Towards a minimum L^2-norm exact control of the Pauli equation

Gabriele Ciaramella*

Abstract

A computational framework for the exact-control of the magnetic state and the spin of an electron is presented. The evolution of this quantum system is governed by the Pauli equation, that is a system of Schrödinger equations coupled by the action of magnetic fields. The magnetic fields are used as controls in order to steer the quantum system from an initial state to a desired target state at a given final time. This control framework is based on a minimum norm optimization formulation of exact-controllability quantum problems, that allows the application of efficient Krylov-Newton optimization techniques. In order to provide this framework with an adequate initialization, a continuation procedure is discussed. Results of numerical experiments demonstrate the effectiveness of the proposed framework.

Introduction

The purpose of the present work is the exact control of the Pauli equation that governs the dynamics of an electron immersed in a spatially uniform magnetic field $\vec{B} = (B_x, B_y, B_z)$. In spherical coordinates (r, θ, ϕ), the Pauli equation is given by the following; see, e.g., [9];

(0.1)
$$i\hbar \frac{\partial}{\partial t}\vec{\psi} = \begin{pmatrix} H_0 + g\mu_B B_z & g\mu_B(B_x - iB_y) \\ g\mu_B(B_x + iB_y) & H_0 - g\mu_B B_z \end{pmatrix} \vec{\psi} \, ,$$

where $\vec{\psi} = \big(\psi_+, \psi_-\big)$ is called spinor and represents the wavefunction describing the state of an electron with spin. In particular, ψ_+ and ψ_- are the wavefunctions corresponding to the spin-up and spin-down conditions. The quantities g and μ_B are two physical constants called g-factor and nuclear magneton, respectively. The component of the magnetic B_z is assumed to be constant, while B_x and B_y are time dependent and represent the control functions. The free Hamiltonian H_0 is given by the following

(0.2)
$$H_0 = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{2\mu r^2} L^2 - \frac{e}{4\mu c}\vec{B}\cdot\vec{L} + V(r) \, ,$$

where e and μ are the charge and the mass of the electron, respectively, c is the speed of light, and $V(r)$ is an external confining potential, that can be, for instance, a zero-potential, a Coulomb potential for describing the behaviour of an Hydrogen atom, a quadratic potential corresponding to an harmonic oscillator, and an infinite spherical well; see, e.g., [4, 5, 9]. The operator $\vec{L}$ is given by

(0.3)
$$\vec{L} = \big(L_x, L_y, L_z\big) \, ,$$

with

(0.4)
$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

(0.5)
$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

(0.6)
$$L_z = -i\hbar\frac{\partial}{\partial\phi} \, .$$

Consequently, L^2 is the following

(0.7)
$$L^2 = L_x^2 + L_y^2 + L_z^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \, .$$

Our goal is the following. Given an initial eigenstate $\vec{\psi}_0$, we seek control magnetic field components B_x and B_y that are capable to steer the trajectory governed by the Pauli equation exactly into a desired target state $\vec{\psi}_d$. This is expressed by the following scheme

(0.8)
$$\vec{\psi}_0 \xrightarrow[\text{Pauli eq. (0.1)}]{(B_x, B_y)} \vec{\psi}_d \, .$$

In order to solve the Pauli equation (0.1), we consider a spectral method that allows to obtain a finite-dimensional system. We consider the following ansatz

(0.9)
$$\vec{\psi}(t, r, \theta, \phi) = \sum_{n=0}^{\infty}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} R_{n,\ell}(r) Y_\ell^m(\theta, \phi) a^{n,\ell,m}(t) \, ,$$

where $a^{n,\ell,m}(t) \in \mathbb{C}^2$. The functions Y_ℓ^m are spherical-harmonics satisfying [9]

(0.10)
$$L^2 Y_\ell^m(\theta, \phi) = \hbar^2 \ell(\ell+1) Y_\ell^m(\theta, \phi) \, ,$$

and the radial functions $R_{n,\ell}(r)$ are eigenfunctions of

(0.11)
$$\left\{-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} + V(r)\right\} R_{n,\ell}(r) = \lambda_{n,\ell} R_{n,\ell}(r) \, .$$

*Institut für Mathematik, Universität Würzburg Emil-Fischer-Strasse 31, 97074 Würzburg, Germany.

We remark that, the ansatz (0.9) is justified for specific choices of the potential $V(r)$, which guarantee that (0.11) admits suitable solutions. In particular, we recall that analytic solutions to (0.11) are known in the following important cases; see, e.g., [4, 5, 9];

- $V(r) = 0$;
- $V(r) = -\frac{e^2}{r}$, which is the Coulomb potential, used for describing the behaviour of an Hydrogen atom;
- $V(r) = \frac{1}{2}\mu\omega^2 r^2$ where ω is a positive constant; this potential is used for defining a three dimensional harmonic oscillator;
- $V(r) = \begin{cases} \infty & \text{if } r > b \\ 0 & \text{if } r \leq b \end{cases}$ with $b > 0$, which is the so-called infinite spherical well.

Notice that in the literature it is possible to find solutions to (0.11) for other potentials of physical interest, see, e.g., [6].

The indexes n, ℓ, m are called quantum numbers, and $R_{n,\ell}Y_\ell^m$ are eigenstates of the free-Hamiltonian operator H_0; see, [9] and references therein. By considering the ansatz (0.9) and using equations (0.10) and (0.11), one notice that, for a given initial state corresponding to the quantum numbers (n_0, ℓ_0, m_0) and to the spin orientation $s_0 \in \mathbb{C}^2$, that is $\vec{\psi}_0 = R_{n_0,\ell_0}Y_{\ell_0}^{m_0}s_0$, the magnetic field components B_x and B_y allow only transition between m quantum numbers and spin orientation s. Hence, the scheme (0.8) become as follows

$$(0.12)\quad (n_0, \ell_0, m_0, s_0) \xrightarrow[\text{Pauli eq.}]{(B_x,B_y)} (n_0, \ell_0, m_d, s_d)\,,$$

where (n_0, ℓ_0, m_d, s_d) identifies the desired target state, that is $\vec{\psi}_d = R_{n_0,\ell_0}Y_{\ell_0}^{m_d}s_d$. In these settngs, for fixed $n = n_0$ and $\ell = \ell_0$, the Pauli equation (0.1) becomes a finite-dimensional dynamical system, given by the following

$$(0.13)\qquad i\hbar\dot{a} = \Big[\tilde{H}_0 + B_x\tilde{H}_x + B_y\tilde{H}_y\Big]a\,,$$

where $a(t) \in \mathbb{C}^{2\ell_0+1}$, $\tilde{H}_0 \in \mathbb{R}^{2\ell_0+1\times 2\ell_0+1}$ is a diagonal matrix, $\tilde{H}_x \in \mathbb{R}^{2\ell_0+1\times 2\ell_0+1}$ is a symmetric matrix, and $\tilde{H}_y \in \mathbb{C}^{2\ell_0+1\times 2\ell_0+1}$ is a Hermitian matrix. These matrix are given as follows

$$(0.14)\qquad \tilde{H}_0 = \Big[\lambda_{n_0,\ell_0}I_{4\ell_0+2} + \Big(\hbar I_2 \otimes M_{\ell_0} + g\mu_B I_z \otimes I_{2\ell_0+1}\Big)B_z\Big]\,,$$

$$(0.15)\qquad \tilde{H}_x = \Big[g\mu_B I_x \otimes I_{2\ell_0+1} + I_2 \otimes K_+^{\ell_0}\Big]\,,$$

and

$$(0.16)\qquad \tilde{H}_y = \Big[g\mu_B I_y \otimes I_{2\ell_0+1} + I_2 \otimes iK_-^{\ell_0}\Big]\,,$$

where I_x, I_y and I_z are the Pauli matrices, $I_{4\ell_0+4}$, $I_{2\ell_0+1}$ and I_2 are identities of dimensions $4\ell_0 + 2 \times 4\ell_0 + 2$, $2\ell_0 + 1 \times 2\ell_0 + 1$ and 2×2, respectively; the matrix M_{ℓ_0} is given by $M_{\ell_0} = \mathrm{diag}(-\ell_0, \ldots, \ell_0)$; the matrices $K_+^{\ell_0}$ and $K_-^{\ell_0}$ are in $\mathbb{R}^{2\ell_0+1\times 2\ell_0+1}$ and given by the following

$$(0.17)\qquad K_+^{\ell_0} = \begin{pmatrix} 0 & K^+_{\ell_0,-\ell_0} & & & \\ K^+_{\ell_0,-\ell_0} & 0 & K^+_{\ell_0,-\ell_0+1} & & \\ & K^+_{\ell_0,-\ell_0+1} & 0 & K^+_{\ell_0,-\ell_0+2} & \\ & & \ddots & & \\ & & & K^+_{\ell_0,\ell_0-1} & 0 \end{pmatrix},$$

and

$$(0.18)\qquad K_-^{\ell_0} = \begin{pmatrix} 0 & K^+_{\ell_0,-\ell_0} & & & \\ -K^+_{\ell_0,-\ell_0} & 0 & K^+_{\ell_0,-\ell_0+1} & & \\ & -K^+_{\ell_0,-\ell_0+1} & 0 & K^+_{\ell_0,-\ell_0+2} & \\ & & \ddots & & \\ & & & -K^+_{\ell_0,\ell_0-1} & 0 \end{pmatrix},$$

with $K^+_{\ell,m} = \sqrt{\ell(\ell+1) - m(m+1)}$. We remark that, for fixed n_0 and ℓ_0, the eigenvalue λ_{n_0,ℓ_0} of the radial equation (0.11) plays the role of a constant in the discrete free Hamiltonian $\tilde{H}_0$. In the sequel we consider $V(r) = 0$ with $\lambda_{n_0,\ell_0} = 0$. Notice that, the dynamics generated by (0.13) is norm-preserving, that is $\|a(t)\|_2 = \|a_0\|_2$ for $t \in [0, T]$, where $\|\cdot\|_2$ is the Euclidean norm.

A method for the exact control of the Pauli (0.13) equation, in dimensionless units, with minimum L^2-norm control is described in the next section. This framework is based on the methodologies developed in [2, 3] for spin systems and in the following extended to the control of the Pauli equation.

1 Minimum L^2-norm exact control of the Pauli equation

In this section, we discuss a method for the exact control of the Pauli equation by means of minimum L^2-norm controls. In particular, in the first part, we formulate a minimum L^2-norm exact control problem, and we notice that its minimizers are characterized by a first order optimality system, in which the terminal condition of the adjoint equation is unknown. This fact is used to reformulate the first order optimality system of the minimum norm problem as an optimization problem that can be addressed by means of shooting type methods. For the sake of clarity, we anticipate this part in the following steps

1. Formulate the L^2-minimum norm exact control problem (1.19);
2. Consider the first-order optimality system of (1.19), that is given by (1.20);

3. Reformulate the optimality system (1.20) as the optimization problem (1.22).

Furthermore, we report results from [3] concerning regularity properties of the optimization problem (1.22) in a neighbourhood of a solution. This regularity allows to address successfully the problem in a neighbourhood of a solution by means of efficient second-order methods.

In the second part, we discuss a continuation procedure for obtaining an approximation of a minimum L^2-norm exact control. This approximation is used to initialize the minimum norm problem solver. The continuation procedure consists in the solution of a sequence of optimal control problems, whose optimal control solutions form a sequence which is proved to converge to a minimum L^2-norm exact control.

1.1 A method for the minimum L^2-norm exact control of the Pauli equation A minimum L^2-norm exact-control problem can be stated as follows

(1.19)
$$\begin{aligned} \min_{a,u} \quad & J(a,u) := \frac{1}{2}\|u\|_{L^2}^2 \\ \text{s.t.} \quad & \dot{a} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]a \ , \ t \in (0,T] \ , \\ & a(0) = a_0 \ , \ a(T) = a_d \ , \end{aligned}$$

where $a \in H^1((0,T);\mathbb{C}^{2\ell_0+1})$ and $u = (B_x, B_y) \in L^2((0,T);\mathbb{R}^2)$. In particular, assuming that the desired target state a_T is reachable at time T, we seek a control $\tilde{u} = (\tilde{B}_x, \tilde{B}_y)$ that steers the quantum state governed by the Pauli equation from an initial state to a given target state exactly. Furthermore, $\tilde{u}$ has to posses a minimum norm, in the following sense

$$\|\tilde{u}\|_{L^2} \leq \|\hat{u}\|_{L^2} \ ,$$

for any exact-control function $\hat{u}$. Controllability results can be found in, e.g., [7, 10].

Standard results in optimization based on the convexity and regularity of the functional and regularity of the constraint of (1.19), ensure that a minimizer of (1.19) is characterized by the following first-order optimality system; see, e.g., [2, 8];

$$\dot{a} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]a \quad , \quad a(0) = a_0 \tag{1.20a}$$
$$a(T) = a_T \tag{1.20b}$$
$$\dot{p} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]p \quad , \quad p(T) = p_T \tag{1.20c}$$
$$\nu B_x + 2\mathbb{R}e\big(\langle p, iH_x a\rangle_{\mathbb{C}}\big) = 0 \tag{1.20d}$$
$$\nu B_y + 2\mathbb{R}e\big(\langle p, iH_y a\rangle_{\mathbb{C}}\big) = 0 \ , \tag{1.20e}$$

where the existence of the adjoint p and its terminal condition $p_T \in \mathbb{C}^{2\ell_0+1}$ is assumed. Notice that, the unknown of the optimality system (1.20) are the control $u = (B_x, B_y)$, and the terminal state of the adjoint equation p_T. In order to solve (1.20), we define the following functions

(1.21)
$$\begin{aligned} g_{B_x}(u,p_T) &:= \nu B_x + 2\mathbb{R}e\big(\langle p(u,p_T), iH_x a(u)\rangle_{\mathbb{C}}\big) \\ g_{B_y}(u,p_T) &:= \nu B_y + 2\mathbb{R}e\big(\langle p(u,p_T), iH_y a(u)\rangle_{\mathbb{C}}\big) \ . \end{aligned}$$

Henceforth (1.20) can be reformulate as the following optimization problem [3]

(1.22)
$$\begin{aligned} \min_{u,p_T} \quad & G(u,p_T) := \frac{1}{2}\|a(T) - a_T\|_2^2 \\ & \qquad + \frac{1}{2}\|g_{B_x}(u,p_T)\|_{L^2}^2 + \frac{1}{2}\|g_{B_y}(u,p_T)\|_{L^2}^2 \\ \text{s.t.} \quad & \dot{a} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]a \ , \ t \in (0,T] \\ & \dot{p} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]p \ , \ t \in [0,T) \ , \end{aligned}$$

where $a, p \in H^1((0,T);\mathbb{C}^{2\ell_0+1})$ with $a(0) = a_0$ and $p(T) = p_T$, and $u = (B_x, B_y) \in L^2((0,T);\mathbb{R}^2)$. Notice that a minimizer of G is characterized by an optimality system given by 4 dynamical systems and 2 gradient components.

The next result, proved in [3], shows the relationships between stationary points of (1.19) and minimizers of (1.22), and states local regularity properties of (1.22).

THEOREM 1.1. *The following holds*

- *the elements (a,u,p) with $a = a(u,a_0)$ and $p = p(u,p_T)$, satisfy $G(u,p_T) = 0$ if and only if they are a stationary point of* (1.19)*;*
- *let (u,p_T) be a solution to* (1.22) *with $G(u,p_T) = 0$, then the Hessian $\nabla^2 G(u,p_T)$ is positive semi-definite;*
- *let (u,p_T) be a solution to* (1.22) *with $G(u,p_T) = 0$. Let $M_1 := \|H_x\|$, $M_2 := \|H_y\|$, $M := M_1 + M_2$ and*

$$\begin{aligned} \tilde{K}_n &:= M_n \|a_0\|_2 \sqrt{T} \\ K_n &:= 1 - 4MTM_n\|p_T\|_2\|a_0\|_2 \ , \end{aligned} \tag{1.23}$$

and assume that

$$\begin{aligned} 1 + \tilde{K}_n\Big(16TM^2\|p_T\|_2^2\tilde{K}_n - 8\sqrt{T}M\|p_T\|_2 \\ - 1 + 4\sqrt{T}M\|p_T\|_2\tilde{K}_n\Big) > 0 \ , \end{aligned} \tag{1.24}$$

and

$$\tilde{K}_n + 4\sqrt{T}M\tilde{K}_n\|p_T\|_2 - 1 > 0 \ , \tag{1.25}$$

for $n = 1, 2$. Then, the Hessian $\nabla^2 G(u,p_T)$ is coercive;

- *minimum points of* (1.19) *are isolated points.*

Notice that Theorem 1.1 ensures local convexity of G and regularity of the corresponding Hessian operator. This properties are important for the numerical solution of (1.19). In particular, we address this problem by means of a shooting-type Newton method, considering that the unknowns of the problem are the control u and the terminal adjoint state p_T, which is used as a shooting variable.

We remark that, Theorem 1.1 guarantees regularity in a neighbourhood of a solution. For this reason an adequate initialization for a numerical solver is an important issue. This issue is addressed in the next section, in which we discuss a continuation method.

1.2 A continuation method for the asymptotic exact-control of the Pauli equation In this section, a continuation method for obtaining an approximation to the exact-control problem (1.19) is discussed. To this purpose, consider the following optimal control problem

(1.26)
$$\begin{aligned} \min_{a,u} \quad & J_\nu(a,u) := \frac{1}{2}\|a(T)-a_T\|_2^2 + \frac{\nu}{2}\|u\|_{L^2}^2 \\ \text{s.t.} \quad & \dot a = -i\Big[H_0 + B_xH_x + B_yH_y\Big]a \ , \ t\in(0,T] \\ & a \in H^1((0,T);\mathbb{C}^{2\ell_0+1}) \ , \ a(0)=a_0 \\ & u=(B_x,B_y)\in L^2((0,T);\mathbb{R}^2) \ , \end{aligned}$$

and notice that a solution to (1.26) for $\nu\to 0$ is sought with the aim to obtain an exact control function. Hence, consider a sequence of weight parameters $\nu_k\to 0$, and denote with $\{J_{\nu_k}\}_k$ the corresponding sequence of cost functionals. This sequence converges to $J_0=\frac{1}{2}\|a(T)-a_T\|_2^2$, and $J_0=0$ corresponds to exact-control. The sequence $\{J_{\nu_k}\}_k$ generates a series of optimal control problems, and $\{u^k\}_k$ is the corresponding sequence of optimal controls solutions, that is u^k solves (1.26) with $\nu=\nu_k$.

Our continuation method is implemented with the following algorithm.

Algorithm 1 (Continuation Method)

Require: u^0, $k=1$, k_{max}, $\gamma\in(0,1)$, ν_1;
while $k<k_{max}$ **do**
1. Solve (1.26) and compute $u^k(\nu_k)$ (using u^{k-1} as starting condition);
2. Set $\nu_{k+1}=\gamma\nu_k$;
3. Set $k=k+1$;

end while

A feature of this continuation method is that the solution at the step k is computed considering as a starting guess the solution obtained at the step $k-1$.

The next theorem states the existence of a subsequence of $\{u^k\}_k$ that converges strongly to an exact control solution u^0 [2]. Moreover, the limit of such a sequence is a minimum-norm solution.

THEOREM 1.2. *Assume that a_T is reachable from a_0 at time T, which means that there exists a control $\tilde u$ such that $J_0=0$. Let $\{\nu_k\}_k$ be a sequence of $\nu_k>0$ such that $\nu_k\to 0$ as $k\to\infty$. Denote with u^k a solution to* (1.26) *corresponding to $\nu=\nu_k$. Then there exists a convergent subsequence, that is $u^{k_j}\to\hat u$ in $L^2((0,T);\mathbb{R}^{N_C})$ as $j\to\infty$, and $\hat u$ is an exact control solution ($J_0(\hat u)=0$) with minimum L^2-norm, that is*

$$\|\hat u\|_{L^2}\le\|\tilde u\|_{L^2} \ ,$$

for all exact-control functions $\tilde u$ such that $J_0(\tilde u)=0$.

Furthermore, it is proved in [2] that the sequence $\{u^k\}_k$ converges to an exact control function $\tilde u$ according to the following estimate

$$\|\tilde u - u_\nu\|_{L^2} = O(\sqrt{\nu}) \ \text{ for } \ \nu\to 0 \ . \tag{1.27}$$

Next, a Krylov-Newton method for the solution to (1.26) is illustrated. This method is used in the step 1 of Algorithm 1.

In order to obtain the first-order optimality system of (1.26), we consider the following Lagrangian function; see, e.g., [1, 11] and references therein;

$$\begin{aligned} L(a,u,p) &= J(a,u) \\ &+ 2\mathbb{R}e\langle p, \dot a + i\Big[H_0+B_xH_x+B_yH_y\Big]a\rangle_{L^2} \ . \end{aligned} \tag{1.28}$$

Consequently, the optimality system is given by

(1.29a)
$$\dot a = -i\Big[H_0+B_xH_x+B_yH_y\Big]a \ , \ a(0)=a_0$$
(1.29b)
$$\dot p = -i\Big[H_0+B_xH_x+B_yH_y\Big]p \ , \ p(T)=-\frac{1}{2}(a(T)-a_T)$$
(1.29c)
$$\nabla_{B_x}L(a,u,p)=0 \ , \ \nabla_{B_y}L(a,u,p)=0$$
(1.29d)
$$\nabla_{B_x}L(a,u,p)=\nu B_x + 2\mathbb{R}e\big(\langle p, iH_xa\rangle_{\mathbb{C}}\big)$$
(1.29e)
$$\nabla_{B_y}L(a,u,p)=\nu B_y + 2\mathbb{R}e\big(\langle p, iH_ya\rangle_{\mathbb{C}}\big) \ ,$$

where (1.29a) and (1.29b) are referred to as the forward state equation and backward adjoint equation, respectively, and (1.29d) and (1.29e) are the gradient components.

Next, we denote $\eta = (a, B_x, B_y, p)$ and write the problem of finding a stationary point as a root problem: find η such that

$$\mathcal{F}(\eta) = 0 \,, \tag{1.30}$$

where $\mathcal{F}(\eta) := \Big(\mathcal{F}_1(\eta), \mathcal{F}_{2,x}(\eta), \mathcal{F}_{2,y}(\eta), \mathcal{F}_3(\eta)\Big)^T$ and

$$\mathcal{F}_1(\eta) := \dot{p} + i\Big[H_0 + B_x H_x + B_y H_y\Big]p \tag{1.31a}$$

$$\mathcal{F}_{2,x}(\eta) := \nu B_x + 2\mathbb{R}e\big(\langle p, iH_x a\rangle_{\mathbb{C}}\big) \tag{1.31b}$$

$$\mathcal{F}_{2,y}(\eta) := \nu B_y + 2\mathbb{R}e\big(\langle p, iH_y a\rangle_{\mathbb{C}}\big) \tag{1.31c}$$

$$\mathcal{F}_3(\eta) := \dot{a} + i\Big[H_0 + B_x H_x + B_y H_y\Big]a \,. \tag{1.31d}$$

In order to solve (1.30), we consider a Newton method, that requires at each iteration to solve the following problem

$$\mathcal{J}(\eta)\delta\eta = -\mathcal{F}(\eta) \,, \tag{1.32}$$

where $\mathcal{J}(\eta)$ is the Jacobian operator evaluated at η. The Newton system (1.32) is given explicitly by the following

$$\begin{pmatrix} \nabla_a\mathcal{F}_1 & \nabla_{B_x}\mathcal{F}_1 & \nabla_{B_y}\mathcal{F}_1 & \nabla_p\mathcal{F}_1 \\ \nabla_a\mathcal{F}_{2,x} & \nabla_{B_x}\mathcal{F}_{2,x} & \nabla_{B_y}\mathcal{F}_{2,x} & \nabla_p\mathcal{F}_{2,x} \\ \nabla_a\mathcal{F}_{2,y} & \nabla_{B_x}\mathcal{F}_{2,y} & \nabla_{B_y}\mathcal{F}_{2,y} & \nabla_p\mathcal{F}_{2,y} \\ \nabla_a\mathcal{F}_3 & \nabla_{B_x}\mathcal{F}_3 & \nabla_{B_y}\mathcal{F}_3 & 0 \end{pmatrix} \begin{pmatrix} \delta a \\ \delta B_x \\ \delta B_y \\ \delta p \end{pmatrix} = - \begin{pmatrix} \mathcal{F}_1 \\ \mathcal{F}_{2,x} \\ \mathcal{F}_{2,y} \\ \mathcal{F}_3 \end{pmatrix} \tag{1.33}$$

where the dependence on η is omitted for brevity.

Notice that the state a and the adjoint p are uniquely determined by the controls B_x and B_y, and we write $a = a(B_x, B_y)$ and $p = p(B_x, B_y)$. This corresponds to $\mathcal{F}_3(\eta) = 0$ and $\mathcal{F}_1(\eta) = 0$, respectively. Consequently, the action of the fourth row of $\mathcal{J}(\eta)$ on the vector of unknowns gives the following initial value problem

$$\dot{\delta a} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]\delta a - i\Big[\delta B_x H_x + \delta B_y H_y\Big]a \,, \tag{1.34}$$

with $\delta a(0) = 0$, which represents the linearization of the forward problem (1.29a). In the same fashion, the action of the first row of $\mathcal{J}(\eta)$, gives the following

$$\dot{\delta p} = -i\Big[H_0 + B_x H_x + B_y H_y\Big]\delta p - i\Big[\delta B_x H_x + \delta B_y H_y\Big]p \,, \tag{1.35}$$

with $\delta p(T) = -\frac{1}{2}\delta a(T)$, that represents the linearization of the backward problem (1.29b). Equations (1.34) and (1.35) are uniquely solvable and their solutions are $\delta a = \delta a(\delta B_x, \delta B_y)$ and $\delta p = \delta p(\delta B_x, \delta B_y)$, respectively. Therefore, the linear system (1.33) becomes as follows

$$\begin{aligned} \big(\mathcal{J}_r(B_x, B_y)(\delta B_x, \delta B_y)\big)_x &= -\mathcal{F}_{2,x}(B_x, B_y) \\ \big(\mathcal{J}_r(B_x, B_y)(\delta B_x, \delta B_y)\big)_y &= -\mathcal{F}_{2,y}(B_x, B_y) \,, \end{aligned} \tag{1.36}$$

where $\mathcal{J}_r(B_x, B_y)$ is the reduced Jacobian operator evaluated in (B_x, B_y); see, e.g. [2, 3, 11]; the only unknowns in (1.36) are δB_x and δB_y. Notice that the action of $\mathcal{J}_r(B_x, B_y)$ on $(\delta B_x, \delta B_y)$ is given by the following

$$\begin{aligned} \big(\mathcal{J}_r(B_x, B_y)(\delta B_x, \delta B_y)\big)_x &:= \nu\delta B_x \\ &\quad + 2\mathbb{R}e\big(\langle \delta p, iH_x a\rangle_{\mathbb{C}} + \langle p, iH_x \delta a\rangle_{\mathbb{C}}\big) \\ \big(\mathcal{J}_r(B_x, B_y)(\delta B_x, \delta B_y)\big)_y &:= \nu\delta B_y \\ &\quad + 2\mathbb{R}e\big(\langle \delta p, iH_y a\rangle_{\mathbb{C}} + \langle p, iH_y \delta a\rangle_{\mathbb{C}}\big) \,. \end{aligned} \tag{1.37}$$

Therefore, the Newton method for solving (1.26) can be written in the following reduced form

(N_1) solve the reduced Newton system (1.36);

(N_2) update the controls, $(B_x, B_y)_{k+1} = (B_x, B_y)_k + (\delta B_x, \delta B_y)_k$.

Implementation details of the Krylov-Newton method for quantum systems are discussed in [2, 3, 11].

2 Exact control algorithm and numerical experiments

In this section, we consider numerical experiments that demonstrates the validity of the presented computational frameworks for the exact control of the Pauli equation. In particular, we initialize the numerical solution by means of the continuation method described in Section 1.2, and then we address problem (1.22) by means of a Krylov-Newton method, where the terminal state of the adjoint p_T is used as a shooting-variable. Notice that, in order to evaluate the quality of the obtained numerical solutions, make use of the so-called fidelity given by the following

$$C := \frac{\langle a(T), a_T\rangle}{\|a(T)\|_2 \|a_T\|_2} \,.$$

This quantity is largely used in physics, and since the dynamics of the Pauli equation is norm-preserving, $C = 1$ means that $a(T) = a_T$. Our numerical strategy is summarized in the following algorithm.

Algorithm 2 (Exact control method)

- call Algorithm 1 to obtain an initialization u_{init} (Theorem 1.2);

while $C < tol$ **do**

- Call a Krylov-Newton solver to solve (1.22) and minimize G;
- Refine the discretization mesh and interpolate the current solution to the new mesh;

end while

We consider numerical experiments in which we want to perform in time $T = 1$ a spin inversion and a transition from $m_0 = -\ell$ to $m_d = \ell$, with $\ell = 1$, 2, 4, 6, 8 and 10.

Some of the controls obtained by the presented computational framework are shown in the next Figure 1. In particular, the left and the right picture show the controls obtained for $\ell = 1$ and $\ell = 10$, respectively. Notice that the obtained control solutions are capable to obtain values of G and C vary close to 0 and 1, respectively, that correspond to the exact control. This is expressed in the next Table 1, in which the value of the fidelity C, the functional G, the norm of the reduced gradient of G, and the number of discretization points for the time interval $[0, T]$ are shown. Moreover, in order to show that the continuation procedure is capable to provide an adequate initialization, the values C_{init} is considered. This correspond to the fidelity obtained by the initialization, performed by means of the continuation procedure (Algorithm 1). We remark that, specific analysis regarding the numerical behaviour of the continuation method are given in [2].

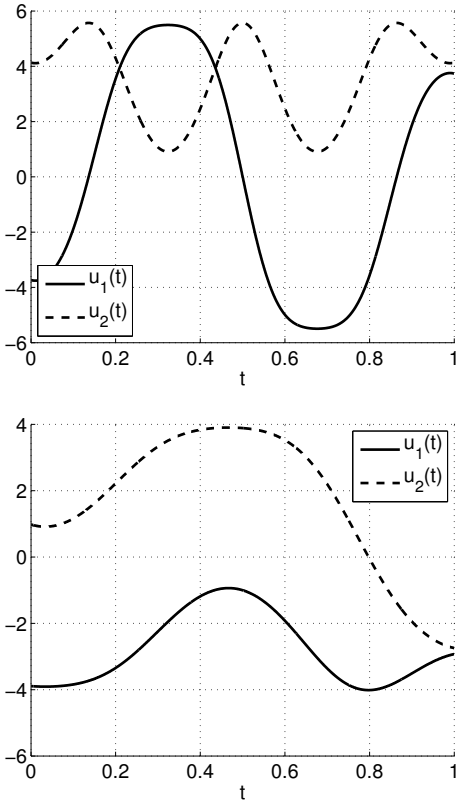

Figure 1: Control functions obtained by means of the presented computational framework in the cases $\ell = 1$ and $\ell = 10$. In particular, the controls in the first picture correspond to $\ell = 1$, and the controls in the second picture correspond to $\ell = 10$. These control functions perform the spin inversion and the transition from $m = -\ell$ to $m = \ell$.

ℓ	C_{init}	C	G	$\|\nabla G_r\|_{L^2}$	N_t
1	0.999763	0.999999	$2.3{\cdot}10^{-11}$	$1.9{\cdot}10^{-11}$	1601
2	0.999951	0.999999	$7.1{\cdot}10^{-11}$	$8.2{\cdot}10^{-11}$	1601
4	0.999875	0.999999	$1.4{\cdot}10^{-9}$	$9.4{\cdot}10^{-12}$	1601
6	0.999928	0.999999	$5.1{\cdot}10^{-10}$	$6.4{\cdot}10^{-11}$	3201
8	0.999772	0.999999	$3.4{\cdot}10^{-10}$	$2.9{\cdot}10^{-9}$	4801
10	0.999818	0.999999	$8.6{\cdot}10^{-10}$	$2.4{\cdot}10^{-9}$	4801

Table 1: Results obtained from the numerical experiments. In particular, C_{init} is the fidelity corresponding to the control obtained by the initialization procedure (continuation method in Algorithm 1); C is the fidelity corresponding to the control solution obtained by Algorithm 2; G is the value of the cost functional of the problem (1.22) evaluated in the computed controls; $\|\nabla G_r\|_{L^2}$ is the norm of the reduced gradient of (1.22); N_t is the number of the points used for the discretization of the time interval $[0, T]$.

Acknowledgements The author wants to thank Alfio Borzì, for his continuous encouragement and his inestimable support, and Greg von Winckel, for his help in understanding the Pauli equation and its discretization. A special thank goes to Gunther Dirr, Julien Salomon and Daniel Wachsmuth, for their contribution to the development of our computational framework, and for many helpful discussions. Finally, a thank goes to Martin Sprengel for his patience during our visit in Nottingham in which this work was written.

References

[1] A. Borzì, *Quantum optimal control using the adjoint method*, Nanoscale Systems: Mathematical Modeling, Theory and Applications, 1 (2012), 93-111.

[2] G. Ciaramella, A. Borzì, G. Dirr, D. Wachsmuth, *Newton methods for the optimal control of closed quantum spin systems*, (2015) SIAM Journal on Scientific Computing (SISC), 37(1), pp. A319-A346;

[3] G. Ciaramella, J. Salomon, A. Borzì, *A method for solving exact-controllability problems governed by closed quantum spin systems*, (2015) International Journal of Control (IJC), 88(4), pp. 682-702;

[4] S. Gasiorowicz, *Quantum Physics - Third Edition*, Wiley and Sons (2003);

[5] D. J. Griffiths (1995) *Introduction to Quantum Mechanics*, Prentice Hall;

[6] S. M. Ikhadir, R. Sever, *Exact solutions of the radial Schrödinger equation for some physical potentials*, Central Eur.J.Phys. 5(2007), 516;

[7] V. Jurdjevic, H. Sussmann, *Control systems on Lie groups*, Journal Diff. Eqns., 12 (1972), 313-329;

[8] E. B. Lee, L. Markus, *Foundations of Optimal Control Theory*, Robert E. Krieger Publishing Company, Malabar, Florida (1986);

[9] B. Thaller, *Advanced Visual Quantum Mechanics*, Springer, New York, 2005;

[10] G. Turinici, *On the controllability of bilinear quantum systems*, Mathematical models and methods for ab initio Quantum Chemistry, 2000;

[11] G. von Winckel, A. Borzì, S. Volkwein, *A globalized Newton method for the accurate solution of a dipole quantum control problem*, SIAM J. Sci. Comput., 31 (2009), pp. 4176-4203;