Prelude Processes

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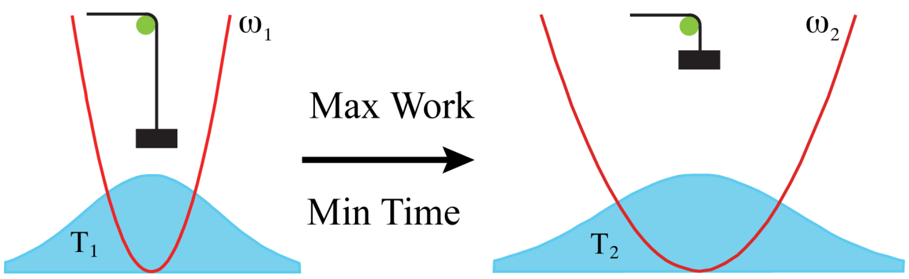
Optimization At A Small Scale

UCSD 2009



Questions of Finite Time Thermodynamics

- What is the maximum power that can be delivered by a heat engine in finite time?

$$\eta_{\mathrm{Max}P} = 1 - \sqrt{\frac{T_C}{T_H}}$$

- Given A_{init}, A_{final}, and τ , what is the minimum entropy that must be produced in changing the state of system A from A_{init} to A_{final} in time τ ?

$$\Delta S_u \geq L^2/2n$$

- Given A_{init} and A_{final}, what is the minimum time for changing the state of system A from A_{init} to A_{final}?

- How fast can we approach T=0?

"The Quantum Refrigerator: The quest for absolute zero",
Y. Rezek, P. Salamon, K.H. Hoffmann, and R. Kosloff,
Europhysics Letters, 85, 30008 (2009)

"Maximum Work in Minimum Time from a Conservative Quantum System",
P.Salamon, K.H. Hoffmann, Y. Rezek, and R. Kosloff,
Phys. Chem. Chem. Phys., 11, 1027 - 1032 (2009)

QuickTime and a
decompressor
are needed to see this picture.

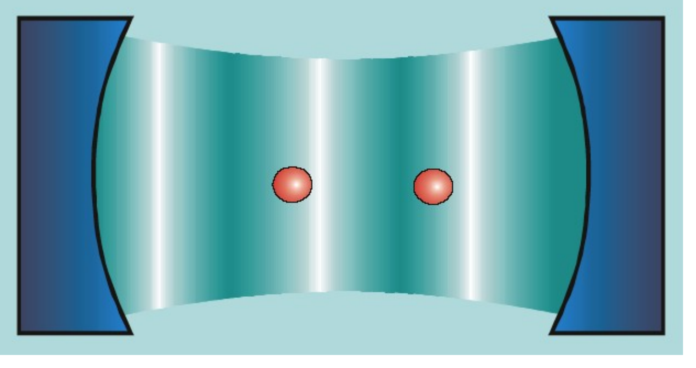
Definition

A prelude process is a reversible process performed as a prelude to a thermal process.

Ensemble of Independent Harmonic Oscillators Sharing a Controlled Frequency ω

$$H = \frac{1}{2}(P^2 + \omega^2 Q^2)$$

Cool atoms in an optical lattice. Lattice created by lasers and having an easily controlled ω .



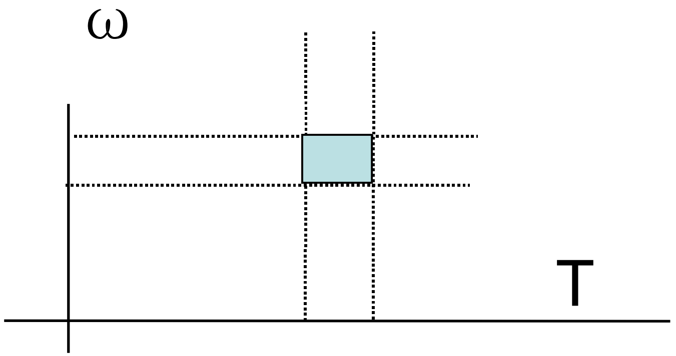
The Heat Engine

Rate Limiting Step

- Contact with $T=T_H$ at $\omega = \omega_1$.
- Adiabatic change from $\omega = \omega_1$ to $\omega = \omega_2$.
- Contact with $T=T_C$ at $\omega = \omega_2$.
- Adiabatic change from $\omega = \omega_2$ to $\omega = \omega_1$.

Controls: It's all in the timing.

Time for thermal contacts and rate at which ω changes on adiabats.



Finite-time Third Law

The second law limits the rate of cooling

For a cycle operating between T_c and T_h and exchanging heat, the net entropy production rate is

$$\sigma = -\dot{\mathcal{Q}}_c/T_c \; + \; \dot{\mathcal{Q}}_h/T_h > 0.$$

For bounded $|\dot{\mathcal{Q}}_h| < C$ this rearranges to give

$$\left(\frac{C}{T_h}\right) T_c > \dot{\mathcal{Q}}_c \propto T^\delta$$

The working fluid: Quantum Harmonic Oscillator

$$H = \frac{1}{2}(P^2 + \omega^2 Q^2) \qquad \text{Hamiltonian}$$

$$L = \frac{1}{2}(P^2 - \omega^2 Q^2) \qquad \text{Lagrangian}$$

$$C = \frac{\omega}{2}(PQ + QP) \qquad \text{Correlation}$$

C is needed to close the Lie algebra

Heisenberg Representation

$$\frac{dA}{dt} = i[H, A] + \frac{\partial A}{\partial t}$$

adiabats

$$\frac{dA}{dt} = i[H, A] + \frac{\partial A}{\partial t} + \mathcal{L}_D^*(A)$$

thermal contacts

with Lindblad operator

$$\mathcal{L}_D(\rho) = k_\downarrow(a^\dagger \rho a - \frac{1}{2}\{aa^\dagger, \rho\}) + k_\uparrow(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\})$$

Dynamics on Adiabats

$$\begin{aligned}\dot{E} &= \frac{\dot{\omega}}{\omega}(E-L)\\ \dot{L} &= -\frac{\dot{\omega}}{\omega}(E-L) - 2\omega C\\ \dot{C} &= 2\omega L + \frac{\dot{\omega}}{\omega}C\end{aligned}$$

$$\omega_{\min} \leq \omega \leq \omega_{\max}$$

$$-\infty \leq \dot{\omega} \leq \infty$$

or, using sudden jumps $\omega_i \longrightarrow \omega_f$

$$\begin{pmatrix} E \\ L \\ C \end{pmatrix}_{\omega_f} = \frac{1}{2}\begin{pmatrix} 1+(\frac{\omega_f}{\omega_i})^2 & 1-(\frac{\omega_f}{\omega_i})^2 & 0 \\ 1-(\frac{\omega_f}{\omega_i})^2 & 1+(\frac{\omega_f}{\omega_i})^2 & 0 \\ 0 & 0 & \frac{2\omega_f}{\omega_i} \end{pmatrix}\begin{pmatrix} E \\ L \\ C \end{pmatrix}_{\omega_i}$$

Sudden adiabats not optimal due to quantum friction.

Fixed omega dynamics

$$\begin{aligned}
\omega(t) &= \omega(0) \\
E(t) &= E(0) \\
L(t) &= \cos(2\omega t)L(0) - \sin(2\omega t)C(0) \\
C(t) &= \sin(2\omega t)L(0) + \cos(2\omega t)C(0)
\end{aligned}$$

Dynamics for Heat Exchange

- Lindblad dynamics

$$E(t) = e^{-\Gamma t}(E(0) - E_{eq}(T)) + E_{eq}(T)$$

$$\begin{pmatrix} L(t) \\ C(t) \end{pmatrix} = e^{-\Gamma t} \begin{pmatrix} \cos(2\omega t) & -\sin(2\omega t) \\ \sin(2\omega t) & \cos(2\omega t) \end{pmatrix} \begin{pmatrix} L(0) \\ C(0) \end{pmatrix}$$

where $\Gamma = k_{\downarrow} - k_{\uparrow}$

Heat bath = coherence decay

Quantum Entropy

The Von Neumann entropy

$$S_{VN} = \mathrm{Tr}\left(\rho \log(\rho)\right)$$

is conserved.

Effective entropy in contact with the heat bath is the energy entropy

$$S_E = \sum_n P_n \log(P_n)$$

where P=diag(ρ_E) and ρ_E is the density matrix in an energy basis.

$$S_{VN} \leq S_E$$

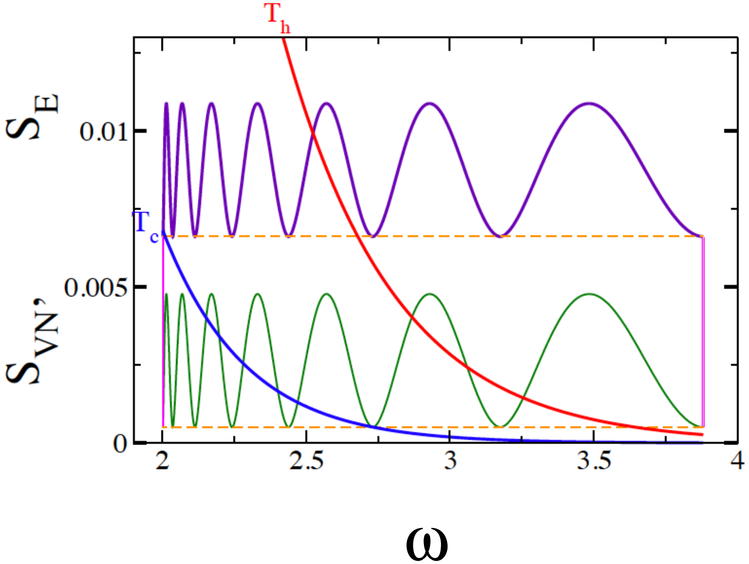
Quantum Friction

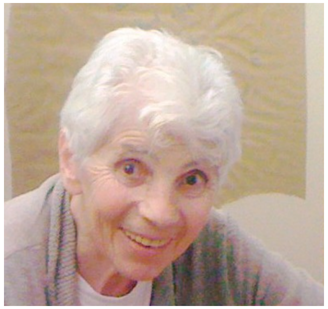
Problem: Changing ω at a finite rate or jumping from

$$\omega_i \longrightarrow \omega_f$$

creates "extra" entropy by increasing S_E.

During a heat exchange, the energy in the LC oscillation becomes heat. This is Feldmann & Kosloff's quantum friction





Adiabatic Switching

If we change ω infinitely slowly,
we can keep S_{VN} constant.

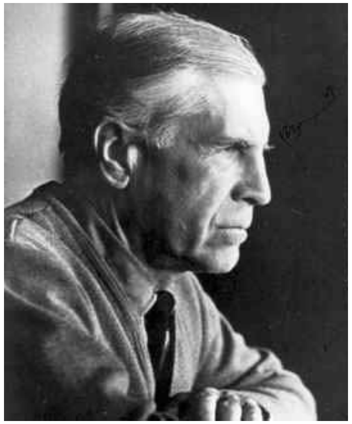
$$S_{\mathrm{VN}} = \ln\left(\sqrt{X - \frac{1}{4}}\right) + \sqrt{X}\,\mathrm{asinh}\left(\frac{\sqrt{X}}{X - \frac{1}{4}}\right)$$

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

Sets energy minimum

Thermal equilibrium at L=C=0

Optimal Control



Easier and more powerful calculus of variations.

The Problem:

$$\frac{dx}{dt} = f(x,u); \qquad \int f_0(x,u)dt \quad \to \mathrm{Min}$$

The Tool:

$$H(x,\lambda,u) = \sum_{i=0}^{n} \lambda_i f_i \quad \begin{cases} \dfrac{dx}{dt} = \dfrac{\partial H}{\partial \lambda} \\ \dfrac{d\lambda}{dt} = -\dfrac{\partial H}{\partial x} \end{cases}$$

The Optimality Conditions:

$$H \text{ constant in time}$$
$$H \text{ maximum in } u \text{ at each } t$$

Optimal Adiabats

Problem: How to choose ω(t)?

$$\begin{aligned}\dot{E} &= \frac{\dot{\omega}}{\omega}(E-L)\\ \dot{L} &= -\frac{\dot{\omega}}{\omega}(E-L)-2\omega C\\ \dot{C} &= 2\omega L+\frac{\dot{\omega}}{\omega}C\end{aligned}$$

augment with

$$\dot{\omega} = u\omega$$

Optimal control Hamiltonian

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

Linear in u!!!

Singular Control Problems

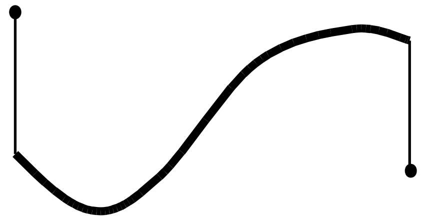
$$H = \sigma(x,\lambda)u + \alpha(x,\lambda)$$

σ = switching function

σ > 0; $u = u_{Max}$

σ < 0; $u = u_{Min}$

σ = 0; u=?



This structure usually leads to turnpike theorems.

Theorem: Optimal control of the harmonic oscillator is bang-bang.

Singular branches are never used.

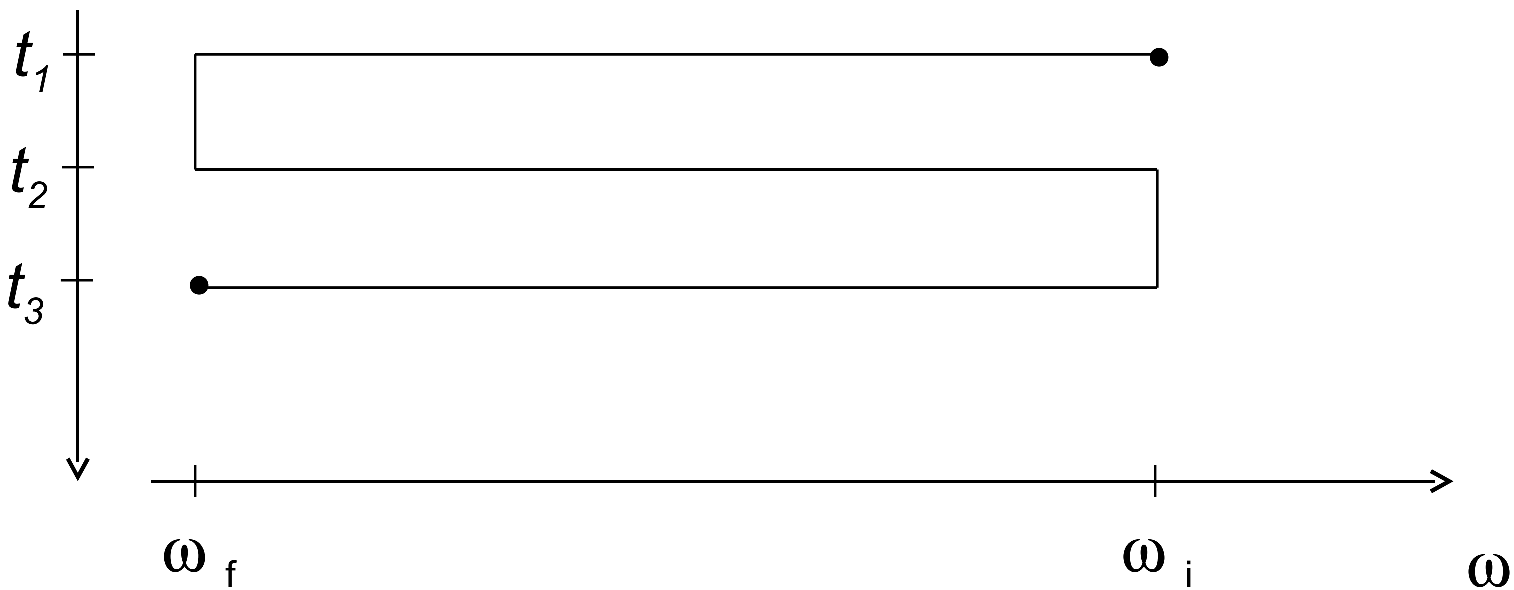
Best Adiabat

$$\omega_f \leq \omega_1, \omega_2 \leq \omega_i \quad \Longrightarrow \quad \begin{aligned} \omega_1^{\text{opt}} &= \omega_f \\ \omega_2^{\text{opt}} &= \omega_i \end{aligned}$$

$$t_3 - t_2 = \frac{1}{2\omega_2} \text{Arccos}\left(\frac{\omega_i^2 + \omega_f^2}{(\omega_i + \omega_f)^2}\right)$$

$$t_2 - t_1 = \frac{1}{2\omega_1} \text{Arccos}\left(\frac{\omega_i^2 + \omega_f^2}{(\omega_i + \omega_f)^2}\right)$$

Total time on the order of one oscillation !!!



The Magic

- Fast(est) adiabatic switching.
- Can only extract the full maximum work available from the change if

  time > min time

  else must create parasitic oscillations.

  -- New type of finite-time Availability
- Time limiting branch in a heat cycle to cool system toward T=0.
  - Implies

$$\dot{Q}_c \propto T^{\frac{3}{2}}$$