Using Optimal Control Theory to Improve Adiabatic Quantum Trajectories

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Motivation

- In adiabatic quantum computation (AQC), the system is kept in the instantaneous ground state $|\phi_0(t)\rangle$ of a slowly varying Hamiltonian $H(t)$, which provides inherent protection against dephasing and relaxation in the energy eigenstate basis.
- However, this protection does not guarantee full fault tolerance, since there still exist some types of noise, which can drive undesirable transitions out of the ground state.
- Therefore, it would be desirable to try decreasing the accumulation of errors by performing a computation in a shorter time. However, how to reconcile faster evolution with the requirement of adiabaticity?
- Our approach: (1) consider Hamiltonians containing multiple control functions and (2) use quantum optimal control theory (QOCT) to find control sets which achieve the target state with a high fidelity while simultaneously maximizing the degree of adiabaticity.
- Exploring properties of optimal adiabatic trajectories in few-qubit model systems elucidates the dynamic mechanisms which suppress unwanted excitations from the ground state.

Controlled quantum adiabatic evolution

- Consider a Hamiltonian with two independent control functions:

$$H(t) = u_{\mathrm{i}}(t)H_{\mathrm{i}} + u_{\mathrm{f}}(t)H_{\mathrm{f}}, \tag{1}$$

- $H_{\mathrm{i}} = H(0)$ is the initial Hamiltonian, whose ground state, $|\phi_0^{(\mathrm{i})}\rangle = |\phi_0(0)\rangle$, is the initial state of the system;
- $H_{\mathrm{f}} = H(T)$ is the final Hamiltonian, whose ground state, $|\phi_0^{(\mathrm{f})}\rangle = |\phi_0(T)\rangle$, encodes the solution to the computational problem;
- $u_{\mathrm{i}}(t)$ and $u_{\mathrm{f}}(t)$ are control functions which satisfy boundary conditions: $u_{\mathrm{i}}(0) = 1$, $u_{\mathrm{f}}(0) = 0$, $u_{\mathrm{i}}(T) = 0$, $u_{\mathrm{f}}(T) = 1$.
- More generally, the Hamiltonian is: $H(t) = H(\{u_k(t)\})$, where $\{u_k(t)\}_{k=1}^{K}$ are control functions which satisfy boundary conditions: $H(\{u_k(0)\}) = H_{\mathrm{i}}$ and $H(\{u_k(T)\}) = H_{\mathrm{f}}$.
- A choice of the control set $u(\cdot) = \{u_k(t)\,|\,k = 1,\ldots,K;\ t \in [0,T]\}$ determines the dynamic trajectory $\psi(\cdot) = \{|\psi(t)\rangle\,|\,t \in [0,T]\}$, where $|\psi(t)\rangle = U(t)|\phi_0^{(\mathrm{i})}\rangle$ is the system's state at time t and $U(t) \equiv U(t,0)$ is the time-evolution operator.

Formulation of quantum optimal control theory

- Given a finite evolution time T, we use QOCT to identify control sets which maximize an objective J composed of a weighted sum of two terms: one is the target-state fidelity, F, and the other is the average ground-state population during evolution, $\overline{P_0}$, i.e.

$$J = F + \alpha\overline{P_0} = |\langle\phi_0^{(\mathrm{f})}|\psi(T)\rangle|^2 + \frac{\alpha}{T}\int_0^T P_0(t)dt, \tag{2}$$

- $P_0(t) = |\langle\phi_0(t)|\psi(t)\rangle|^2$ is the instantaneous ground-state population at time t;
- $\alpha > 0$ is a positive weight factor which determines the relative importance of the two terms.
- The objective is a functional of the controls: $J = J[u(\cdot)]$, and the QOCT problem may be stated as the search for $J^\star = \max_{u(\cdot)} J[u(\cdot)]$. A set of optimal controls, which maximizes the objective, is denoted as $u^\star(\cdot)$, so that $J[u^\star(\cdot)] = J^\star$.
- To implement the search for $u^\star(\cdot)$, we use a gradient-based algorithm.

Model system

- In numerical simulations, we use a one-qubit Hamiltonian:

$$H(t) = x(t)\sigma_x + z(t)\sigma_z, \tag{3}$$

- $x(t)$ and $z(t)$ are the control functions,
- σ_x and σ_z are the Pauli matrices.
- The energy gap between the ground state and the first excited state:

$$g(t) = 2\sqrt{x^2(t) + z^2(t)}. \tag{4}$$

- We apply QOCT to two AQC problems:

$$\text{(i)}\quad H_{\mathrm{i}} = \sigma_x, \quad H_{\mathrm{f}} = \sigma_x + \sigma_z, \tag{5a}$$

$$\text{(ii)}\quad H_{\mathrm{i}} = \sigma_x, \quad H_{\mathrm{f}} = \sigma_z. \tag{5b}$$

Adiabatic condition

- According to the adiabatic theorem, the population loss from the ground state $|\phi_0(t)\rangle$ can be made arbitrarily small: $1 - P_0(t) \leq 4\epsilon^2$, where $\epsilon \ll 1$, if the Hamiltonian change is sufficiently slow:

$$\frac{|\langle\phi_1(t)|\partial H/\partial t|\phi_0(t)\rangle|}{g^2(t)} \leq \epsilon, \tag{6}$$

- For the one-qubit Hamiltonian (3), the equality in the adiabatic condition (6) can be recast into the form:

$$\frac{|x\dot{z} - z\dot{x}|}{4(x^2+z^2)^{3/2}} = \epsilon. \tag{7}$$

- If $x(t)$ and $z(t)$ are independent functions, then, in general, equation (7) has an infinite number of solutions. We can sample various solutions of (7), by imposing different constraints that eliminate one of the two functions from the equation.

Initial and optimal control sets

- The control landscape corresponding to the composite objective $J = F + \alpha\overline{P_0}$ is expected to possess multiple local optima.
- Selecting an initial control set that results in a good optimal solution becomes itself a part of the QOCT problem.
- One possibility is initializing searches at control sets that satisfy (7).
- To illustrate how the adiabatic condition (7) complements QOCT, consider, for example, the AQC problem (ii) and three control sets:

(a) The linear interpolation ($s = t/T$ is the scaled time):

$$\{x(s) = 1 - s,\ z(s) = s\}.$$

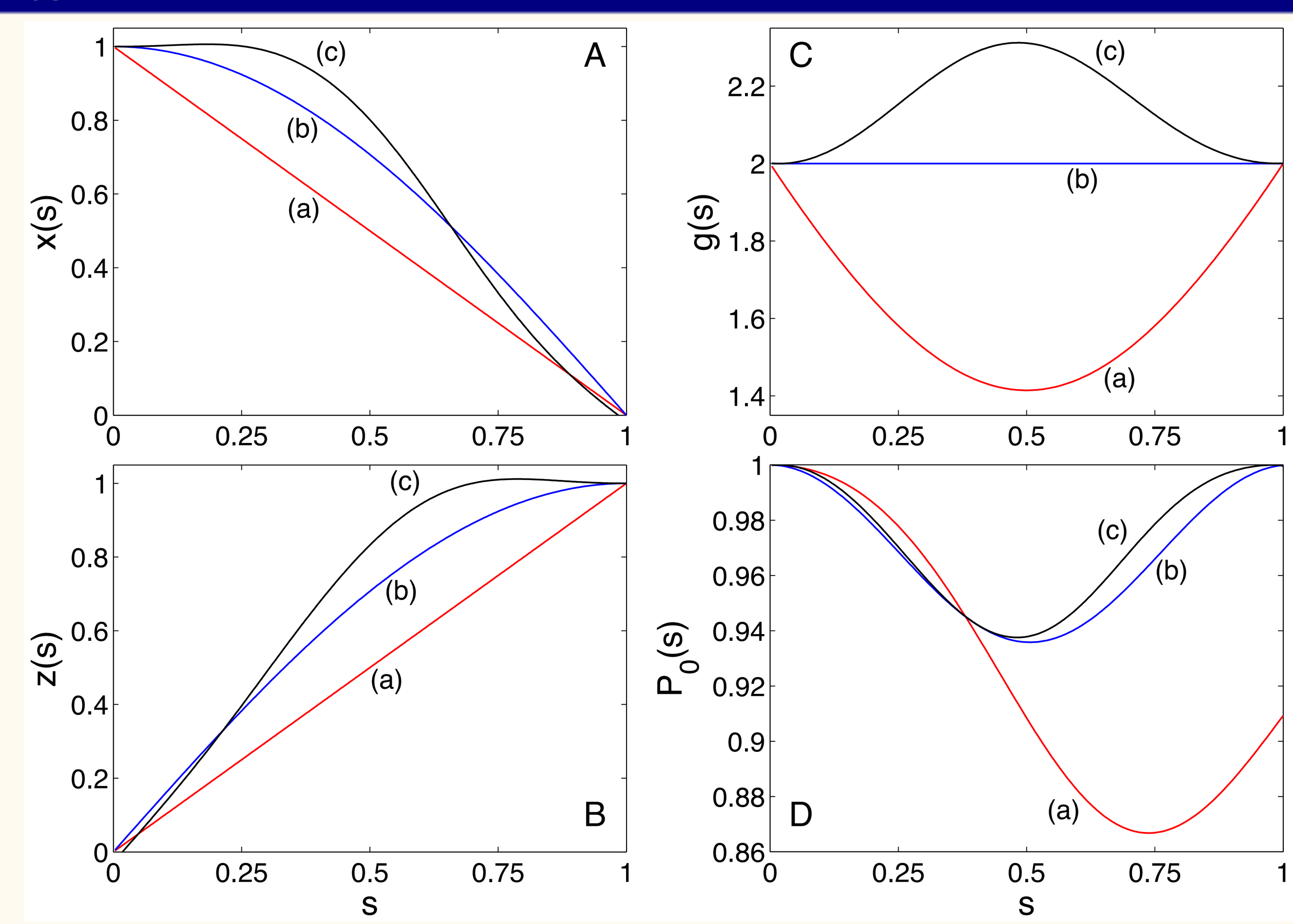
(b) A non-linear interpolation:

$$\{x(s) = \cos(\pi s/2),\ z(s) = \sin(\pi s/2)\},$$

which is a solution of the adiabatic condition (7), obtained by imposing the constraint $x^2(s) + z^2(s) = 1$.

(c) An optimal control set $\{x^\star(s),\ z^\star(s)\}$ maximizing the objective (2) with $\alpha = 0.1$ and $T = 3$, which is found by the numeric search starting from the set (b) used as the initial guess.

Optimization results



Results for the AQC problem (ii) with $H_{\mathrm{i}} = \sigma_x$ and $H_{\mathrm{f}} = \sigma_z$.

(a) The linear interpolation, $\{x(s) = 1 - s,\ z(s) = s\}$: $1 - F \approx 9.1 \times 10^{-2}$, $\overline{P_0} \approx 0.925$.

(b) A non-linear interpolation, $\{x(s) = \cos(\pi s/2),\ z(s) = \sin(\pi s/2)\}$: $1 - F \approx 1.1 \times 10^{-4}$, $\overline{P_0} \approx 0.968$.

(c) An optimal control set $\{x^\star(s),\ z^\star(s)\}$: $1 - F \approx 3.8 \times 10^{-7}$, $\overline{P_0} \approx 0.972$.

Conclusions and future directions

- By combining QOCT with the initial-set selection via the adiabatic condition, it is possible to significantly improve both the target-state fidelity and the degree of adiabaticity during evolution.
- There exists a very rich variety of dynamic trajectories associated with different multi-function control sets, and a proper search can discover solutions with a substantially improved performance.
- The use of a composite objective and a gradient-based optimization method, while simple and numerically efficient, gives only a snapshot of accessible dynamics.
- More insight into the attainable control performance can be gained by applying global search methods.
- Although numerical optimizations have to be restricted to few-qubit systems, they are likely to significantly expand our understanding of dynamical mechanisms which help to enhance the adiabaticity.
- Furthermore, global optimization methods are applicable directly in the laboratory through the use of adaptive feedback control.
- For more details on this work see: C. Brif, M. D. Grace, M. Sarovar, and K. C. Young, "Exploring adiabatic quantum trajectories via optimal control," New J. Phys. **16**, 065013 (2014).

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