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ANALYTICAL AND NUMERICAL SOLUTION OF A SUB-RIEMANNIAN OPTIMAL CONTROL PROBLEM WITH APPLICATIONS TO QUANTUM SPIN SYSTEMS*

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Abstract. Experiments in nuclear magnetic resonance (NMR) spectroscopy and NMR quantum computing require control of ensembles of quantum mechanical systems. The controlled transfer of coherence along a one-dimensional chain of spin systems plays a key role in NMR spectroscopy of proteins, and spin chains have also been proposed for NMR quantum information processing. The problem of time-optimal or energy-optimal control of these systems corresponds to finding optimal paths on Lie groups in which evolution in only certain directions on the group can be directly controlled. In this paper, we consider energy-optimal control of a three-spin system; this turns out to be a sub-Riemannian optimal control problem on SO(4). The goal of this optimal control problem is: given the initial configuration and the desired final configuration as the identity element in SO(4), design three control inputs that steer the system from the initial configuration to the identity $I \in \mathrm{SO}(4)$ along an extremal trajectory. We first obtain necessary conditions for the normal extremal trajectories for both the continuous time system, and then for its discrete counterpart obtained from a discrete variational scheme. We also obtain expressions for the control inputs, and provide a numerical algorithm for the system which can be used to carry out accurate numerical simulations.

1. Introduction.

Experiments in nuclear magnetic resonance (NMR), such as NMR spectroscopy and NMR quantum computing, require control of ensembles of quantum mechanical systems. In particular, the NMR spectroscopy of proteins involves transfer of coherent states along one-dimensional chains of spin systems [1]. Spin chains have been also proposed for the implementation of solid-state NMR quantum computers [2]. In practice, the transfer time should be as short as possible to minimize the effects of decoherence due to interaction with the laboratory environment, and to optimize the sensitivity of the experiments.

In [3], Yuan, Glaser and Khaneja present a method for efficient transfer of coherence along a linear chain of n-spin systems. The initial step in this method is

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