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Optimal control in a quantum cooling problem

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ABSTRACT

The optimal control for cooling a quantum harmonic oscillator by controlling its frequency is considered. It is shown that this singular problem may be transformed with the proper choice of coordinates to an equivalent problem which is no longer singular. The coordinates used are sufficiently simple that a graphical solution is possible and eliminates the need to use a Weierstrass-like approach to show optimality. The optimal control of this problem is of significance in connection with cooling physical systems to low temperatures. It is also mathematically significant in showing the power and limitations of coordinate transformations for attacking apparently singular problems.

The optimal control of a quantum harmonic oscillator is a problem of considerable interest in connection with the cooling of physical systems to lower and lower temperatures [1,2]. We have previously considered the control achievable by varying only the frequency of the oscillator—the classical parametric oscillator. The findings in [2] present several surprises. The optimal control is a fast adiabatic process, i.e. a process in which populations in each quantum state end up unchanged despite requiring much less time than traditional adiabatic following. Although the process is reversible, one can associate with it a potential dissipation that will ensue if the process is to be used as a prelude to a thermalization process. This dissipation is exactly the deviation from adiabaticity in the quantum sense [2] and comes with an associated minimum time below which some parasitic oscillations must remain in the system and add to the heat contributions in any ensuing contact with a heat bath. Schmiedl et al. [3] consider the same problem without requiring the squared frequency, ω^2, to remain non-negative. They find that as a limit, the adiabatic process can be achieved in arbitrarily short times by going to sufficiently negative ω^2. Similar findings were reported by Chen et al. [4]. All these findings contribute to the general field of optimally controlling physical systems and processes, which is of importance not only for technical applications [5–7] but also for mathematical algorithms like simulated annealing [8–10].

The purpose of this letter is to present a much simpler proof of the main technical result in [2] which was forced to resort to a lengthy argument reminiscent of the construction of the Weierstrass E-function to show directly that the solution is of the bang–bang type for this singular problem. The proof in [2] relies on explicitly replacing sufficiently small portions of any curve using an intermediate value of the control parameter by a small bang–bang portion operating between the endpoints. Here we show that by using a clever change of coordinates one can circumvent most of the difficulties including the need to proceed to the limit $\dot{\omega} \to \pm\infty$ to achieve the required jumps in ω. The literature on singular optimal control [11,12] suggests that problems often *appear* singular due to apparent extra degrees of freedom which are in fact constrained by some function of the state variables being constant. As shown below, this proves to be the case for the optimal control of a quantum oscillator for which the von Neumann entropy S_{vN} must remain constant. This letter shows how to implement

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a change of coordinates that eliminates one of the degrees of freedom by using the constancy of S_{vN}. The result is a two-dimensional problem which is no longer singular and for which the solution can be obtained in a geometrically clear manner. The proof that all optimal solutions are of the bang–bang type also follows easily.

Physically, the problem that we treat represents an ensemble of non-interacting quantum oscillators bound by a shared harmonic potential. We control the curvature of the potential $\omega(t)$. The energy of an individual particle is represented by the Hamiltonian

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

where m is the mass of the particle, and $\hat{\boldsymbol{Q}}$ and $\hat{\boldsymbol{P}}$ are the momentum and position operators. For convenience, we set the mass $m = 1$ below.

The dynamics is generated by the externally driven time dependent Hamiltonian $\hat{\boldsymbol{H}}(\omega(t))$. Our description is based on the Heisenberg picture in which our operators are time dependent. Generalized canonical states [13–17] are fully characterized by the frequency ω and the expectation values of three time dependent operators:

$$\hat{\boldsymbol{H}} = \frac{1}{2}\hat{\boldsymbol{P}}^2 + \frac{1}{2}\omega^2\hat{\boldsymbol{Q}}^2 \quad \text{Hamiltonian} \tag{2}$$

$$\hat{\boldsymbol{L}} = \frac{1}{2m}\hat{\boldsymbol{P}}^2 - \frac{1}{2}m\omega^2\hat{\boldsymbol{Q}}^2 \quad \text{Lagrangian} \tag{3}$$

$$\hat{\boldsymbol{C}} = \frac{\omega}{2}(\hat{\boldsymbol{Q}}\hat{\boldsymbol{P}} + \hat{\boldsymbol{P}}\hat{\boldsymbol{Q}}) \quad \text{position-momentum correlation.} \tag{4}$$

These three operators form a Lie algebra and thus completely characterize the time evolution generated by $\hat{\boldsymbol{H}}(\omega(t))$ which is an element of this algebra. Thermal equilibrium for the ensemble is characterized by $\langle\hat{\boldsymbol{L}}\rangle = 0$ (equipartition) and $\langle\hat{\boldsymbol{C}}\rangle = 0$ (no correlation).

It is enough to follow the expectation values $E = \langle\hat{\boldsymbol{H}}\rangle$, $L = \langle\hat{\boldsymbol{L}}\rangle$, and $C = \langle\hat{\boldsymbol{C}}\rangle$ of these operators. These expectation values obey the dynamical equations

$$\dot{E} = u(E - L) \tag{5}$$

$$\dot{L} = -u(E - L) - 2\omega C \tag{6}$$

$$\dot{C} = uC + 2\omega L \tag{7}$$

$$\dot{\omega} = u\omega \tag{8}$$

where, for convenience, we have set $u = \dot{\omega}/\omega$. u represents our (unbounded!) control for steering the system from a given initial state

$$E(0) = E_i, \tag{9}$$

$$L(0) = L_i = 0, \tag{10}$$

$$C(0) = C_i = 0, \tag{11}$$

$$\omega(0) = \omega_i, \tag{12}$$

to a state of minimum final energy, $E(\tau) \to \min$ with $\omega_f \le \omega(t) \le \omega_i$, for all $0 \le t \le \tau$, where τ is the process duration.

The von Neumann entropy S_{vN} of the system is given by a monotonically increasing function of the Casimir invariant

$$X = \frac{E^2 - (L^2 + C^2)}{\omega^2} \tag{13}$$

of the Lie algebra associated with the dynamics [2]. S_{vN} and X are constant for the time evolution; their values are determined by the initial conditions.

Minimality of the final energy subject to fixed X implies that the final values $C(\tau) = C_f$ and $L(\tau) = L_f$ should be equal to zero while $\omega(\tau)$ should be minimum and hence equal to ω_f. The value of $E(\tau) = E_f$ is then expressed as

$$E_f = \omega_f\sqrt{X} = \frac{\omega_f}{\omega_i}E_i. \tag{14}$$

So, initial and final states of the system are given.

Many controls $u(t)$ exist that achieve this control for sufficiently large τ, while for τ below a critical value $\tau_{\min}$, no controls can reach the desired final state. Accordingly, we seek the value of the control u that minimizes the process duration $\tau \to \min$.

We begin by introducing new variables [18]

$$z_1 = \frac{E - L}{\omega^2}; \qquad z_2 = E + L; \qquad z_3 = \frac{C}{\omega} \tag{15}$$

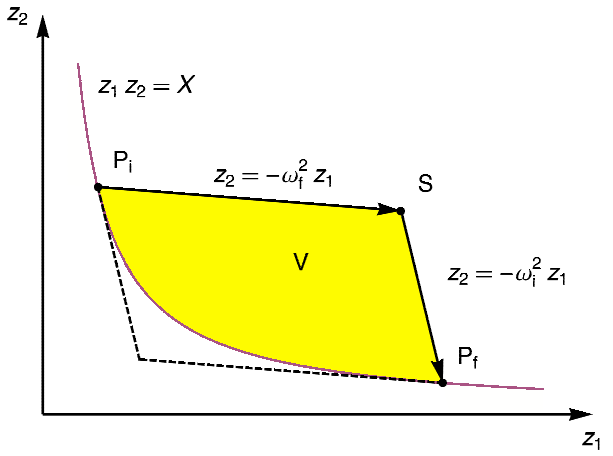

Fig. 1. The feasible region V and the optimal solution $P_i \to S \to P_f$.

which can be used to express the old variables

$$E = (z_2 + \omega^2 z_1)/2; \qquad L = (z_2 - \omega^2 z_1)/2; \qquad C = \omega z_3; \qquad X = z_1 z_2 - z_3^2. \tag{16}$$

Let us express z_3 as a function of X, z_1, z_2 and rewrite the system of the dynamical equation (5) using our variables, taking into account (15), (16). The result is the following:

$$\dot{z}_1 = 2z_3 = 2\sqrt{z_1 z_2 - X}, \tag{17}$$

$$\dot{z}_2 = -2\omega^2 z_3 = -2\omega^2 \sqrt{z_1 z_2 - X}. \tag{18}$$

The choice of the sign on the square root in these equations is determined by the sign of C which is positive for the case $\omega_f < \omega_i$ discussed here. Note that the control u does not appear in these equations. In fact since u is effectively $\dot{\omega}$, and is unconstrained, we can achieve any desired $\omega(t)$ (including jump discontinuities) and use $v = \omega^2$ as our new control. Thus our change of variables has reduced the number of state variables to two and we further have

$$\frac{dz_2}{dz_1} = -\omega^2 = -v. \tag{19}$$

The boundary conditions for variables z_1 and z_2 are

$$z_{1i} = \frac{E_i}{\omega_i^2}, \qquad z_{1f} = \frac{E_f}{\omega_f^2} = \frac{\sqrt{X}}{\omega_f}, \qquad z_{2i} = E_i, \qquad z_{2f} = E_f = \omega_f \sqrt{X}, \tag{20}$$

where we have made use of the final state conditions from above. Note that since $\omega_f < \omega_i, z_{1f} > z_{1i}$.

This transformation of state space simplifies the problem so much that it is possible to illustrate the solution graphically. The duration of the transition of the system from the initial to the final state is

$$\tau = \int_{z_{1i}}^{z_{1f}} \frac{dz_1}{2\sqrt{z_1 z_2 - X}}. \tag{21}$$

It can be calculated once we have chosen $z_2(z_1)$. It follows from (21) that z_2 for each z_1 should maximize the product $z_1 z_2$ along the optimal solution $z_2^*(z_1)$ subject to the restrictions on v:

$$\omega_f^2 \le v \le \omega_i^2. \tag{22}$$

Consider the graph of our feasible region V shown in Fig. 1. It follows from (19) and (22) that V must be contained in the parallelogram bounded by lines with slopes $-\omega_i^2$ and $-\omega_f^2$ emanating from the initial and final points. In addition, the fact that z_3 must be real implies that V includes only the portion of this parallelogram above the hyperbola $z_1 z_2 = X$. Here $P_i = (z_{1i}, z_{2i})$ is the initial state and $P_f = (z_{1f}, z_{2f})$ is the final state. Both points are on the hyperbola $z_1 z_2 = X$. It follows from (21) that the optimal solution $\tau \to \min$ lies on the upper boundary of V for arbitrary initial and final points on $z_1 z_2 = X$.

The optimal solution thus proceeds by an initial jump $\omega_i \to \omega_f$, keeping $\omega = \omega_f$ until we reach the switch point S, switching ω to $\omega = \omega_i$ until we reach P_f and then switching to $\omega = \omega_f$. The bang–bang nature of the solution can alternatively be obtained from Pontryagin's maximum principle, but the geometrically clear solution was chosen here for its simplicity.

The coordinates of the switching point $S = (z_{1S}, z_{2S})$ can be found as a solution of the equations

$$z_{2S} = z_{2i} - \omega_f^2(z_{1S} - z_{1i}), \qquad z_{2S} = z_{2f} - \omega_i^2(z_{1S} - z_{1f}). \tag{23}$$

The result is

$$z_{1S} = \frac{\omega_i^2 z_{1f} - \omega_f^2 z_{1i} + z_{2f} - z_{2i}}{\omega_i^2 - \omega_f^2} \tag{24}$$

$$z_{2S} = \frac{\omega_i^2 z_{2i} - \omega_f^2 z_{2f} + \omega_i^2\omega_f^2(z_{1i} - z_{1f})}{\omega_i^2 - \omega_f^2}. \tag{25}$$

We can use the results to evaluate the integrals

$$\tau_{\min} = \frac{1}{2}\left(\int_{z_{1i}}^{z_{1S}} \frac{dz_1}{\sqrt{[z_{2i} - \omega_f^2(z_1 - z_{1i})]z_1 - X}} + \int_{z1S}^{z_{1f}} \frac{dz_1}{\sqrt{[z_{2f} - \omega_i^2(z_1 - z_{1f})]z_1 - X}}\right), \tag{26}$$

which eventually simplifies to

$$\tau_{\min} = \frac{1}{2\omega_f}\arccos\left(\frac{\omega_i^2 + \omega_f^2}{(\omega_i + \omega_f)^2}\right) + \frac{1}{2\omega_i}\arccos\left(\frac{\omega_i^2 + \omega_f^2}{(\omega_i + \omega_f)^2}\right) \tag{27}$$

for the minimal duration $\tau_{\min}$ of cooling the quantum oscillator to $E = E_f$.

The above arguments show that with a carefully chosen coordinate change that takes advantage of the constancy of the von Neumann entropy of a quantum system one can resolve the apparently singular nature of the optimal control of a quantum harmonic oscillator. In the transformed variables, the solution becomes simple and geometrically clear. The simplicity achieved here however is lost once one tries to extend this approach to arbitrary initial and final states rather than the equilibrium states used here. In that case the two-to-one nature of the transformation requires the appropriate sign of the square root corresponding to the signs of C_i and C_f, and the cone of controllability can point the wrong way requiring a traversal to and from the hyperbola $z_1z_2 = X$. The consideration of this more general problem is left for a future effort.

The solution obtained achieves the equivalent of a quantum adiabatic process in fast time—on the order of one oscillation. By contrast, the traditional adiabatic-following approach takes infinite time and is obtained by traversing along the $z_1z_2 = X$ hyperbola in Fig. 1.

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