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Time-optimal controls for frictionless cooling in harmonic traps

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Image: Ornamental multiplication of space-time figures of temperature transformation rules (adapted from T. S. Bíró and P. Ván 2010 EPL 89 30001; artistic impression by Frédérique Swist).
The third law of thermodynamics is also called the unattainability principle [1–4]. In a dynamical interpretation absolute zero is unattainable as the cooling rate from a thermal bath with falling temperature declines as well and approaches zero together with an appropriate power of the temperature [5]. The relation of the cooling rate to the bath temperature depends crucially on the thermodynamic cooling process used. In particular, the times needed for cooling processes in an adiabatic fashion are important. In that context the frictionless cooling of particles in harmonic traps, which gained a lot of recent attention (see [6–16] and references therein), are of relevance. Here the interesting question is how these processes can be performed in the minimum time. A number of different methods have been suggested and implemented [6–8,10,17]. We feel it fair to say that the problem has turned out to be much richer than initially imagined. Our previous study considered only the case where the particles are confined by attractive harmonic potentials [17]. It turns out that allowing the potential to become repelling during the process can achieve even shorter times [6–8,10,11]. When the potentials can become arbitrarily strong, frictionless transfer can be achieved in zero time [6,7,11]. We note however that this would require the energy of the oscillator to become infinite. It is natural to set bounds on the strength, i.e. the curvature, of achievable potentials but at large values of such a bound a new complication arises. Stefanatos et al. [11] have shown that the structure of the minimum time solution changes at sufficiently large values of the bound insofar as more jumps in the frequency outperform the three-jump solutions that are optimal for more moderate values of the largest frequency achievable in the control. Here we focus on such problems for which three-jump controls are optimal. This applies for example when the initial frequency coincides with the maximum allowed frequency, the case of interest for refrigeration. As argued in [5] the maximum allowed frequency is used as the initial
state for the adiabatic cooling branch to ensure maximum population in the ground state. Our previous solution was correct for this case, provided imaginary frequencies are used in the formulas (28) and (29) presented in [17].

The aim of this paper is twofold. Our first aim is to discuss the implications of the optimal three-jump bang-bang control on the cooling rate of a quantum refrigerator. Contrary to the restrictions in [17] we here allow the potential to become repelling, which leads to much larger cooling rates.

The second aim of this paper is to consider the addition of continuity requirements for the controls. Such requirements have been implemented by a number of authors based on Ermakov invariants added to the control problem and have resulted in smooth controls which have been tested empirically [7,8,10,11,15]. Here we take a different approach which directly constrains the rate with which the potential can be changed. We present a special type of optimal control, which we call ramped bang-bang. Such ramped bang-bang control considerably shortens the time needed to achieve a frictionless transition from one thermal state to one at a different temperature when compared to continuous controls obtained from the approach advocated by Chen et al. [7,8] based on Ermakov invariants.

In this paper we analyze the parametric harmonic oscillator, i.e. a particle of mass \( m \) in a quadratic, time-dependent potential. Its Hamiltonian is given by

\[
\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{1}{2} k(t) \hat{Q}^2.
\]  
(1)

As we will allow the potential to become repelling we use the force constant \( k(t) \) instead of the frequency \( \omega(t) = \sqrt{k(t)/m} \) which will become imaginary in that case.

The dynamics can be completely described by the expectation values of three time-dependent operators: namely the expectation values of the momentum squared \( \langle \hat{P}^2 \rangle \), the position squared \( \langle \hat{Q}^2 \rangle \), and the correlation \( \langle \hat{D} \rangle = \langle \hat{Q} \hat{P} + \hat{P} \hat{Q} \rangle \). These will be collective labelled as \( x = \langle \hat{P}^2 \rangle, \langle \hat{Q}^2 \rangle, \langle \hat{D} \rangle \). Substituting these operators into the Heisenberg-equation and taking expectation values leads to three linear coupled differential equations, describing the dynamics that we need to control

\[
\langle \hat{P}^2 \rangle = f_1(x,k) = -k(t) \langle \hat{D} \rangle,
\]  
(2)

\[
\langle \hat{Q}^2 \rangle = f_2(x,k) = \langle \hat{D} \rangle / m,
\]  
(3)

\[
\langle \hat{D} \rangle = f_3(x,k) = 2\langle \hat{P}^2 \rangle / m - 2k(t) \langle \hat{Q}^2 \rangle.
\]  
(4)

Starting from a thermal equilibrium with \( k_i \), our goal is to reach the target state, thermal equilibrium with \( k_f \), in minimal time

\[
\int_{t_1}^{t_f} f_0(x,k) dt = \int_{t_1}^{t_f} dt.
\]  
(5)

Thermal equilibrium implies \( \langle \hat{D} \rangle(t_{1,f}) = 0 \) and \( \langle \hat{P}^2 \rangle(t_{1,f}) \) and \( \langle \hat{Q}^2 \rangle(t_{1,f}) \) have to fulfill the equipartition requirement, i.e. \( \langle \hat{P}^2 \rangle(t_{1,f}) / m = k(t_{1,f}) \langle \hat{Q}^2 \rangle(t_{1,f}) \).

For the parametric oscillator the desired state transition is achieved by a suitable control of the force constant \( k(t) \). We first turn to the case where the control \( k(t) \) is limited in size by \( k_{\text{min}} \leq k(t) \leq k_{\text{max}} \). Experimentally this amounts to a maximum confining potential in a harmonic trap, or conversely, to a maximum repelling potential. Thus the control is free to vary within these constraints, but cannot exceed them.

In order to find the fastest adiabatic transition we solve an optimal control problem, with the dynamics eqs. (2)–(4) as constraints. The technical details of that problem were discussed in [17], so we here restrict ourselves to the important features of that control problem. The objective of the control problem \( f_0(x,k) = 1 \) is especially simple. The linear dependence of the dynamics on the control \( k(t) \) leads to a linear dependence of the control Hamiltonian \( \mathcal{H} \),

\[
\mathcal{H} = \sum_{n=0}^{3} \lambda_n f_n(x,k) \equiv \mathcal{H}_0 + \sigma k,
\]  
(6)

where the \( \lambda_n \) are the adjoint variables, and \( \mathcal{H}_0 \) and \( \sigma k \) are the two terms of \( \mathcal{H} \), which are zeroth and first order in \( k \) respectively. The Pontryagin maximality principle [18] requires that the value of the control must maximize \( \mathcal{H} \). Thus when the switching function \( \sigma \), i.e. the coefficient of the control, is positive, \( k \) must be as large as possible and when \( \sigma \) is negative, \( k \) must be as small as possible. Since away from the constraints set by the inequalities \( k_{\text{min}} \leq k(t) \leq k_{\text{max}} \) the value of \( k \) is not constrained, this amounts in our problem to jumps in \( k \). Such jumps must terminate on the boundary arcs \( k(t) = k_{\text{max}} \) or \( k(t) = k_{\text{min}} \) 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 [17,19,20], along which the switching function \( \sigma \) vanishes identically over a time interval. 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 \( k \)'s. The proof is presented in [17,21], which shows that continuously varying \( k(t) \) can never be part of an optimal control. For a further discussion of singular control problems we refer the reader to [22] for quantum problems in general and to [23,24] for spin control problems in particular, for classical systems see [25,26].

The number of jumps needed to reach our target state turns out to be three. However, depending on the size of \( k_{\text{max}} \) multi-jump bang-bang controls with more than three jumps can outperform the three-jump control [27]. For the discussion here, we restrict ourselves to the three-jump control which allows a closed-form description and which is the only case of interest for use in refrigeration for which we always want \( k_i = k_{\text{max}} \). Cooling the system by a three-jump control requires a jump from the initial \( k_i \) to the minimum possible \( k_1 = k_{\text{min}} \), hold \( k \) constant for a wait time \( \tau_1 \), then jump to the maximum possible \( k_2 = k_{\text{max}} \), hold \( k \) constant for a wait time \( \tau_2 \), and finally
the optimal three-jump bang-bang solution is to reach the target state in the minimum time. Summarizing bang-bang controls were used in a quantum refrigerator to determine the temperature dependence of the cooling rate as the temperature of the cold bath approaches zero. As already pointed out, both times can become arbitrarily small if \( k_1 = -k_2 \) approaches infinity for fixed \( k \). However, if we choose fixed \( k_1 \) and \( k_2 \) and then vary \( k \) things are different. In that case it can be shown that \( \tau_1 \) diverges with \(-\log k_1\) as the leading term while \( \tau_2 \) remains finite. For the special choice \( k_1 = -k_2 \) and \( k_2 = -k_1 \) one obtains

\[
\tau_1 = \frac{-\log(k_1/k_2)}{4\sqrt{k_1/m}},
\]

\[
\tau_2 = \frac{\pi}{4\sqrt{k_1/m}}.
\]

This leads to implications for the cooling rate \( R \). Let \( \tau_c \) and \( \tau_h \) be the times spent in contact with the cold and hot heat bath, respectively, and let \( \tau_{adi} = 2(\tau_1 + \tau_2) \) be the time needed for the adiabats. Further denote the population (i.e. the expectation of the number operator) for a system in equilibrium with the cold or hot \(( i = c, h)\) temperature bath by

\[
n_{e}^{ci}(\omega_i, T_i) = 1/(e^{\frac{\hbar}{\Gamma_{e}c}T_i} - 1).
\]

Following the same approach as in [5] one finds

\[
R = F(\tau_c, \tau_h, \tau_{adi})G(\omega_c, \omega_h, T_c, T_h),
\]

with

\[
G(\omega_c, \omega_h, T_c, T_h) = \hbar \omega_c (n_{e}^{ci} - n_{h}^{ci})
\]

and

\[
F(\tau_c, \tau_h, \tau_{adi}) = \frac{(e^{\Gamma_{e}c} - 1)(e^{\Gamma_{h}} - 1)}{(e^{\Gamma_{e}c} + e^{\Gamma_{h}} - 1)(\tau_{adi} + \tau_c + \tau_h)},
\]

where \( \Gamma \) is the relaxation rate for establishing thermal equilibrium while in contact with a bath. Maximizing \( F \) with respect to the relative size of the isochoric times leads to \( \tau_c = \tau_h \), which allows us to introduce \( z \equiv \Gamma_{e}c = \Gamma_{h} \). We can now ask how much time we should spend on the isochores \(( z)\) for a given time spent on the adiabats \(( \tau_{adi})\), by setting the derivative of \( F \) with respect to \( z \) to zero. This yields the equation

\[
2z + \Gamma_{adi} = \text{Sinh}(z).
\]

Taking the limit where the time spent on the adiabats is long, this equation becomes \( \Gamma_{adi} \approx e^2 / 2 \). Within that approximation we can rewrite \( R \) as

\[
R^* = G(\omega_c, \omega_h, T_c, T_h)/\tau_{adi}.
\]

We now want to find an upper bound on \( R^* \) for \( T_c \) decreasing towards zero. To find such a bound we maximize \( R^* \) for fixed \( T_h \) and \( \omega_h \) with respect to \( \omega_c \). Note that \( G \) as

\[
k_\text{optimal}(t) = \begin{cases} k_1, & \text{for } t = 0, \\ k_1, & \text{for } 0 < t \leq \tau_1, \\ k_2, & \text{for } \tau_1 < t < \tau_1 + \tau_2, \\ k_1, & \text{for } t = \tau_1 + \tau_2. \end{cases}
\]

For any values of the intermediate frequencies \( k_1 \) and \( k_2 \), the values of \( \tau_1 \) and \( \tau_2 \) given in [17] can be used by allowing \( \omega \) to become negative

\[
\tau_1 = \frac{1}{2\sqrt{-k_1/m}} \text{Arccosh}(r_1),
\]

\[
\tau_2 = \frac{1}{2\sqrt{k_2/m}} \text{Arccosh}(r_2),
\]

where

\[
r_1 = \frac{2k_1(k_2 + k_1)\sqrt{k_1} - (k_1 + k_2)(k_1 + k_1)\sqrt{k_1}}{(k_2 - k_1)\sqrt{k_1}(k_1 - k_1)},
\]

\[
r_2 = \frac{2k_2(k_1 + k_1)\sqrt{k_1} - (k_1 + k_2)(k_2 + k_1)\sqrt{k_2}}{(k_1 - k_2)\sqrt{k_2}(k_2 - k_2)}.
\]

Here we made already use of the fact that in the following \( k_1 < 0 \). For the case of cooling \( \sqrt{k_1/m} = \omega_f < \omega_1 = \sqrt{k_1/m} \), the smaller \( k_1 \) and the larger \( k_2 \) are, the faster the process. The fastest three-jump process with \( \tau_1 = \tau_2 = 0 \) is obtained in the limit \(-k_1 = k_2 \rightarrow \infty \). In order to make contact with experiments [28] the following values were used by [7]: \( \omega_1 = 250 \times 2\pi \) Hz and \( \omega_f = 2.5 \times 2\pi \) as well as \( \gamma = \sqrt{\omega_1/\omega_f} = 10 \).

In fig. 1 we show how the times \( \tau_1 \) and \( \tau_2 \) change as a function of \( k_f \) for the case \( k_2 = -k_1 \). The choice to set \( k_1 = -k_2 \) is motivated by the fact that the same harmonic potential can be made repelling or attractive by a phase shift in case it is created by an optical lattice.

The bang-bang control presented above is of relevance in a dynamical interpretation of the third law. In [5] optimal bang-bang controls were used in a quantum refrigerator.
quantum refrigerator decreases close to linearly with decreasing frequencies. Such requirements lead to the same limitations on the time averaged energies of the oscillator levels during the adiabatic move are discussed showing that limits on the time-averaged energies of the oscillator levels could be reached for smaller $\tau_{adi}$ due to the second law, and on the adiabatic cooling process might lead to slower cooling rates than $R_{opt}$ for small $T_c$. Figure 2 shows $\omega_{c,opt}$ as a function of $T_c$. The close to diagonal graph supports the above suggestion. Inserting $\omega_{c}\propto T_c$ into $R^*$ would then lead to $R^* \propto -T_c/\log T_c$. This is checked in fig. 3, where

$$A^{opt} = \frac{-\log T_c}{T_c} R^{opt}$$

is shown as a function of $T_c$, showing the slightly lower decrease within the range analyzed. This is consistent with the hypothesis that the third law constrains the cooling rate beyond the requirements due to the second law, and is the closest approach to the rate expected from the second law. We note however that further requirements on the adiabatic cooling process might lead to slower cooling rates than $R^{opt}$ or $-T_c/\log T_c$. In [8] the effect of limits on the time-averaged energies of the oscillator levels during the adiabatic move are discussed showing that such requirements lead to the same limitations on the cooling rate as the requirement of positive intermediate frequencies.

We now turn to our second aim, namely controls with a continuity requirement. In a recent paper by Chen et al. [7,8] a smooth control was suggested which allows an adiabatic transition between thermal states of a harmonic oscillator in finite time. Such controls have also been used experimentally [10]. The control is based on the existence of invariants of motion [29–32] for a harmonic oscillator. These invariants depend on a function of time $b(t)$, which is intimately connected to the time-dependent frequency of the oscillator via an Ermakov equation

$$\bar{b} + \omega(t)^2 b = \omega_i^2/b^3.$$  

(21)

The function $b(t)$ is dimensionless and scales with the time $t$, which is available to change the system from a thermal equilibrium state at $t = 0$ with $\omega(0)^2 = \omega_i^2 = k(0)/m = k_i/m$ to the final equilibrium state at $t = t_f$ with $\omega(t_f)^2 = \omega_f^2 = k(t_f)/m = k_f/m$. The reduction in the frequency ratio corresponds to the reduction in temperatures and is characterized by $\gamma = \sqrt{\omega_i/\omega_f}$. In order to ensure a continuous $k(t) = m\omega(t)^2$ at $t = 0$ and at $t = t_f$ with $k(t) = k_i$ for $t < t_f$ and $k(t) = k_f$ for $t > t_f$ $b(t)$ must fulfill $b(0) = 1$, $\dot{b}(0) = 0$, and $\ddot{b}(0) = 0$ as well as $b(t_f) = \gamma$, $\dot{b}(t_f) = 0$, and $\ddot{b}(t_f) = 0$. In [7] a polynomial ansatz fulfilling the above conditions is presented $b(t) = 6(\gamma - 1) (t/t_f)^3 - 15(\gamma - 1)(t/t_f)^4 + 10(\gamma - 1)(t/t_f)^5 + 1$. Based on this ansatz the ensuing continuous control $k_C(t,t_f)$ —called C-control in the following— can be determined from eq. (21). Note that $k_C(t,t_f)$ will depend on $t$ and $t_f$ separately, and not only on $t_f$.

For each $t_f$ this control can now be compared to the optimal three-jump bang-bang control. As both controls allow the transition in arbitrarily short time provided that also a negative $k$, i.e., a repelling potential, is allowed, one needs to compare the controls for the same system constraints. These constraints are given by the ability to control $k(t)$ during the transition, i.e., the extreme values reachable for $k$.

For a given $k_C(t,t_f)$ we thus define $k_C^{max}(t_f) = \max_{0 \leq t \leq t_f} k_C(t,t_f)$ and $k_C^{min}(t_f) = \min_{0 \leq t \leq t_f} k_C(t,t_f)$. Then we input these as $k_1 = k_C^{min}(t_f)$ and $k_2 = k_C^{max}(t_f)$ together with $k_i$ and $k_f$ into eqs. (8) and (9) and obtain the time $t_1$ corresponding to $t_f$ for the optimal bang-bang control.

To highlight the savings in time fig. 4 (top) shows a comparison between $k_C(t)$ and $k_{33}(t)$ as a function of time. Here the process duration $t_f = 3$ was preset, then the corresponding minimal and maximal $k$ were obtained and these were used to construct $k_{33}(t)$. Note that the time required to achieve the same transition within the same $k$-limits is only $t_1 = 2.154$ for the optimal bang-bang solution.

In fig. 4 (bottom) the ratio $t_1/t_f$ is shown, which stresses the fact that the time needed for the optimal control is indeed shorter than for the continuous invariant control. Note that for shorter times $t_1$ the ratio seems to become constant. The corner in the ratio occurs where $k_C^{max}(t_f)$ becomes larger than 1. As already said above, we expect that usually the range of controllability for $k(t)$ is the same for positive and negative values. Then the advantages of the bang-bang solution become even more apparent. In that case the comparison requires the use of a bang-bang control which
has $k_2 = -k_1 = \max(k_{C}^{\max} (t_f), |k_{C}^{\min} (t_f)|)$ and which we call symmetric bang-bang $k_{RR}(t)$. This comparison is depicted in fig. 5 (top). The time savings now are even larger and $\tau_f = 1.679$.

If this procedure is repeated for all $t_f$, the resulting $\tau_f$ to $t_f$ ratio is shown in fig. 5 (bottom).

In this section we turn to the control problem which ensues if one insists on having a continuous control. In that case the bang-bang solution is no longer an option, and the control problem has to be recast with the constraint that the derivative of $k(t)$ is bounded $\dot{k}_{\min} < \dot{k}(t) < \dot{k}_{\max}$. To handle this scenario one introduces $u(t) \equiv \dot{k}(t)$ as a new control and supplements the state variables with $k(t)$. It turns out that the resulting control problem is again linear in the control $u(t)$ and thus the optimal control will consist of arcs with the limitations on $\dot{k}$ active, arcs with the limitations on $k(t)$ active, and in principle also further interior trajectories. However, as each part of an optimal control is optimal for the restricted problem, it follows from the non-existence of interior solutions in the unbounded problem that they do not exist in this case as well. We term such optimal controls ramped bang-bang solutions. As any continuous control with the same restriction on its time derivative is within the set of possible controls, ramped bang-bang solutions will always be superior to any continuous control out of that set. Thus a more generalized C-control will not lead to faster solutions, as long as the derivative stays within the constraints given.

In fig. 6 (top) a comparison of the C-control $k_C$ with the ramped bang-bang solution is shown. The limitations are taken from the C-control and the figure shows that also for this continuous control a shorter process time
can be obtained. Compared to the time needed for the C-control $t_f = 3$ we here find a overall time of $\tau_f = 2.370$.

The gain in time becomes even larger, if one uses the symmetrized ramped bang-bang control. This is shown in fig. 6 (bottom). Here the process times compare as $t_f = 3$ vs. $\tau_f = 1.916$.

In summary we showed that also for harmonic traps which can implement repelling potentials the use of three-jump bang-bang controls are time optimal for refrigeration [27]. In particular the process times are shorter than for comparable continuous controls based on invariants. In addition we showed that the requirement of continuous controls leads to ramped bang-bang controls which also outperform the comparable continuous controls. Of course, such controls will approach the performance of the ramped bang-bang one if the appropriate $b(t)$ are chosen.

We mention that the same basic principles can be used to create controls which have an even smoother transition at the initial and final times of the process. Especially that the existence of three-jump bang-bang controls for systems allowing repelling potentials provide scaling properties of the cooling rate of a quantum refrigerator in the context of the third law.

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