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# Time-optimal processes for interacting spin systems

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**Abstract** – Reversible adiabatic processes connecting thermal equilibrium states are usually considered to be infinitely slow. Recently, fast reversible adiabatic processes for quantum systems have been discussed. Here we present time-optimal processes for a paradigmatic ensemble of two interacting spin-$\frac{1}{2}$ systems in an external magnetic field, which previously had been employed as working fluid in a quantum refrigerator. These processes are realized by appropriate bang-bang or quasi–bang-bang controls of the external magnetic field. Explicit control protocols including the necessary times for a transition connecting thermal equilibrium states depending on the limiting conditions on the magnetic field strength are presented.



Optimal control of quantum systems has attracted considerable interest in recent years [1–7]. Sources of interest in the area are manifold and range from quantum computing and control of chemical reactions to manipulating Bose-Einstein condensates. Our present interest in such control stems from the quest to attain lower and lower temperatures with more and more complicated systems [8]. Heat pumps that reach such extreme temperatures perforce require quantum treatment.

Lossless control of the working fluid can be achieved in the adiabatic limit which requires slow operation. Due to heat leaks from the surroundings, the objective for heat pumping from extremely low temperatures is not the coefficient of performance but rather the rate of heat removal from the system being cooled. That is not to say that irreversibilities do not play an important role for such engines. Quite the contrary, any irreversibility in the branch cooling the working fluid will limit the temperature that the working fluid can attain as well as the subsequent rate of heat transfer out of the cooled system. Thus, the branch of the cooling cycle during which the working fluid is cooled is the natural focus for optimal control. Fast cooling of working fluids runs into the problem of exciting internal degrees of freedom, a phenomenon also termed quantum friction [9,10]. Surprisingly, however, we have found [11] that there exist very fast effectively adiabatic processes, *i.e.*, processes that begin and end at states that the adiabatic process would connect thereby eliminating the quantum frictional irreversibilities. In a previous effort [8,11], we have exhibited such processes for cooling a working fluid made of harmonic oscillators. In the present work, we show that such fast effectively adiabatic cooling can also be achieved for a working fluid composed of two coupled spins – the original system for studying quantum friction. Whether such fast effectively adiabatic processes exist for other quantum systems is an important open problem. This paper presents a second example.

Optimal control of spin systems has a long history [4,12,13]; the resultant controls have a rich and well–worked-out structure, which are important for NMR [1,4]. In general, the structure of the achievable controls depends strongly on the type of control one assumes possible. For example, the controls applied in [12] had more degrees of freedom than those used in the present paper.

The present effort also deviates somewhat from the standard problem in the field in its view of the initial and final states as well as the natural constraints on the allowed controls. Rather than considering arbitrary transfer of populations between excited and ground states, we focus on controls that carry our system from one thermal state to another. This makes it natural to consider the problem of minimum time transfer using external fields constrained to operate between initial and final frequencies. We carry

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out the analysis explicitly for this case which is simpler than the full optimal control and which gives explicit formulas for the minimum time. We conclude by discussing the more general case where these constraints on the external field are relaxed.

The thermodynamic system we investigate was introduced by [10]. It is an ensemble of non-interacting spin systems, each consisting of two interacting spin-$\frac{1}{2}$ particles. The Hamiltonian of these systems is

$$\mathcal{H} = \mathcal{H}^{\text{int}} + \mathcal{H}^{\text{ext}}(\omega), \tag{1}$$

where

$$\mathcal{H}^{\text{int}} = \frac{1}{2}\hbar j(\sigma_x^1 \otimes \sigma_x^2 - \sigma_y^1 \otimes \sigma_y^2) =: \hbar j \mathcal{B}_2, \tag{2}$$

$$\mathcal{H}^{\text{ext}} = \frac{1}{2}\hbar\omega(t)(\sigma_z^1 \otimes \mathcal{I}^2 + \mathcal{I}^1 \otimes \sigma_z^2) =: \hbar\omega(t)\mathcal{B}_1. \tag{3}$$

$\mathcal{H}^{\text{int}}$ represents the interaction between the two spins and $\mathcal{H}^{\text{ext}}$ the interaction of the spins with an external magnetic field $\omega$. Here $\sigma$ is the Pauli spin operator, $j$ scales the strength of the inter-particle interaction and $\omega(t)$ is the time-dependent strength of the external magnetic field which is considered to be in the $z$-direction. The energy levels of one of the spin systems are

$$E_1 = -\hbar\Omega, \qquad E_2 = E_3 = 0, \qquad E_4 = \hbar\Omega \tag{4}$$

with $\Omega(t) = \sqrt{\omega^2 + j^2}$.

The operators $\mathcal{B}_1$ and $\mathcal{B}_2$ together with $\mathcal{B}_3 = \frac{1}{2}(\sigma_y^1 \otimes \sigma_x^2 + \sigma_x^1 \otimes \sigma_y^2)$ generate a Lie algebra, which is isomorphic to the $\mathfrak{su}(2)$ Lie algebra [14]. This has the consequence that in the Heisenberg picture the time derivatives of these operators,

$$\dot{\mathcal{B}}_1 = 2j\mathcal{B}_3, \tag{5}$$

$$\dot{\mathcal{B}}_2 = -2\omega\mathcal{B}_3, \tag{6}$$

$$\dot{\mathcal{B}}_3 = -2j\mathcal{B}_1 + 2\omega\mathcal{B}_2, \tag{7}$$

can be written as linear combinations of these same operators. Due to the linearity of eqs. (5)–(7) one obtains equivalent equations for the expectation values of the operators $b_i = \langle \mathcal{B}_i \rangle$ by tracing over the density matrix $\rho$,

$$\dot{b_1} = f_1(\vec{b}, \omega) = 2jb_3, \tag{8}$$

$$\dot{b_2} = f_2(\vec{b}, \omega) = -2\omega b_3, \tag{9}$$

$$\dot{b_3} = f_3(\vec{b}, \omega) = -2jb_1 + 2\omega b_2. \tag{10}$$

Note that these equations imply that

$$X = b_1^2 + b_2^2 + b_3^2 \tag{11}$$

is a constant of the motion for an arbitrary control $\omega$.

If $\rho$ is a thermodynamic equilibrium state then the corresponding expectation values $b_i^{\text{eq}}$ obey [10]

$$b_3^{\text{eq}} = 0, \tag{12}$$

$$b_1^{\text{eq}} j = b_2^{\text{eq}} \omega, \tag{13}$$

which can be obtained as stationary values of (8)–(10) for a time-independent $\omega$.

Here we are interested in the problem whether one can connect two different thermodynamic equilibrium states without friction and in a finite time by appropriately controlling $\omega$ and how such control can be achieved. In [10] it was shown that controls exist which allow a transition in finite time. Below we present time-optimal controls, *i.e.*, they generate the fastest transition between two different thermodynamic equilibrium states.

Using the optimal control theory, (see, for instance, [15]) we minimize the cost function

$$\tau = \int_{t_\text{i}}^{t_\text{f}} 1 \mathrm{d}t \tag{14}$$

under the constraints given by the equations of motion (8)–(10). In the following we assume that the control is limited by $\omega_{\min} \leqslant \omega(t) \leqslant \omega_{\max}$ and no conditions on the continuity of the control are given as in [16]. Here the process starts at the initial time $t_\text{i}$ and finishes at the yet unknown final time $t_\text{f}$. The control Hamiltonian $H_\text{C}$ is linear in $\omega$,

$$H_\text{C} = \lambda_0 + \sum_{i=1}^{3} \lambda_i \cdot f_i(\vec{b}, \omega) = \sigma(\vec{\lambda}, \vec{b})\omega + \alpha(\vec{\lambda}, \vec{b}), \tag{15}$$

where $\vec{\lambda} = (\lambda_0, \lambda_1, \lambda_2, \lambda_3)$ is the vector of the adjoint variables, and

$$\sigma(\vec{\lambda}, \vec{b}) = 2(\lambda_3 b_2 - \lambda_2 b_3), \tag{16}$$

$$\alpha(\vec{\lambda}, \vec{b}) = \lambda_0 + 2j(\lambda_1 b_3 - \lambda_3 b_1). \tag{17}$$

Moreover, $H_\text{C}$ has no explicit time dependence, which leads to $H_\text{C} = 0$ along an optimal trajectory [15]. Finally, provided the constant $\lambda_0 \neq 0$, it is often chosen to be $\lambda_0 = 1$, thus setting the scale and sign of $\vec{\lambda}$.

From the control Hamiltonian we get the dynamics for the state variables $b_i$ and for the adjoints $\lambda_i$,

$$\dot{b}_i = \frac{\partial H_\text{C}}{\partial \lambda_i} \quad \text{and} \quad \dot{\lambda}_i = -\frac{\partial H_\text{C}}{\partial b_i}. \tag{18}$$

Pontryagin's maximum principle requires $H_\text{C}$ to be maximized for given $b$'s and $\lambda$'s, *i.e.*, $\omega = \omega_{\max}$ for $\sigma > 0$ and $\omega = \omega_{\min}$ for $\sigma < 0$. For $\sigma = 0$ one has to distinguish two cases: If this occurs only at one point of time, the control can be chosen arbitrarily at that instant, but if $\sigma = 0$ during a whole interval of time, things are different: For such so-called singular arcs, one can then try to obtain conditions on $\omega$ from $\sigma = 0$, $\dot{\sigma} = 0$, $\ddot{\sigma} = 0$, etc. Here this procedure does not lead to the desired result, as one can show that the system stays on a singular arc once it is on one.

Instead, we turn to a different approach based on a graphical representation of the processes. Due to the existence (see eq. (11)) of the invariant $X$, a process can be described by a path on a sphere with radius $\sqrt{X}$. The path $\mathcal{P}(t) = (b_1(t), b_2(t), b_3(t))$ can then be projected

from the sphere into the $(b_1, b_2)$-plane and one gets a curve $\mathcal{C}(t) = (b_1(t), b_2(t))$ with

$$b_3 = b_3(b_1, b_2) = \pm\sqrt{X - (b_1^2 + b_2^2)}. \tag{19}$$

The sign of $b_3$ depends on the process. Following eq. (8), with $j > 0$ in mind, positive $b_3$ will lead to an increase of $b_1$ in time and negative $b_3$ will lead to a decrease of $b_1$ in time. Because of continuity $b_3$ can only change sign by crossing zero.

Based on the projection described above we will now discuss processes as curves in the $(b_1, b_2)$-plane. First we note that the total time for a process can be obtained from (8), (14) and (19) by

$$\frac{\mathrm{d}b_1}{\mathrm{d}t} = 2jb_3 \quad \Rightarrow \quad \tau = \frac{1}{2j}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \frac{\mathrm{d}b_1}{\sqrt{X - (b_1^2 + b_2^2)}}. \tag{20}$$

Thus, in a fashion similar to the one used in [17] we find the time-optimal evolution by choosing paths which for any $b_1$ minimize $b_2^2$ along the way. In fig. 1 in the upper left the graphical consequence of that fact is shown. The solid line represents a process path which takes less time than the dashed one.

In a second step we note that by dividing (9) by (8) one finds that boundary arcs are represented by lines with constant slope,

$$\frac{\mathrm{d}b_2}{\mathrm{d}b_1} = -\omega/j. \tag{21}$$

In our figures $\omega$ is given in units of $j$, while in our equations we keep the $j$-dependence. In fig. 1 in the lower part the graphical consequence is that the optimal path consists of boundary arcs. In the upper right one sees that, in addition, $\omega = 0$ arcs can occur. In more complex situations we have thus to expect that the general control is a quasi–bang-bang solution:

$$\omega(t) = \begin{cases} \omega_\mathrm{max}, \\ 0, \\ \omega_\mathrm{min}. \end{cases} \tag{22}$$

We now turn to the case where we connect two thermal equilibrium states characterized by $\omega_\mathrm{i}$ and $\omega_\mathrm{f}$. Following [18] we limit $\omega$ to positive values with $0 < \omega_\mathrm{i} \leqslant \omega \leqslant \omega_\mathrm{f}$. Note that this forces the intial and final states to be within the first quadrant. The situation is shown in fig. 2. We note that there exists a path with two switching points which can connect the initial and the final state by an appropriate choice of the intermediate $\omega$. However, this $\omega$ is not optimal. The path is shown in fig. 2 as a dashed line.

Geometrically, as we move from $b_1$ to $b_1 + \mathrm{d}b_1$, the smaller $b_2^2$, the better. Thus, the best path is to start in the initial state at $P_\mathrm{i}$ by switching from $\omega_\mathrm{i}$ to the largest magnetic field strength $\omega_\mathrm{f}$. After waiting the time $t_1$ one switches at the switch point $P_\mathrm{S}$ to $\omega_\mathrm{i}$, waits the time $t_2$, and finally switches at $P_\mathrm{f}$ to $\omega_\mathrm{f}$ thus reaching the final equilibrium state.

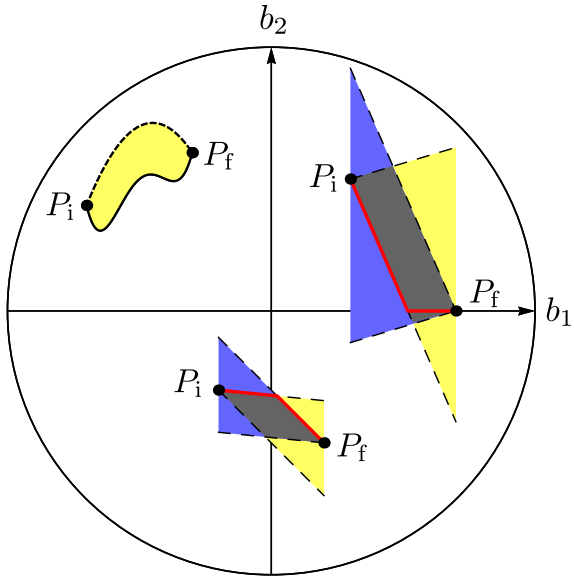


Fig. 1: (Colour on-line) In this figure the circle of thermal equilibrium states is shown. In the upper left two possible paths connecting the same initial point $P_\mathrm{i}$ and final point $P_\mathrm{f}$ are depicted. The path represented by the solid black line is traversed in a shorter time than the dashed path, as for all $b_1$ values the corresponding $b_2^2$ is always smaller for the solid path than for the dashed one. In the lower half the light cone represents the states which can be reached from the initial point by a bounded control, *i.e.*, $-\infty < \omega_\mathrm{min} \leqslant \omega \leqslant \omega_\mathrm{max} < \infty$. The dark cone shows states from which the final point can be reached. The overlap area is where possible paths connecting the initial and the final point can be located. The fastest path is the one with the smallest $b_2^2$ possible, here depicted by the solid line. This path consists only of boundary arcs. In the upper right a similar situation is shown; note that here the time-optimal path does not lie on the boundary of the feasible values but contains an $\omega = 0$ arc.

In that case the solid path seen in fig. 2 is obtained. If the magnetic field strength is unlimited, but positive, the dotdashed path would be time-optimal. As one is able to integrate eq. (20) analytically, the resulting waiting times are obtained as

$$\tau_1 = \frac{1}{2\Omega_\mathrm{f}}\mathrm{a}\cos(\phi), \quad \tau_2 = \frac{1}{2\Omega_\mathrm{i}}\mathrm{a}\cos(\phi), \tag{23}$$

$$\phi = \frac{\Omega_\mathrm{i}\Omega_\mathrm{f}(j^2 + \omega_\mathrm{i}\omega_\mathrm{f}) - (j^2 + \omega_\mathrm{i}\omega_\mathrm{f})^2}{j^2(\omega_\mathrm{i} - \omega_\mathrm{f})^2} \tag{24}$$

with the total time $\tau = \tau_1 + \tau_2$.

We now enlarge the set of possible $\omega$ values by allowing the reversal of the magnetic field. It is natural to restrict ourselves to the case $|\omega| \leqslant \omega_\mathrm{max}$. Figure 3 shows that by allowing negative $\omega$ values, paths with a positive inclination become possible. If one enlarges the allowed $\omega$ set from $\omega_\mathrm{i} \leqslant \omega \leqslant \omega_\mathrm{f}$ to $|\omega| \leqslant \omega_\mathrm{f}$ the former optimal path, drawn long-dashed in fig. 3, is no longer optimal, instead the dashed drawn path is the optimal solution. One also sees that if $\omega_\mathrm{max}$ is large enough, one can reach

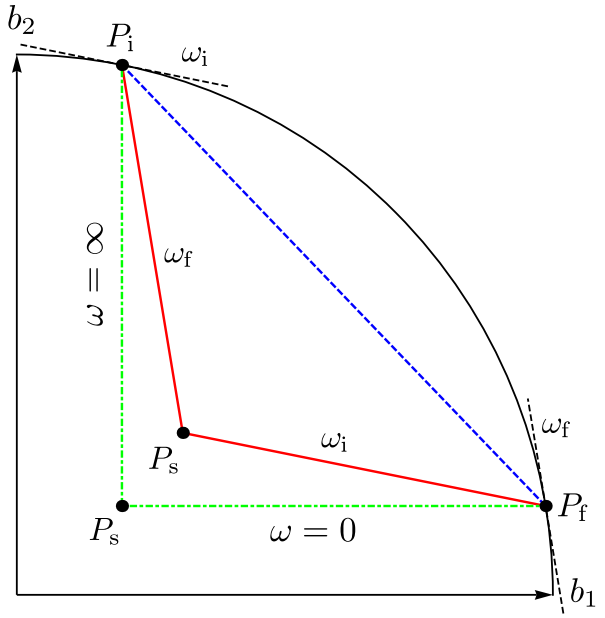


Fig. 2: (Colour on-line) Restricting the magnetic field strength to $\omega > 0$, the dynamics is limited to the first quadrant. Shown are the time-optimal path (solid line) for $\omega_\mathrm{i} \leqslant \omega \leqslant \omega_\mathrm{f}$, and the unlimited time-optimal path (dot-dashed line). The non-optimal path (dashed line) connects $P_\mathrm{i}$ and $P_\mathrm{f}$ directly. Note that for the solid time-optimal path the slopes of the arcs match the slopes of the tangents at the initial and final points.

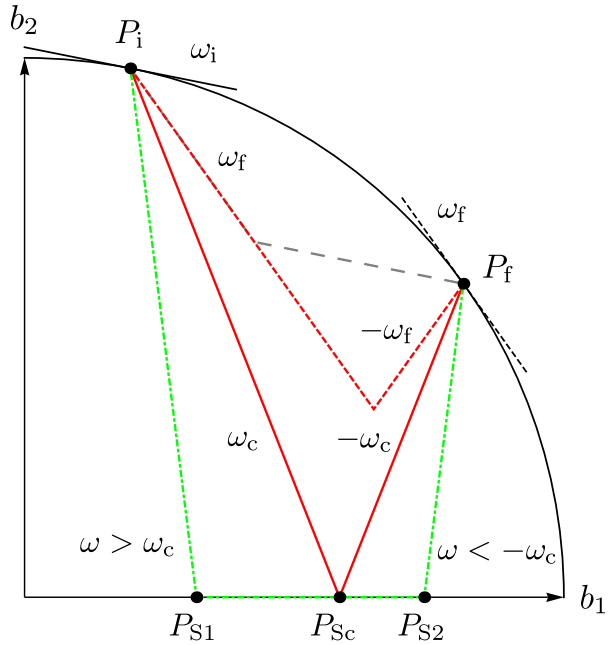


Fig. 3: (Colour on-line) Optimal paths for controls allowing the reversal of the controlling magnetic field are shown for progressively larger values of the field. The original optimal path for $\omega > 0$ is no longer optimal, instead for $|\omega| \leqslant \omega_\mathrm{f}$ the dashed path becomes optimal, with increasing $\omega_\mathrm{max}$, the switching point moves towards $b_2 = 0$. If the field reaches a critical size $\omega_\mathrm{c}$, the solid path becomes time-optimal; for fields larger than the critical value a four–switching-point solution $(P_\mathrm{i}, P_\mathrm{S1}, P_\mathrm{S2}, P_\mathrm{f})$ is the best solution.

the line $b_2 = 0$ within the process. Crossing the line $b_2 = 0$ and using negative $b_2$ would make the process slower than staying on the line $b_2 = 0$. We thus find solutions of the quasi–bang-bang type. These solutions have a path with four switching points $(P_\mathrm{i}, P_\mathrm{S1}, P_\mathrm{S2}, P_\mathrm{f})$. The unknown switching points $P_\mathrm{S1}$ and $P_\mathrm{S2}$ can be calculated from the previously obtained characteristics of the quasi–bang-bang solution,

$$P_\mathrm{S1} = \left(\frac{\omega_\mathrm{max}\omega_\mathrm{i} + j^2}{\omega_\mathrm{max}\Omega_\mathrm{i}}, 0\right), \quad P_\mathrm{S2} = \left(\frac{\omega_\mathrm{max}\omega_\mathrm{f} - j^2}{\omega_\mathrm{max}\Omega_\mathrm{f}}, 0\right). \tag{25}$$

It turns out that these solutions occur if the maximal magnetic field strength $\omega_\mathrm{max}$ is greater than the critical-field strength $\omega_\mathrm{c}$, with

$$\omega_\mathrm{c} = j^2 \frac{\Omega_\mathrm{i} + \Omega_\mathrm{f}}{\omega_\mathrm{f}\Omega_\mathrm{i} - \omega_\mathrm{i}\Omega_\mathrm{f}}. \tag{26}$$

We refrain from giving the waiting times which can still be determined analytically. Also, with the current restriction $|\omega| \leqslant \omega_\mathrm{max}$ paths starting from $P_\mathrm{i}$ in the $-b_1$ direction are possible. One can show that these paths take more time than the optimal solution given. The proof of this fact will be given elsewhere.

In conclusion we analyzed the problem of finding fast processes connecting thermal equilibrium states of an interacting spin system by using control theory. We obtained time-optimal solutions to move the system from a given initial state to a given final state. The time-optimal solutions may be bang-bang solutions, or depending on the initial and final states, they may also contain arcs with vanishing magnetic field. We were able to analytically calculate the times needed for the arcs as well as the total time of the process. If one limits the magnetic field strength $|\omega| \leqslant \omega_\mathrm{max}$, a characteristic magnetic field strength $\omega_\mathrm{c}$ appears. Depending on the size of $\omega_\mathrm{max}$ optimal processes exist with three or four switching points. In all cases the initial and final states are among them. Finally, we note that we have shown that interacting spins can also be controlled to undergo fast, effectively adiabatic processes.

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