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Quantum Pontryagin Neural Networks in Gamkrelidze Form Subjected to the Purity of Quantum Channels

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Abstract— **We investigate a time and energy minimization optimal control problem for open quantum systems, whose dynamics is governed through the Lindblad (or Gorini-Kossakowski-Sudarshan-Lindblad) master equation. The dissipation is Markovian time-independent, and the control is governed by the Hamiltonian of a quantum-mechanical system. We are specifically interested to study the purity in a dissipative system constrained by state and control inputs. We deal with the state constraints through Gamkrelidze revisited method, while handling control constraints through the idea of saturation functions and system extensions. This is the first time that quantum purity conservation is formulated in such framework. We obtain the necessary conditions of optimality through the Pontryagin Minimum Principle. Finally, the resulted boundary value problem is solved by a Physics-Informed Neural Network (PINN) approach, a technique that is also new in quantum control context. We show that these PINNs play an effective role in learning optimal control actions.**

I. Introduction

One of the extremely important subjects in quantum information processing is state purity preservation. In this regard, an Optimal Control Problem (OCP) of quantum dissipative dynamics can be formulated such that the dissipation is Markovian time-independent. This means that the memory effects are neglected and the dynamics of the quantum system under study is only dependent on the current state not the past history. Therefore, we can describe the density operator evolution by the Lindblad master equation. In such dynamics, there is an interaction of the controllable part of the system, the Hamiltonian (or conservative) term, and the uncontrollable part, the non-Hamiltonian (or dissipative) term. Under most conditions, dissipation leads to an increase in entropy (or a decrease in purity) of the system. However, proposing a strategy to control the Hamiltonian term of the system evolution with the intent that the non-Hamiltonian term causes an increase in purity is a matter of debate.

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There have been several efforts in the literature aiming to preserve the quantum state purity, e.g. [1, Chapter 12]. In [2], a time- and energy-minimum global OCP has been studied for open quantum systems, however, their results are presented based on having fast control of the Hamiltonian and unbounded control signals as it is stressed by the authors. In [3], a time minimum quantum OCP has been studied aiming at achieving a target state with maximum purity for a quantum state transition problem applicable for a two-level system. However, their method is a two-level specific (not easy to extend) and, as the authors claim, it is sensitive to the initial guess. In this paper, we address the limitations of previous strategies by exploiting new techniques in the context of quantum optimal control problems.

A. Main Contributions

We investigate a minimum time-energy OCP for dissipative quantum systems interacting with the environment, whose dynamics is governed by the Lindblad equation, and is subjected to preserve the state purity in a quantum state transition process. Our contributions are listed as follows:

- We consider the purity of quantum channels as state constraints, such that the purity is preserved within some bounds. The technique to deal with this problem leans upon the revisited method of Gamkrelidze's version of Pontryagin's Minimum Principle (PMP) [4], which is novel in quantum control context. The feasibility of using the Gamkrelidze approach can be found in [5], but in a coherence preservation setting.
- We address the constrained control restriction through the technique of saturation functions and system extensions by extending [6] to the quantum context, and show its compatibility with the Gamkrelidze version of PMP.
- We derive the necessary optimality PMP conditions, and show that they are also sufficient conditions for (local) optimality. We then solve the resulted Boundary Value Problem (BVP) via a recently developed neural network approach known as Pontryagin Neural Networks (PoNNs) derived from the Theory of Functional Connection (TFC) [7]. In particular, we exploit the PoNNs method for the Gamkrelidze version of PMP by introducing an additional multiplier and extra optimality conditions. We also apply the technique of saturation functions presented in [8]-[9] to PoNNs, by showing its compatibility with Gamkrelidze version of PMP.

Overall, the combination of these three techniques is new for an OCP, specially in the context of quantum control.

The structure of the work is as follows: In Section II, we introduce the Lindblad master equation and provide a linear isomorphism such that the transformed system is linear in the state and real. Section III formulates the optimal control problem of minimum time and energy, and in the next section, we present the Pontryagin's Minimum Principle in Gamkrelidze form with saturation functions. We solve the resulted BVP through a physics-informed neural network approach, explained in section V. The simulation results have been shown for the quantum state transfer problem in a two-level system in section VI. The paper ends with conclusion and an overview on prospective research challenges.

B. Notation

For a general continuous-time trajectory x, the term $x(t)$ indicates the trajectory assessed at a specific time t. We use the superscripts T and $\dagger$ to show the transpose and conjugate transpose of a matrix (or vector), respectively. To denote the wave functions as vectors, we use the Dirac notation $|\psi\rangle = \sum_{k=1}^{n} \alpha_k |\hat{\psi}_k\rangle$, where $|\psi\rangle$ indicates a state vector, α_k are the complex-valued expansion coefficients, and $|\hat{\psi}_k\rangle$ are basis vectors that are fixed. Dirac's bra notation is defined such that $\langle\psi| = |\psi\rangle^\dagger$. In addition, the notation $|\rho\rangle\rangle$ indicates the vectorized form of the density operator in the Fock-Liouville space, and the vectorization operator is shown by *vec*, such that $|\rho\rangle\rangle = vec(\rho)$, and $vec(|\psi\rangle\langle\xi|) = |\xi\rangle \otimes |\psi\rangle$, in which $\otimes$ indicates the tensor product. We denote partial derivatives using subscripts, i.e., for f being a function of n variables including x, then f_x denotes the partial derivative relative to the x input. The notation $[\cdot,\cdot]$ represent a commutator and $\{\cdot,\cdot\}$ is a Poisson bracket. The imaginary unit is shown by $i = \sqrt{-1}$. A vector with all elements equal to zero is represented as $\mathbf{0}$.

II. The Lindbladian dynamics equation

The general mathematical tool to describe our knowledge of the state of an n-level quantum system is through the density operator ρ, which is a Hermitian positive semi-definite operator of trace one acting on the Hilbert space $\mathbb{H}$ of the system. In quantum mechanics, the evolution of density operator through the Lindblad (or Gorini-Kossakowski-Sudarshan-Lindblad) master equation represents the most extensive generator of Markovian dynamics which takes the form, [10],

$$\dot{\rho} = -i[H,\rho] + \sum_k \gamma_k \left[L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right] \qquad (1)$$

in which the first term represents the unitary evolution of the quantum system, where H is a Hermitian operator called the quantum-mechanical Hamiltonian defined as

$$H = diag(E_1, E_2, \cdots, E_n) + \sum_{l=1}^{m} u_l(t) H_l$$

where the diagonal term implies that the basis corresponds to the eigenvectors, and E_i represents a real number concerning the energy level. The control $u_l(t) \in \mathbb{R}$ demonstrates a set of external functions coupled to the quantum system via time independent interaction Hamiltonians H_l. The second term of (1) represents the dissipative part of the state evolution, where L_k indicates the sequence of arbitrary Lindblad operators, and $\gamma_k \geq 0$ is the damping rate. Master equations can be bothersome due to the commutation term and the Poisson bracket. Since convex combination gives the preservation of the trace and positive definiteness, it is possible to create a Hilbert space of density operators via defining a scalar product. The next result provides a linear space of density operators, called Fock-Liouville space, by which we present a solution of the master equation via vectorization such that the resulting Liouvillian superoperator is governed by a linear system.

Proposition 1: Consider the Lindbladian dynamical system (1). There exists a linear isomorphism, coordinate transformation, such that the transformed system is linear in the states and real.

Proof: We show the results by providing a coordinate transformation given by the following composition of 3 linear isomorphisms (whose notation is defined in the sequel):
i) $\mathscr{L}: \ \rho \mapsto \mathscr{L}\rho$, ii) $|\cdot\rangle\rangle: \ \rho \mapsto |\rho\rangle\rangle$,
iii) $\tilde{\cdot}: \ v \mapsto \tilde{v} := \begin{bmatrix} \mathrm{Re}(v) & \mathrm{Im}(v) \end{bmatrix}^T$
and finally $\tilde{\mathscr{L}} = (\tilde{\cdot}) \circ |\cdot\rangle\rangle \circ \mathscr{L} \circ |\cdot\rangle\rangle^{-1} \circ (\tilde{\cdot})^{-1}$. To obtain i, we apply the Choi-Jamiolkowski isomorphism for vectorization, through the mapping $|\cdot\rangle\rangle: \ |i\rangle\langle j| \mapsto |j\rangle \otimes |i\rangle$, to (1) obtaining the Liouville superoperator acting on the Hilbert space of density operator as $|\dot{\rho}\rangle\rangle = \mathscr{L}|\rho\rangle\rangle$ where

$$\begin{aligned} \mathscr{L} = &-i\left(I \otimes H - H^T \otimes I\right) \\ &+ \sum_k \gamma_k \left[L_k^* \otimes L_k - \frac{1}{2} I \otimes L_k^\dagger L_k - \frac{1}{2}\left(L_k^\dagger L_k\right)^T \otimes I \right] \end{aligned}$$

in which I is the identity matrix. To show ii, note that, for an arbitrary density operator $\rho = \sum_{i,j} \rho_{i,j} |i\rangle\langle j|$, its vectorized form is given by $|\rho\rangle\rangle = \sum_{i,j} \rho_{i,j} |j\rangle \otimes |i\rangle$. Finally to get iii, we implement the system state and superoperator as

$$|\tilde{\rho}\rangle\rangle = \begin{bmatrix} \mathrm{Re}\left(|\rho\rangle\rangle\right) \\ \mathrm{Im}\left(|\rho\rangle\rangle\right) \end{bmatrix}, \quad \tilde{\mathscr{L}} := \begin{pmatrix} \mathrm{Re}\left(\mathscr{L}\right) & -\mathrm{Im}\left(\mathscr{L}\right) \\ \mathrm{Im}\left(\mathscr{L}\right) & \mathrm{Re}\left(\mathscr{L}\right) \end{pmatrix}$$

so that we obtain

$$|\dot{\tilde{\rho}}\rangle\rangle = \tilde{\mathscr{L}}|\tilde{\rho}\rangle\rangle \qquad (2)$$

■

We consider (2) as the system dynamics in the rest of paper.

III. Optimal control formulation

This section describes the problem formulation. To this end, we have first to describe the state constraint that arises from the concept of quantum purity.

A. Quantum purity

Quantum purity is a fundamental property of a quantum state. For pure states, the purity $P = 1$, while $P < 1$ shows that the quantum state is mixed. In dissipative quantum systems, a state may be initialized as pure, i.e., $\rho = |\psi\rangle\langle\psi|$, and then

due to the interaction with the environment and through a channel χ is decohered and mapped to a mixed state. A quantum channel χ over the space $\mathbb{H}$ represents a completely positive trace-preserving quantum map, i.e., $\chi \in CPTP(\mathbb{H})$. Hence, the purity of the channel χ is considered as just the purity of the state ρ. Therefore, one can write

$$P(\rho) = tr\left(\chi(\rho)^2\right) = tr\left(\rho^2\right) = \left(vec\left(\rho^\dagger\right)\right)^\dagger vec\left(\rho\right)$$

which leads to $\tilde{P}(\rho) = \left\langle\left\langle \tilde{\rho}^\dagger \,|\tilde{\rho}\,\right\rangle\right\rangle$. Preservation or maximization of the purity of a state transmitted through a quantum channel, i.e., a dissipative quantum system, is an important objective in quantum information processing. To do so, several decoherence-reduction techniques, such as quantum error correcting codes, and decoherence-free subspaces have been developed. In this work, following the study in [1, Chapter 12] that imposes an equality state constraint, we use a less restricted form by keeping the quantum purity above some predefined level, i.e., $\bar{\alpha}P_0 \leq \tilde{P}(\rho) \leq P_0$ with $0 < \bar{\alpha} < 1$, where $P_0 = P(\rho_0)$ is the purity of the initial state.

B. Problem Formulation

Quantum operations such as quantum state transition need to be done in the shortest possible time. However, due to the inverse relation between control time and amplitude, a fast operation may cause a very large control amplitude, which is practically impossible. The methods to design the quantum optimal controller vary according to the choice of the cost functional, the construction of the Pontryagin-Hamiltonian function, and the computation scheme to solve the PMP optimality conditions. We deal with a time-energy minimization state constrained OCP (P) with bounded control aiming to transfer the initial state $|\,\tilde{\rho}(t_0)\rangle\rangle = \rho_0$ to a desired target state $\left|\,\tilde{\rho}(t_f)\right\rangle\rangle = \rho_f$. The problem casts as the following:

$$(P)\begin{cases} \min\limits_{u,t_f}\left\{J = \Gamma t_f + \eta\int_{t_0}^{t_f} u^2(t)\,dt\right\} \\ \text{subject to} \\ \left|\,\dot{\tilde{\rho}}(t)\right\rangle\rangle = \tilde{\mathscr{L}}\,|\tilde{\rho}\,\rangle\rangle \;\text{ a.e. } t \in [t_0,t_f] \\ |\,\tilde{\rho}(t_0)\rangle\rangle = \rho_0 \in \mathbb{R}^{4n} \\ u(t) \in \mathscr{U} := \{u \in L_\infty : u(t) \in \Omega \subset \mathbb{R}\} \\ \Omega = [u_{\min}, u_{\max}] \text{ a.e. } t \in [t_0,t_f] \\ h(|\,\tilde{\rho}(t)\rangle\rangle) \leq 0 \text{ for all } t \in [t_0,t_f] \end{cases}$$

where Γ and η in the performance index J are positive coefficients, and t_f shows the free final time to be optimized. The second term of J is a common choice for the cost functional in molecular control, which measures the energy of the control field in the interval $[t_0,t_f]$. The control is represented as a measurable bounded function. The inequality $h(|\,\tilde{\rho}(t)\rangle\rangle) \leq 0$ defines the state constraints for the density operator - see the specific example in (5). In this setup, we assume that all the sets are Lebesque measurable and the functions are Lebesgue measurable and Lebesgue integrable. The goal is to obtain a pair $(\rho^\star, u^\star)$ which is optimal in the sense that the value of cost functional is the minimum over the set of all feasible solutions.

Remark 1: It is important to assert the existence of a solution to problem (P) in the class of measurable controls. Following the Filippov's theorem, [11], since the right-hand side of the dynamical system is linear with respect to the control, and the set of control values is convex and compact, then one can conclude that there exists a feasible control process to this problem.

IV. Pontryagin's Minimum Principle in Gamkrelidze Form with Saturation Functions

To deal with the indicated problem, one can identify two Lagrangian multipliers: μ, and λ, where

- μ is bounded variation, non-increasing $\mu : \left[t_0,t_f\right] \to \mathbb{R}^2$, such that $\mu(t)$ is constant on the time interval in which the state constraint is inactive.
- $|\,\lambda\rangle\rangle : \left[t_0,t_f\right] \to \mathbb{R}^{4n}$ is the time-varying Lagrange multiplier vector, whose elements are called the costates of the system.

We handle control constraints with saturation functions, [6], such that the indicated inequality-constraint for control is transformed into a new equality-constraint. To do so, we define a new unconstrained control variable $\nu(t)$, and substitute the control constraint with a smooth and monotonically increasing saturation function $\phi : \mathbb{R} \to (u_{\min}, u_{\max})$ such that

$$\phi(\nu) = u_{max} - \frac{u_{max} - u_{min}}{1 + \exp(s\nu)} \quad \text{with} \quad s = \frac{c}{u_{\max} - u_{\min}}$$

in which $c > 0$ is a constant parameter, useful for modifying the slope of $\phi(\nu)$ at $\nu = 0$. The advantage of using a saturation function is that it is defined within the range of Ω, and asymptotically approaches the saturation limits for $\nu \to \pm\infty$. The next steps are the following:

- We add a regularization term to the cost functional J via a regularization parameter α, and define the new cost functional as $\tilde{J} = J + \alpha\int_{t_0}^{t_f} \nu^2(t)dt$, and solve the OCP successively by decreasing α_k. We use the result that if u_{k+1} and u_k are the optimal control inputs for $\alpha_{k+1} < \alpha_k$, then with $\lim\limits_{k\to\infty} \alpha_k = 0$, $\tilde{J}(u_k, \alpha_k)$ converges to a non-increasing optimal cost, [6], i.e., by bringing α closer to 0, we approach to the original problem.
- We consider an additional optimality condition for the new control variable by minimizing the Pontryagin-Hamilton function with respect to ν. Moreover, we need to consider the constraint equation
$$u(t) - \phi(\nu) = 0 \tag{3}$$
for the boundary value problem.
- We introduce a multiplier $\beta : \left[t_0,t_f\right] \to \mathbb{R}$ to take the equality constraint into account.

In this new setup, we will now obtain the optimality conditions. To this end, we first construct the Pontryagin Hamiltonian $\mathscr{H}$ defined for all $t \in \left[t_0,t_f\right]$ by

$$\begin{aligned}\mathscr{H}(\rho,\lambda,u,\nu,\delta,\alpha,\beta,t) = &\left(|\,\lambda(t)\rangle\rangle - 2\delta(t)\,|\,\tilde{\rho}(t)\rangle\rangle\right)^T \tilde{\mathscr{L}}\,|\,\tilde{\rho}(t)\rangle\rangle \\ &+ \eta u^2(t) + \alpha\nu^2(t) + \beta(t)\left(u(t) - \phi(\nu)\right)\end{aligned} \tag{4}$$

where $\delta(t) = \left[\,1\;\;-1\,\right]\mu(t)$.

Proposition 2: Consider the OCP (P1) that is given by (P), but with cost function $\tilde{J}$, and the additional constraint (3). Let $u^\star(t)$ be an optimal control and $\tilde{\rho}^\star(t)$ the corresponding state trajectory response. Then, there exist the multiplier $\lambda^\star(t)$ that together with $\delta,\beta:[t_0,t_f]\to\mathbb{R}$ satisfy the PMP necessary conditions. More precisely,

$$\mathscr{H}(\rho^\star,\lambda^\star,u^\star,\nu,\mu,\alpha,\beta,t)\leq\mathscr{H}(\rho^\star,\lambda^\star,u,\nu,\mu,\alpha,\beta,t)$$

for all $t\in[t_0,t_f]$, and all feasible controls $u\in\Omega$. Moreover,

$$\frac{\partial\mathscr{H}}{\partial u}=(|\lambda^\star\rangle\rangle-2\delta|\tilde{\rho}^\star\rangle\rangle)^T\tilde{\mathscr{L}}_u|\tilde{\rho}^\star\rangle\rangle+2\eta u^\star+\beta=0$$
$$\frac{\partial\mathscr{H}}{\partial\nu}=2\alpha\nu-\beta\frac{\partial\phi(\nu)}{\partial\nu}=0$$

The remaining first-order necessary conditions for the state and costate variables are given as

$$\left|\dot{\tilde{\rho}}^\star\right\rangle\rangle=\frac{\partial\mathscr{H}}{\partial|\lambda\rangle\rangle}=\tilde{\mathscr{L}}|\tilde{\rho}^\star\rangle\rangle,\quad|\tilde{\rho}^\star(t_0)\rangle\rangle=\rho_0$$
$$\left|\dot{\lambda}^\star\right\rangle\rangle^T=\frac{-\partial\mathscr{H}}{\partial|\tilde{\rho}\rangle\rangle}=\tilde{\mathscr{L}}^T|\lambda^\star\rangle\rangle-4\delta\tilde{\mathscr{L}}|\rho^\star\rangle\rangle,\left|\lambda^\star\left(t_f\right)\right\rangle\rangle=\lambda_f=\mathbf{0}$$

In addition, the transversality condition imposes that

$$\mathscr{H}\left(t_f\right)+\Gamma=0$$

Proof: Following similar arguments as in [4] for the indicated set of conditions, the extended Hamilton-Pontryagin function is

$$\mathscr{H}(\rho,\lambda,u,\nu,\mu,\alpha,\beta,t)=(|\lambda(t)\rangle\rangle-\mu^T(t)\nabla_{\tilde{\rho}}h(|\tilde{\rho}(t)\rangle\rangle))^T$$
$$\tilde{\mathscr{L}}|\tilde{\rho}(t)\rangle\rangle+\eta u^2(t)+\alpha\nu(t)^2+\beta(t)(u(t)-\phi(\nu))$$

where the state constraint $h(|\tilde{\rho}(t)\rangle\rangle)$ and multiplier $\mu(t)$ are

$$h(|\tilde{\rho}(t)\rangle\rangle)=\begin{pmatrix}\tilde{P}[\chi(\rho)]-P_0\\ \bar{\alpha}P_0-\tilde{P}[\chi(\rho)]\end{pmatrix}\leq 0,\quad \mu(t)=\begin{pmatrix}\mu_1(t)\\ \mu_2(t)\end{pmatrix}\tag{5}$$

Therefore, the gradient is given by

$$\nabla_{\tilde{\rho}}h(|\tilde{\rho}(t)\rangle\rangle)=\begin{pmatrix}\nabla_{\tilde{\rho}}\tilde{P}[\chi(\rho)] & -\nabla_{\tilde{\rho}}\tilde{P}[\chi(\rho)]\end{pmatrix}^T$$

where $\nabla_{\tilde{\rho}}\tilde{P}[\chi(\rho)]=2|\tilde{\rho}(t)\rangle\rangle$. Then, the Pontryagin Hamiltonian forms as written in (4) from which the necessary conditions according to the PMP have been indicated. ■

Proposition 3: Let $\rho^\star(t)$, $u^\star(t)$, $\lambda^\star(t)$ be an optimal trajectory of (P1). Then, $\rho^\star(t)$, $u^\star(t)$, $\lambda^\star(t)$ is a local minimizer of the Pontryagin Hamiltonian (4) as long as α satisfies the condition

$$\alpha>\frac{\beta}{2}\varepsilon\tag{6}$$

where $\varepsilon=\max_{\nu\in\mathbb{R}}|\frac{\partial^2\phi(\nu)}{\partial\nu^2}|$ is a finite bound.

Proof: A similar case of obtaining the second-order sufficient condition for local optimality is indicated in [12], however, in our case since we have two control variables $\bar{u}=(u,\nu)$, the second derivative of our Pontryagin Hamiltonian is a 2×2 matrix rather than a scalar. Accordingly, if the Pontryagin Hamiltonian has a positive definite Hessian with respect to $\bar{u}$, then it is guaranteed that $u^\star(t)$ is the local minimizer of the Hessian, i.e., the generalized Legendre-Clebsch condition guarantees that over a singular arc, the Pontryagin Hamiltonian is minimized. In this case, the Hessian is given by $\mathscr{H}_{\bar{u}\bar{u}}=\begin{pmatrix}2\eta & 0\\ 0 & 2\alpha-\beta\frac{\partial^2\phi}{\partial\nu^2}\end{pmatrix}>0$. Clearly, it is positive definite since η is positive, $\frac{\partial^2\phi}{\partial\nu^2}$ is bounded and α satisfies (6). ■

Algorithm 1 Modelling and training the PoNN (main steps)

1: Morphing transformation

$$\tau=\tau_0+c(t-t_0)\leftrightarrow t=t_0+\frac{1}{c}(\tau-\tau_0),\quad c>0$$

2: Derive the approximated formulations for $y(t)$

$$\hat{y}(\tau)=g(\tau)+\sum_{n=1}^{k}\Omega_k(\tau)(y(\tau_k)-g(\tau_k))\tag{8}$$

3: Obtain a new equation as a function of the independent variable τ, $g(\tau)$, and its derivative

$$F(\tau,\hat{y}(\tau),\dot{\hat{y}}(\tau))=\tilde{F}(\tau,g(\tau),\dot{g}(\tau))=0\tag{9}$$

4: Formulate $g(\tau)$ through a single layer neural network

$$g(\tau)=\sum_{l=1}^{L}\xi_l\sigma(\omega_l\tau+b_l)=\boldsymbol{\sigma}^T(\tau)\boldsymbol{\xi}\tag{10}$$

in which $\boldsymbol{\sigma}^T(\tau)=\sigma^T(\tau)\otimes I_{n\times n}$, where $\sigma^T(\tau)=[\sigma(\omega_1\tau+b_1),\ldots,\sigma(\omega_L\tau+b_L)]$, and $\boldsymbol{\xi}=vec([\xi_1,\ldots,\xi_L])$.

5: Compute the derivatives of $g(\tau)$ as $\dot{g}(\tau)=c\boldsymbol{\sigma}'^T(\tau)\boldsymbol{\xi}$ where $\boldsymbol{\sigma}'=\frac{d\boldsymbol{\sigma}(\tau)}{d\tau}$ and obtain (9) in terms of unknowns, so $\tilde{F}(\tau,\boldsymbol{\xi})=0$.

6: Discretize τ into N points, and express the obtained set of differential equations as loss functions at each point as $\mathbb{L}^T(\boldsymbol{\xi})=\left[\tilde{F}(\tau_0,\boldsymbol{\xi}),\ldots,\tilde{F}(\tau_N,\boldsymbol{\xi})\right]$ and obtain the unknown $\boldsymbol{\xi}$, by computing the solution of $\mathbb{L}=\mathbf{0}$.

V. Physics-Informed Neural Networks Based on the Theory of Functional Connections

In this section, we exploit the newly developed Pontryagin PINN method derived from the theory of functional connection, [7], [8]. We give a short overview on how physics-informed neural networks derived from TFC can be used to solve BVPs. Consider a generic differential equation

$$F(t,y(t),\dot{y}(t))=\mathbf{0},\quad y(t_k)=y_{t_k},\quad k\in\emptyset\cup\{1,2,\ldots\}\tag{7}$$

where $F:\mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}^n$ is a given map, and $y(t)\in\mathbb{R}^n$ is the state variable that has known values at instant of time t_k. Note that here we utilize a unified process to resolve problems involving initial, boundary, or multiple values, so $k\in\emptyset$ refers to the boundary-free functions. The goal is to obtain the (approximated) solution $\hat{y}(\cdot)$ of (7) along time. Algorithm 1 describes (an adaptation of) the main steps of the application of TFC method. The first step is to apply a morph transformation (change of time) so that the problem can be written in the domain of the activation functions to be used in the next steps. Next, we impose the solution to be on the form of (8), where $g(\cdot):\mathbb{R}\to\mathbb{R}^n$ indicates a user-specified function, and Ω is the so-called switching function. The free function $g(\cdot)$, as developed in [13] based on the theory of extreme learning machine (ELM), is modeled by a single hidden layer feedforward neural network (10), where the summation is over all L hidden neurons, and $\sigma(\cdot)$ is the activation function. In (10), ξ_l, ω_l and b_l denote the output weight, input weight, and bias of the lth hidden node,, respectively. These parameters correspond to the learning factors to be updated in the training phase. We then obtain a new set of equations $\tilde{F}(\tau,\boldsymbol{\xi})$, solved via the augmented loss

function $\mathbb{L}$. Now, let proceed with the solution of optimality conditions obtained for (P_1). We approximate the state and costate as

$$|\tilde{\rho}\rangle\rangle(\tau,\boldsymbol{\xi}_\rho) = \left(\boldsymbol{\sigma}_{\tilde{\rho}}(\tau) - \Omega_1(\tau)\boldsymbol{\sigma}_{\tilde{\rho}}(\tau_0) - \Omega_2(\tau)\boldsymbol{\sigma}_{\tilde{\rho}}(\tau_f)\right)^T\boldsymbol{\xi}_{\tilde{\rho}} + \Omega_1(\tau)\rho_0 + \Omega_2(\tau)\rho_f$$

$$|\lambda\rangle\rangle(\tau,\boldsymbol{\xi}_\lambda) = \left(\boldsymbol{\sigma}_\lambda(\tau) - \Omega_2(\tau)\boldsymbol{\sigma}_\lambda(\tau_f)\right)^T\boldsymbol{\xi}_\lambda + \Omega_2(\tau)\lambda_f$$

where the switching functions are described by $\Omega_1(\tau) = 1 + \frac{2\Delta\tau^3}{\Delta\tau_f{}^3} - \frac{3\Delta\tau^2}{\Delta\tau_f{}^2}$ and $\Omega_2(\tau) = -\frac{2\Delta\tau^3}{\Delta\tau_f{}^3} + \frac{3\Delta\tau^2}{\Delta\tau_f{}^2}$ with $\Delta\tau = \tau - \tau_0$ and $\Delta\tau_f = \tau_f - \tau_0$, [9]. By taking the derivatives of the above expressions, we obtain

$$|\dot{\tilde{\rho}}\rangle\rangle(\tau,\boldsymbol{\xi}_\rho) = c\left(\boldsymbol{\sigma}'_{\tilde{\rho}}(\tau) - \Omega'_1(\tau)\boldsymbol{\sigma}_{\tilde{\rho}}(\tau_0) - \Omega'_2(\tau)\boldsymbol{\sigma}_{\tilde{\rho}}(\tau_f)\right)^T\boldsymbol{\xi}_{\tilde{\rho}} + \Omega'_1(\tau)\rho_0 + \Omega'_2(\tau)\rho_f$$

$$|\dot{\lambda}\rangle\rangle(\tau,\boldsymbol{\xi}_\lambda) = c\left(\boldsymbol{\sigma}'_\lambda(\tau) - \Omega'_2(\tau)\boldsymbol{\sigma}_\lambda(\tau_f)\right)^T\boldsymbol{\xi}_\lambda + \Omega'_2(\tau)\lambda_f$$

Regarding the control variables, the following functional approximation are introduced

$$u(\tau,\boldsymbol{\xi}) = \boldsymbol{\sigma}_u^T(\tau)\boldsymbol{\xi}_u, \quad \nu(\tau,\boldsymbol{\xi}) = \boldsymbol{\sigma}_\nu^T(\tau)\boldsymbol{\xi}_\nu$$

We also expand the equality constraint multiplier $\beta(\tau,\boldsymbol{\xi}) = \boldsymbol{\sigma}_\beta^T(\tau)\boldsymbol{\xi}_\beta$. In addition, the state constraint multipliers are

$$\mu_1(\tau,\boldsymbol{\xi}) = \boldsymbol{\sigma}_{\mu_1}^T(\tau)\boldsymbol{\xi}_{\mu_1}, \quad \mu_2(\tau,\boldsymbol{\xi}) = \boldsymbol{\sigma}_{\mu_2}^T(\tau)\boldsymbol{\xi}_{\mu_2}$$

In line with the ELM algorithm, [13], for the free final time problems, the vector of PoNNs' parameters to be learned is constructed as $\boldsymbol{\zeta} = [\boldsymbol{\xi}_{\tilde{\rho}}\ \boldsymbol{\xi}_\lambda\ \boldsymbol{\xi}_u\ \boldsymbol{\xi}_\nu\ \boldsymbol{\xi}_\beta\ \boldsymbol{\xi}_{\mu_1}\ \boldsymbol{\xi}_{\mu_2}\ c]^T$. Now, we express the set of loss functions to be minimized as

$$\begin{aligned}
&\mathbb{L}_{\tilde{\rho}} = |\dot{\tilde{\rho}}\rangle\rangle - \tilde{\mathscr{L}}|\tilde{\rho}\rangle\rangle\\
&\mathbb{L}_\lambda = |\dot{\lambda}\rangle\rangle^T - (\tilde{\mathscr{L}}^T|\lambda\rangle\rangle - 4\delta\tilde{\mathscr{L}}|\tilde{\rho}\rangle\rangle)\\
&\mathbb{L}_u = (|\lambda\rangle\rangle - 2\delta|\tilde{\rho}\rangle\rangle)^T\tilde{\mathscr{L}}_u|\tilde{\rho}\rangle\rangle + 2\eta u + \beta\\
&\mathbb{L}_\nu = 2\alpha\nu - \beta\phi'(\nu), \quad \mathbb{L}_\phi = u - \phi(\nu)\\
&\mathbb{L}_{\mathscr{H}} = \mathscr{H}(t_f) + \Gamma\\
&\mathbb{L}_{\mu_1} = \tilde{P}[\chi(\rho)] - P_0, \quad \mathbb{L}_{\mu_2} = \bar{\alpha}P_0 - \tilde{P}[\chi(\rho)]
\end{aligned}$$

leading to an augmented form of the loss function as

$$\mathbb{L} = \begin{bmatrix}\mathbb{L}_{\tilde{\rho}} & \mathbb{L}_\lambda & \mathbb{L}_u & \mathbb{L}_\nu & \mathbb{L}_\phi & \mathbb{L}_{\mathscr{H}} & \mathbb{L}_{\mu_1} & \mathbb{L}_{\mu_2}\end{bmatrix}^T \quad (11)$$

Equation (11) can be solved by a numerical minimization scheme, and the PoNN's parameter will be learnt during the procedure. The iterative least-square method has proved to be an efficient scheme for such problem, [8]. Through this method, the estimation of $\boldsymbol{\zeta}$ is adjusted and refined to improve accuracy and convergence towards the desired outcome at $k+1$th iteration, such that $\boldsymbol{\zeta}_{k+1} = \boldsymbol{\zeta}_k + \Delta\boldsymbol{\zeta}_k$, where $\Delta\boldsymbol{\zeta}_k = -\left(\mathbb{J}(\boldsymbol{\zeta}_k)^T\mathbb{J}(\boldsymbol{\zeta}_k)\right)^{-1}\mathbb{J}(\boldsymbol{\zeta}_k)^T\mathbb{L}(\boldsymbol{\zeta}_k)$, in which $\mathbb{J}$ is the Jacobian matrix, compiling the partial derivatives of the loss function with respect to each unknown parameter, and, therefore provides a complete representation of the sensitivity of the losses to changes in the unknowns. The iterative procedure continues to be repeated until the convergence criteria is satisfied, meaning that for a predefined tolerance $\bar{\varepsilon} > 0$, we reach to $L_2[\mathbb{L}(\boldsymbol{\zeta}_k)] < \bar{\varepsilon}$.

VI. Simulation Results

In the following, we show the feasibility of our results in a numerical study. Let consider a quantum system consisting of a two-level atom and a vacuum environment. The dissipation is captured via the decay of the atom through a photon emission, which is a result of the atom - environment interaction. The environment in this case is the surrounding vacuum state. Therefore, the system dynamics must be expressed through the master equation (1), in which the term $H(u(t))$ describes the total atom-vacuum quantum-mechanical Hamiltonian as

$$H(u(t)) = E|1\rangle\langle 1| + u(t)(|0\rangle\langle 1| + |1\rangle\langle 0|) \quad (12)$$

where $u(t)$ is the driving control coherently switching between the two states. We work with the implemented dynamics in (2). For this problem, the damping rate γ is the atom-vacuum coupling, and the Liouvillian superoperator in the Fock-Liouvillian space is $\mathscr{L} = \begin{pmatrix} 0 & iu & -iu & \gamma \\ iu & -iE-\frac{\gamma}{2} & 0 & -iu \\ -iu & 0 & -iE-\frac{\gamma}{2} & iu \\ 0 & -iu & iu & -\gamma \end{pmatrix}$, which is mapped to the extended superoperator $\tilde{\mathscr{L}}$. The parameters are considered as the following: $N = 40$, $L = 30$, $\eta = 0.1$, $\Gamma = 0.01$, $\gamma = 0.9$, $\bar{\alpha} = 0.99$, $\alpha = 10^{-5}$, $E = 1$. Moreover, we use the Chebyshev orthogonal polynomials as the basis for TFC implementation. Regarding the constraints for the components of the control $u(t)$, they have been set as $u_{min} = -1$ and $u_{max} = +1$. The results are obtained after 48 iterations. For all results, the state is initiated as $\rho_{11} = 1$, with no coherence between different states. First, we neglect the dissipation part, so the solution reduces to the resolution of the Liouville-von Neumann equation, see Fig. 1(a). As the next case, we consider the dissipation while there is no coherent driving. The population of the excited state experiences an exponential decay, see Fig. 1(b). Afterward, it becomes feasible to compute the behavior of a dissipative quantum system that undergoes both coherent driving and decay. In such cases, oscillations and decay co-occur as both behaviors exist simultaneously, see Fig. 1(c). In the following, we plot the state evolution under the action of optimal control. We initiate by the pure state $\rho_{11} = 1$ and target to $\rho_{00} = 1$, while following the constraints on purity preservation. The population evolution is shown in Fig. 1(d). According to the data depicted in the graph, there is a clear trend of exponential decay in the population of the initial state, while there is a corresponding upward trend in the population of the target as time passes. In order to check the security level of reaching the target, we have to calculate the transition probability known as the quantum fidelity, referring to the degree of similarity between two quantum states, typically the system state $\rho(t)$ and target φ. We study fidelity in terms of state purity computed by $\mathscr{F}(\rho,\varphi) = \frac{(tr(\rho\varphi))^2}{P(\rho)P(\varphi)}$, [14]. Since our target φ is a pure state, i.e., $\varphi = |\psi\rangle\langle\psi|$, fidelity can simply be assessed as $\mathscr{F}(\rho,\varphi) = \frac{\langle\psi|\rho|\psi\rangle}{P(\rho)}$. Fig. 2 shows the effects of purity preservation on fidelity.

Remark 2: Recently, the theory of functional connections has been extended to n-dimensions, as described in [15]. Therefore, a natural question is whether the proposed method

using PoNNs is scalable enough to be applied to systems with any number of levels. From this work, we can observe that for an n-level system, the dimension of the Liouville superoperator $\tilde{\mathscr{L}}$ in (2) is $2n^2 \times 2n^2$, which also leads to an increase in the dimension of the augmented loss vector $\mathbb{L}$ in (11), and therefore an overall increase in computational complexity. On the other hand, as pointed out in [16], TFC approach presents a low condition number, and typically is numerically robust, as indeed we could attest from our numerical computations, that revealed good robustness to poor initialization and insensitivity to small changes in the input data. Therefore, the proposed strategy can perform well in practical applications, where there may be noise or other sources of uncertainty in the system.

VII. Conclusion

In this study, we proposed a framework for preserving quantum purity during a quantum state transition problem. Specifically, we aim to minimize both the time and energy required for the transition, while adhering to the Lindblad master equation, which governs the system dynamics. To achieve this goal, we employed a combination of two techniques, namely the Gamkrelidze revisited method and the concept of saturation functions and system extensions. The resulting boundary value problem is then solved using Pontryagin neural networks, which are well-suited for this type of problem formulation. Our approach allows us to preserve the purity of the quantum state during the transition while minimizing the resources required. Furthermore, we analyze the effects of state constraints on the evolution of quantum fidelity, providing a numerical example for a two-level system. As future work, we intend to extend our approach to higher-order dimensional systems, which could yield valuable insights and applications in various fields, including quantum computing and quantum communication. Our results have important implications for the practical implementation of quantum state transitions.

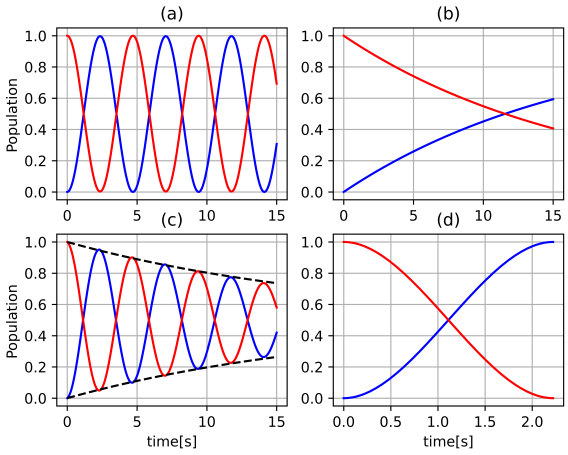

Fig. 1: Population evolution under quantum dynamics. The blue and red lines represent the evolution of ρ_{00} and ρ_{11}, respectively. (a) Coherent driving with no decay. (b) Decay with no coherent driving. (c) Coherent driving and decay. (d) Optimal coherent driving and decay.

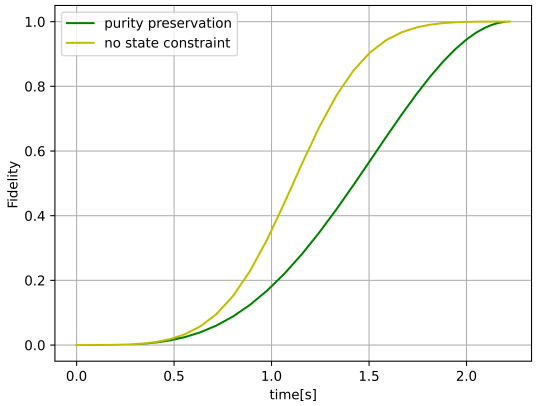

Fig. 2: State transition probability quantified by purity.

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