probability mass from the left to the right potential well. The latter action (or lack of action) entails a cost ΔR, namely, the energy difference in the final state between the right and left potential wells. In the example above $\Delta R \approx 2\bar{x}\ell$. If the probability mass is moved, the "Burgers" velocity $v = \partial_x \psi / \tau$ in the left well can be chosen to be uniform, i.e., $\partial_x \psi(x, t_0) \approx 2\tau\bar{x}/\Delta t$. Balance is then obtained for $4\tau\bar{x}^2/\Delta t \approx 2\bar{x}\ell$ or $\Delta t \approx 2\tau\bar{x}/\ell$. If the duration is much shorter, it "pays" to leave the mass where it is, while if it is much longer, it pays to move. Finding the exact optimal protocol at around the critical time requires solving the variational equations in this Letter, which in one dimension reduce to the equation $0 = \ln|\partial_x^2 \Psi| + \beta R_0(\partial_x \Psi) = R_1(x)$ for the Lagrangian map Ψ entering (17). Solving this equation is certainly not trivial, even in one dimension, and depends on the details of the boundary conditions. Details of this calculation will be reported elsewhere.

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. 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.

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