

Maximum work in minimum time from a conservative quantum system

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This paper considers the problem of obtaining maximum work from a conservative quantum system corresponding to a given change in an external parameter in the Hamiltonian. The example we present is a non-interacting collection of harmonic oscillators with a shared frequency ω which changes from a given initial to a given final value. The example is interesting for its role in experiments at ultra-low temperatures and for probing finite-time versions of the third law of thermodynamics. It is also the simplest system displaying quantum friction, which represents loss mechanisms in any reversible prelude to a thermal process. The example leads to a new type of availability. It is also the first example of a minimum time for transitions between thermal states of a thermodynamic system.

Introduction

The concept of Gibbs free energy is familiar to most readers. The change in free energy is the maximum work that could be captured from allowing some specified change in a thermodynamic system to take place or the minimum work needed to make the change happen. The proviso that the change must happen at constant temperature and pressure is needed. Without this proviso, the change in a more general quantity called the *availability* has this same optimum work characterization.[†] The change of availability equals the work extracted in *any* reversible process between the initial and final states. If any dissipation is present, the change in availability is more than the work extracted; this statement is one form of the second law of thermodynamics.

This paper describes a quantum control problem where a totally new kind of availability appears. It is the availability associated with a specified change in an external parameter in the Hamiltonian describing the system. Such time dependent mechanics is perfectly reversible. The work extracted equals the change in the energy of the system. Yet we find that some ways of carrying out the change *in the external parameter* result in more work extracted than other ways.

Another new feature of our “reversible” availability is that the time duration of the process plays a crucial role. In fact we find that there is a minimum time for achieving this maximum work and without constraining the time, our extension of availability to this situation becomes meaningless. It has previously been pointed out in great generality¹ that finite time constraints typically force us to forego some of the available work from a process. The fact that this applies even

when all processes considered are reversible, goes beyond the considerations in that paper.

The specific example we treat in this paper is the optimal control problem of cooling an ensemble of non-interacting particles in a harmonic potential. The Hamiltonian of this system is controlled by changing the curvature of the confining potential by means of an external field. This amounts to controlling the (shared) frequency ω of the oscillators and is described by the time dependent Hamiltonian $\hat{H}(\omega(t))$.

Since we are dealing with a conservative mechanical system, the change in the energy of the system is the work done by the system. Thus for a given initial state, maximizing the work done is equivalent to minimizing the final energy of the system. The minimum value of the final energy is determined by the value of the von Neumann entropy S_{VN} , which must necessarily stay constant during our reversible process. There are many ways to reach the minimum energy subject to this constraint, the classical example being the quantum adiabatic process² in which ω is changed infinitesimally slowly. Moving at finite rates excites parasitic oscillations in our system; a fact that has been termed *quantum friction*^{3,4} and can be attributed to the Hamiltonian at time t and at time $\neq t$ not commuting, $[\hat{H}(t), \hat{H}(t')] \neq 0$. When the process duration needs to be fast, we cannot avoid quantum frictional processes leaving some energy in parasitic oscillations. This is the reason we fail to capture the full classical availability; some of it is left behind in such oscillations. Its “loss” owes partly to the fact that the reversible process we envision is a prelude to a thermal process and that during thermal processes, the energy in the parasitic oscillations leaves the system as heat. It turns out, however, that there exist fast frictionless controls and we find the fastest such control below: *the minimum time for extracting the maximum work*.

While the problem is interesting in its own right, it plays a pivotal role as the adiabatic branch in a cooling cycle⁵ in which the adiabatic branch is followed by a thermal branch. Such cycles can be used to probe the unattainability of absolute zero.⁶ Our results applied to such cycles imply a finite time version of the third law of thermodynamics. Specifically, they

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[†] Availability is also called exergy.

imply that as the temperature of the cold bath T_c approaches zero, the cooling rate must approach zero as $T_c^{3/2}$.^{6,7}

Our problem is also the first example of another important but until now unconsidered question for thermodynamics: What is the *minimum time* for controlling a system to move between two thermal states? The question is loaded with subtlety; thermal equilibrium is traditionally approached only asymptotically so asking how one can get to another equilibrium state in minimum time should lead only to paradoxes. Not so for our problem and the answer hints at possible ways of attacking the question in general. The minimum time problem has obvious importance in a number of contexts. As a familiar example from solid state chemistry, consider the minimum time problem of inducing a transition from graphite to diamond. Our calculations below find the first closed form expression for the minimum time between two thermal states of any thermodynamic system.

There have been many studies exploring finite time effects on thermodynamic processes.^{8–11} The example we solve here extends our understanding of the finite time third law and of the minimum time problem. It also introduces a new form of finite time availability.

The system

Consider an ensemble of non-interacting particles bound by a shared harmonic potential well. We control the curvature of the potential $\omega(t)$. The energy of an individual particle is represented by the Hamiltonian

$$\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{1}{2} m \omega(t)^2 \hat{Q}^2. \quad (1)$$

where m is the mass of the particle, and \hat{Q} and \hat{P} are the momentum and position operators. We will assume that the system is initially in thermal equilibrium

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}. \quad (2)$$

It then follows that the state of the system at any time during the process is a generalized Gibbs state of the canonical form,^{12–16}

$$\hat{\rho} = \frac{1}{Z} e^{\gamma \hat{a}^2} e^{-\beta \hat{H}} e^{\gamma^* \hat{a}^{\dagger 2}}, \quad (3)$$

where \hat{a}^\dagger and \hat{a} are the (time dependent) raising and lowering operators of the harmonic oscillator. Note that this includes thermal states, which are obtained when $\gamma = 0$.

The dynamics is generated by the externally driven time dependent Hamiltonian $\hat{H}(\omega(t))$. Our description is based on the Heisenberg picture in which our operators are time dependent. The equation of motion for an operator \hat{O} of the working medium is:

$$\frac{d\hat{O}(t)}{dt} = \frac{i}{\hbar} [\hat{H}(t), \hat{O}(t)] + \frac{\partial \hat{O}(t)}{\partial t}. \quad (4)$$

The canonical state (3) is fully characterized by the frequency ω and the expectation values of three time-dependent operators: $\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{1}{2} m \omega^2 \hat{Q}^2$, $\hat{L} = \frac{1}{2m} \hat{P}^2 - \frac{1}{2} m \omega^2 \hat{Q}^2$, and $\hat{C} = \frac{\omega}{2} (\hat{Q}\hat{P} + \hat{P}\hat{Q})$ (the Hamiltonian, the Lagrangian, and a

position-momentum correlation). These three operators form a Lie algebra and thus completely characterize the time evolution generated by $\hat{H}(\omega(t))$ which is an element of this algebra. Thermal equilibrium (Cf. eqn (2)) is characterized by $\langle \hat{L} \rangle = \langle \hat{C} \rangle = 0$.

Substituting these operators into our equation of motion (4) and taking expectation values leads to three linear coupled differential equations, describing the dynamics that we need to control

$$\dot{E} = \frac{\dot{\omega}}{\omega} (E - L) \quad (5)$$

$$\dot{L} = -\frac{\dot{\omega}}{\omega} (E - L) - 2\omega C \quad (6)$$

$$\dot{C} = 2\omega L + \frac{\dot{\omega}}{\omega} C \quad (7)$$

where we have adopted the notation $L = \langle \hat{L} \rangle$ and $C = \langle \hat{C} \rangle$ and switched to $E = \langle \hat{H} \rangle$ to free up the symbol H for our optimal control Hamiltonian in the sections to follow. To cast our equations into the form required by optimal control theory, we augment our dynamical eqns (10)–(12) by introducing an additional dynamical equation

$$\dot{\omega} = \omega u \quad (8)$$

where u is our control variable and $x = (\omega, E, L, C)$ are our state variables. Using this new equation to eliminate $\dot{\omega}$ from eqns (10)–(12) our dynamical equations are all of the form $\dot{x} = f(x, u)$,

$$\dot{\omega} = f_1(x, u) = \omega u \quad (9)$$

$$\dot{E} = f_2(x, u) = u(E - L) \quad (10)$$

$$\dot{L} = f_3(x, u) = -u(E - L) - 2\omega C \quad (11)$$

$$\dot{C} = f_4(x, u) = 2\omega L + uC \quad (12)$$

as required for the formalism of optimal control.

The functions $\omega(t)$ achievable using our control, do not limit the size of $\dot{\omega}$ which means that we will have occasion to consider discontinuous jumps in ω ($u = \pm\infty$). The eqns (9)–(12) do not apply to such jumps. Rather for a jump $\omega_1 \rightarrow \omega_2$ we must require

$$E_2 = \frac{1}{2}(E_1 + L_1) + \frac{1}{2}(E_1 - L_1) \frac{\omega_2^2}{\omega_1^2} \quad (13)$$

$$L_2 = \frac{1}{2}(E_1 + L_1) - \frac{1}{2}(E_1 - L_1) \frac{\omega_2^2}{\omega_1^2} \quad (14)$$

$$C_2 = C_1 \frac{\omega_2}{\omega_1} \quad (15)$$

These equations follow from noting that during the jump \hat{Q} and \hat{P} are constant. Thus we can express $E = \langle \hat{H} \rangle$, $L = \langle \hat{L} \rangle$, and $C = \langle \hat{C} \rangle$ before and after the jump in terms of \hat{Q} and \hat{P} and then eliminate \hat{Q} and \hat{P} from the resultant equations.

A special control corresponding to a “wait” condition $\dot{\omega} = u = 0$ will play an important part in our discussion below. For this case the eqns (9)–(12) integrate to

$$\omega(t) = \omega(0) \quad (16)$$

$$E(t) = E(0) \quad (17)$$

$$L(t) = \cos(2\omega t)L(0) - \sin(2\omega t)C(0) \quad (18)$$

$$C(t) = \sin(2\omega t)L(0) + \cos(2\omega t)C(0). \quad (19)$$

During such waits, the variables L and C oscillate in time with constant $L^2 + C^2$ and with angular frequency 2ω . This is the parasitic oscillation referred to in the introduction.

Since any $\omega(t)$ represents Hamiltonian dynamics, the von Neumann entropy of the system is perforce constant. This entropy is given by⁶

$$S_{\text{VN}} = \ln\left(\sqrt{X - \frac{1}{4}}\right) + \sqrt{X} \operatorname{asinh}\left(\frac{\sqrt{X}}{X - \frac{1}{4}}\right) \quad (20)$$

where

$$X = \frac{E^2 - L^2 - C^2}{\hbar^2 \omega^2}. \quad (21)$$

We would expect the entropy to be a function of a combination of E, L, C which is itself a scalar under unitary transformations induced by the operator set. Such a combination is provided by X (ref. 17, p. 47). We note that since S_{VN} is a monotonic function of X , constancy of S_{VN} implies that X must stay constant.

The minimum energy problem

As noted above, maximizing the work output is equivalent to minimizing the final energy. An optimal control formulation of the minimum final energy problem leads to a singular problem^{18,19} for which the formalism of optimal control gives no answer. This can be understood physically since *any* trajectory is part of an optimal one. To see this, we begin by noting that the minimum energy that can be reached by any control starting from the thermal state $(\omega, E, L, C) = (\omega_i, E_i, 0, 0)$ must have $X = E_i^2/\hbar^2\omega_i^2$. Since X stays constant, the value of ω_f sets the value of $E_f^2 - L_f^2 - C_f^2$. It follows that to make E_f as small as possible, the final state should be another thermal state, *i.e.*, $L_f = C_f = 0$. The minimum final energy is $E_f^* = \frac{\omega_f}{\omega_i} E_i$ for the thermal state with $\beta_f = \frac{\omega_i}{\omega_f} \beta_i$. This energy can be reached by any control that changes the frequency ω infinitely slowly.² Any finite rate control starting from a thermal state moves us away from such a state as seen by examining the dynamical eqns (10)–(12) with $L = C = 0$ but with $\dot{\omega} \neq 0$. The trick to reaching the minimum energy is to move back to a state with $L = C = 0$ at the final time. There are many ways to do this. For example,⁶ we can use the control

$$u(t) = \frac{2 \ln(\omega_f/\omega_i)}{\sqrt{4\pi^2 + [\ln(\omega_i/\omega_f)]^2}} \omega(t) \quad (22)$$

which can be solved analytically for explicit $x(t)$ and reaches the desired final state in time

$$\tau = \frac{(1 - \omega_i/\omega_f) \sqrt{4\pi^2 + [\ln(\omega_i/\omega_f)]^2}}{2\omega_i \ln(\omega_i/\omega_f)}. \quad (23)$$

Once we have one such solution, any trajectory can be part of a trajectory that reaches this final state. For example, we can simply reverse the trajectory and then follow eqns (22)–(23). This is no longer true however when we constrain the time, since then we may not have enough time to reverse the trajectory or perhaps even to follow the trajectory in eqns (22)–(23). In fact, once we ask for the minimum time solution, we get an essentially unique answer. This is described in the following section.

The minimum time problem

Our optimal control problem is then to minimize the time

$$\tau = \int f_0(x, u) dt = \int dt \quad (24)$$

subject to the constraints represented by the dynamical eqns (9)–(12), the inequalities $\omega_{\min} \leq \omega(t) \leq \omega_{\max}$, the initial state $(\omega_i, E_i, 0, 0)$, and the final state $(\omega_f, E_f, 0, 0)$. The argument in the previous section insures that such trajectories exist; here we seek the minimum time trajectory.

The optimal control Hamiltonian²⁰ is

$$\begin{aligned} H &= \sum_{n=0}^4 \lambda_n f_n(x, u) \\ &= \lambda_0 + \lambda_1 u \omega + \lambda_2 u (E - L) - \lambda_3 (u (E - L) + 2\omega C) \\ &\quad + \lambda_4 (2\omega L + u C) \end{aligned} \quad (25)$$

where the λ 's are conjugate variables closely related to the Lagrange multipliers in a Lagrangian formulation. Note that the optimal control Hamiltonian is linear in the control u . To emphasize this, we group the terms containing u and find

$$\begin{aligned} H &= [\lambda_1 \omega + (\lambda_2 - \lambda_3)(E - L)]u + [\lambda_0 + 2\omega(\lambda_4 L - \lambda_3 C)] \\ &= \sigma u + \alpha \end{aligned} \quad (27)$$

where we have introduced the terms $\sigma = \sigma(x, \lambda)$ and $\alpha = \alpha(x, \lambda)$ for the coefficients of H viewed as a linear polynomial in our control u . The Pontryagin maximality principle²⁰ tells us that at any instant, the value of the control must maximize H . Thus when the switching function σ is positive, u must be as large as possible and when σ is negative, u must be as small as possible. Since away from the boundaries set by the inequalities $\omega_{\min} \leq \omega(t) \leq \omega_{\max}$ the value of u is not constrained, this amounts in our problem to jumps in ω . This can be seen by considering the problem with $|u(t)| \leq u_{\max}$ and letting $u_{\max} \rightarrow \infty$. Such jumps must terminate on the boundary arcs $\omega(t) = \omega_{\max}$ or $\omega(t) = \omega_{\min}$ which can be used as segments of the optimal trajectory. In addition to jumps and boundary arcs, the optimal control for such problems can also have singular branches along which the switching function σ vanishes identically over a time interval. These are characterized by $\sigma(t) = \dot{\sigma}(t) = \ddot{\sigma}(t) = \dots = 0$, which usually suffice to determine the optimal control $u^*(t)$ along such arcs. That is not the case here; the equations that result from setting σ and all its derivatives identically to zero do not determine the control. While

such problems are known in the optimal control literature,^{18,19} they are rare. For this problem, however, we can prove directly that singular branches are *never* included in the optimal control which must therefore be of the bang-bang type, jumping between and waiting at the extreme allowed ω 's. The proof is presented in the appendix, which shows that finite, non-zero u can never be part of an optimal control.

The number of jumps needed to reach our target state $(\omega_f, \frac{\omega_f}{\omega_i} E_i, 0, 0)$ turns out to be simply an issue of the number of degrees of freedom. While we can use a single jump to reach ω_f , such a jump will put a considerable amount of energy into the parasitic oscillation, since L_f becomes $E_i(1 - \frac{\omega_f^2}{\omega_i^2})/2$. Similarly, two jumps do not suffice. Three jumps, however, turn out to be enough. Recall that any control must keep the von Neumann entropy constant and thus effectively reduces the dimension of our problem by one. Jumping

$$\begin{aligned}
 &(\omega_i, t = 0) \\
 &\quad \Downarrow_{\text{jump}} \\
 &(\omega_1, t = 0) \\
 &\quad \Downarrow_{\text{wait}} \\
 &(\omega_1, t = t_1) \\
 &\quad \Downarrow_{\text{jump}} \\
 &(\omega_2, t = t_1) \\
 &\quad \Downarrow_{\text{wait}} \\
 &(\omega_2, t = t_1 + t_2) \\
 &\quad \Downarrow_{\text{jump}} \\
 &(\omega_f, t = t_1 + t_2)
 \end{aligned}$$

leaves us with two wait times t_1 and t_2 as adjustable parameters. Adjusting these times and using the specified value of ω_f and the constant value of S_{VN} allows us to solve for the values of t_1 and t_2 which reach the target state. In fact, this combination allows us to reach the target state in the minimum time. More jumps give alternative controls for achieving the same state in the same time, but cannot improve further on the three jump case. For any values of the intermediate frequencies ω_1 and ω_2 , the required values of t_1 and t_2 are

$$t_1 = \frac{1}{2\omega_1} \text{Arccos} \left(\frac{2\omega_1^2(\omega_2^2 + \omega_f^2)\omega_i - (\omega_1^2 + \omega_2^2)(\omega_1^2 + \omega_f^2)\omega_f}{(\omega_2^2 - \omega_1^2)\omega_f(\omega_1^2 - \omega_f^2)} \right) \quad (28)$$

$$t_2 = \frac{1}{2\omega_2} \text{Arccos} \left(\frac{2\omega_2^2(\omega_1^2 + \omega_f^2)\omega_f - (\omega_1^2 + \omega_2^2)(\omega_2^2 + \omega_f^2)\omega_i}{(\omega_1^2 - \omega_2^2)\omega_i(\omega_2^2 - \omega_f^2)} \right) \quad (29)$$

The total time $\tau = t_1 + t_2$ is shown plotted in Fig. 1. For the case of cooling ($\omega_f < \omega_i$), the smaller ω_1 and the larger ω_2 are,

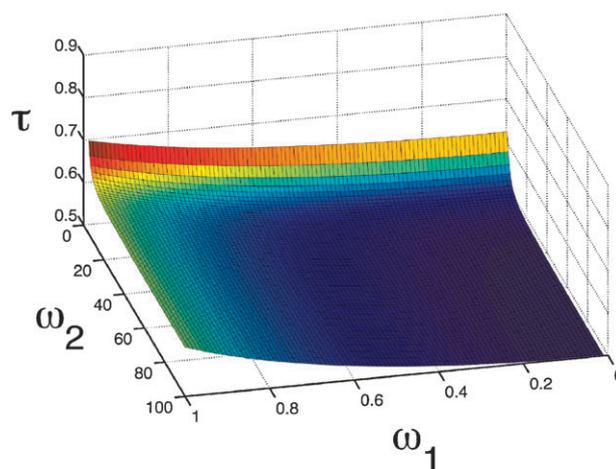


Fig. 1 The total time τ to reach ω_f with energy $E_f = \frac{\omega_f}{\omega_i} E_i$ as a function of the intermediate frequencies ω_1 and ω_2 . Note that the time is monotonic in both ω_1 and ω_2 . The global minimum is at $\omega_1 = 0$ and $\omega_2 = \infty$.

the faster the process. The fastest process is obtained in the limit $\omega_1 \rightarrow 0$ and $\omega_2 \rightarrow \infty$.

$$\tau_{\min}^{**} = \frac{\sqrt{1 - \omega_f/\omega_i}}{\sqrt{\omega_f \omega_i}} \quad (30)$$

When ω_1 and ω_2 are constrained to lie within the interval $[\omega_f, \omega_i]$, the best we can do is to take $\omega_1 = \omega_f$ and $\omega_2 = \omega_i$. For this case, the minimum time to reach $(\omega_f, E_0 \frac{\omega_f}{\omega_i}, 0, 0)$ is given by

$$\tau^* = \frac{1}{2} \left(\frac{1}{\omega_i} + \frac{1}{\omega_f} \right) \text{Arccos} \left(\frac{\omega_i^2 + \omega_f^2}{(\omega_i + \omega_f)^2} \right). \quad (31)$$

The optimal control works by jumping to the final frequency and allowing just enough parasitic oscillation (eqns (18)–(19)) that when added to a similarly timed oscillation after a jump back creates a state that can jump to $L = C = 0$!

We close by noting that if we let $\omega_f \rightarrow 0$ in eqn (32), the time $\tau^* \rightarrow \infty$ as $\tau^* \sim \omega_f^{-1/2}$. This is the result needed for the strengthened version of the third law mentioned in the introduction.

Conclusions

The arguments above presented an example in which the maximum work that accompanies the change in an external parameter of a Hamiltonian system has an associated minimum time. If we try to go faster, some of the availability must be “left behind” as parasitic oscillations. Is the available work left in parasitic oscillations really lost? If, at the completion of our process, we let the system equilibrate to a heat bath, the energy in parasitic oscillations leaves the system as heat. In this sense it will be lost. The minimum time maximum work process described above does not leave any energy in parasitic oscillations. It moves our system to a thermal state. If the initial state is also thermal and we have at least the minimum

time needed, the maximum work equals the change in the *classical* availability. For shorter times this is not the case and our availability deviates from the classical.

As a familiar example, consider a cylinder containing a gas and equipped with a piston. If we decrease the pressure on the outside of the piston infinitely slowly, we get the reversible work which equals the change in availability of the gas. If we drop the pressure instantaneously to its final value, we only recover a portion of the available work. The remainder shows up (at least initially) as a parasitic oscillation of the piston about its equilibrium position. If the piston is frictionless and the gas inviscid, this oscillation will continue undamped. Either friction or viscosity would damp the oscillation, converting the available work to heat. Does there exist a minimum time control of the external pressure that ends up capturing all of the available work for the frictionless piston and inviscid gas? The answer is not known. However, the example treated in this paper makes an affirmative answer likely. More generally, we believe that there exist minimum times for carrying out reversible versions of most thermodynamic processes so as to avoid parasitic oscillations. Our ensemble of harmonic oscillators is the first example in this direction.

Besides its characterization as the maximum work that can be extracted from our system for a given change in its environment, our availability has the property that it is a function of the initial state of the system and the initial and final states of the environment: ω_i and ω_f . For the initial state (E_i, L_i, C_i) of our system, the availability is

$$W_{\max} = E_i - (E_f)_{\min} = E_i - \frac{\omega_f}{\omega_i} \sqrt{E_i^2 - L_i^2 - C_i^2} \quad (32)$$

Note that when the initial state is thermal ($L_i = C_i = 0$), this reduces to the classical change in availability of the system. It comes however with a minimum time; only processes lasting longer than this minimum time can capture all of the availability in (32). Finite time adjustments to availability which must necessarily forego some of the work due to finite time constraints have been discussed previously.¹ Their realization in a Hamiltonian system is surprising.

While some previous work has found some relatively fast ways to achieve the same net effects as a quasistatic process^{21,22} our results are the first proof of a minimum time solution to the transition between two thermal states of a (quantum) thermodynamic system. Since thermal equilibrium is something that is only approached asymptotically according to current dogma, this is a surprising finding. Furthermore, we believe that we have found the in-principle minimum, *i.e.*, there exists no faster control even when additional control modes are introduced.

The control described here is achievable to a good approximation and is of some experimental interest²³ for cold gases in optical lattices. The curvature of the periodic potential can be switched several orders of magnitude faster than the oscillation period so our control can be realized to a good approximation. The control is robust, in the sense that approximate controls approximate the results closely.

Our problem has important implications for our understanding of thermodynamics in finite time.⁸⁻¹⁰ The maximum work we can extract from our ensemble of oscillators as the frequency is changed from its initial to its final value is a finite time *conservative* availability. It is the work obtained only along a certain subset of all the (necessarily reversible!) schedules for changing $\omega(t)$ from ω_i to ω_f . It bears on the strengthened form of the third law and establishes a paradigm for a new and important thermodynamic question: what is the minimum time between thermodynamic states of a system. We believe our results revitalize the thirty-something year old subject of finite time thermodynamics with new, interesting, and fundamental questions that show there is much more to the subject than has met the eye.

Appendix. Proof of optimality

Our proof that *all minimal time solutions are of the bang-bang type* is by contradiction. Assume that an optimal time trajectory uses a twice differentiable control $u(t)$ which does not vanish identically in the time interval $[a, a + t]$. We show that we can replace a small portion of the trajectory with a faster bang-bang trajectory between the same initial and final states. Thus the original trajectory could not have been optimal. The proof proceeds by a direct calculation which needs to be third order to see the effect. We use the dynamical equations and their derivatives to construct a series solution to the equations after a time step t . We then use the initial and final states of this solution to construct a faster bang-bang solution between the same states.

We begin by constructing the series solutions for the state variables. For notational convenience, all unsubscripted quantities refer to the initial state at time $t = a$ of our small time step. The series solutions are easily (although laboriously) constructed by repeated differentiation of both sides of eqns (9)–(12), and then elimination of all derivatives from the right hand sides. Evaluating the first three derivatives of the state functions in this manner, we write down the Taylor series to third order for these functions.

$$\omega_f = \omega + [\omega u]t + 1/2[\omega(u^2 + u')]t^2 + 1/6[\omega(u^3 + 3uu' + u'')]t^3 \quad (33)$$

$$E_f = E + [(E - L)u]t + [1/2((E - L)(2u^2 + u') + 2\omega Cu)]t^2 + 1/6((E - L)(4u^3 + 6uu' + u'') + 4\omega C(2u^2 + u') + 4\omega^2 Lu)]t^3 \quad (34)$$

$$L_f = L + [(L - L)u - 2\omega C]t + [1/2((L - E)(2u^2 + u') - 6\omega Cu - 4\omega^2 L)]t^2 + 1/6(4(L - E)u^3 - 16\omega Cu^2 + 6(L - E)uu' - 24\omega^2 Lu - 8\omega Cu' + (L - E)u'' + 4\omega^2 Eu + 8\omega^3 C)]t^3 \quad (35)$$

We have omitted the Taylor series for C_f since the invariance of the von Neumann entropy forces the value of C once the values of the other three state functions have been specified.

Next we consider a bang-bang solution constructed to go from the same initial state to the same final state. It turns out that we need to distinguish two cases: (1) $uC < 0$, and

(2) $uC > 0$. For the former, we need the three-jump bang-bang solutions employed in the manuscript

$$\omega(t) = \begin{cases} \omega, & \text{for } t = 0 \\ \omega_f, & \text{for } 0 < t \leq \tau_1 \\ \omega, & \text{for } \tau_1 < t < \tau_1 + \tau_2 \\ \omega_f, & \text{for } t = \tau_1 + \tau_2, \end{cases} \quad (36)$$

while for the latter we need a one jump solution

$$\omega(t) = \begin{cases} \omega, & \text{for } 0 \leq t \leq \tau_1 \\ \omega_f, & \text{for } \tau_1 < t \leq \tau_1 + \tau_2. \end{cases} \quad (37)$$

Either way, when the eqn (33) is used in eqns (36) or (37), we end up with expressions for E_f and L_f after the bang-bang move to the same final frequency ω_f . This expression is in terms of τ_1, τ_2, t , and the initial state and control values. Equating these to the expressions for E_f and L_f in eqns (34) and (35) gives two equations for determining τ_1 and τ_2 in terms of the initial state, the value of the control (and its derivatives) and the duration t of the step. It is then a simple matter of comparing $\tau_1 + \tau_2$ to t to determine which step is faster. Unfortunately, while this program is straightforward numerically, it bogs down with technical difficulties. If we expand these equations to first or second order in the small quantities τ_1, τ_2 and t , we find $\tau_1 + \tau_2 = t$. When we try to solve using third order expansions, the best symbolic manipulators (MAPLE and MATHEMATICA) cannot solve the two cubic equations in two unknowns. Changing variables to $\tau_1 = \tau/2 + \varepsilon$ and $\tau_2 = \tau/2 - \varepsilon$ helps. In this case the cubic equation equating the values of E_f is only second order in ε . An explicit solution of this equation for ε in terms of the quadratic formula can then be substituted into the second equation (for L_f) and all of it expanded to third order in τ and t to give a single cubic equation. Since our goal is to compare t and τ , it is expedient to change variables once again using the substitution $\tau = t - \delta$. Since we know that $\delta = 0$ to second order, it is then sufficient to expand the resulting cubic to first order in δ and third order in t . For case 1 ($uC < 0$), this gives

$$5t^3\omega u(E-L) + 12(2L\omega t + C + 2t^2Cu^2 + t^2Cu' + 2tCu + 6t^2\omega Lu - 2\omega^2Ct^2 - 2\omega u t^2E)\delta = 0 \quad (38)$$

and solving this to third order in t gives

$$\delta = -\frac{5t^3\omega u(E-L)}{12C}. \quad (39)$$

Similarly for the second case ($uC > 0$), the equation we get is

$$t^3\omega u(E-L) + 12(t^2\omega uE - C + 2t^2Cu^2 - 2L\omega t - t^2Cu' - 2tCu - 5t^2\omega Lu + 2\omega^2Ct^2)\delta = 0 \quad (40)$$

which results in the solution

$$\delta = \frac{1t^3\omega u(E-L)}{12C}. \quad (41)$$

Noting that t, ω , and $E - L$ are all positive, we find in either case that $\delta > 0$. Since $\delta = t - \tau$, we find that the bang-bang solution proceeds faster between the same two endpoints thereby completing our proof.

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