Quantum Systems: Dynamics and Control[1]

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Outline

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Time-adiabatic approximation without gap conditions[5]

Take $m+1$ Hermitian matrices $n \times n$: $\boldsymbol{H}_0, \ldots, \boldsymbol{H}_m$. For $u \in \mathbb{R}^m$ set $\boldsymbol{H}(u) := \boldsymbol{H}_0 + \sum_{k=1}^m u_k \, \boldsymbol{H}_k$. Assume that u is a slowly varying time-function: $u = u(s)$ with $s = \epsilon t \in [0,1]$ and ϵ a small positive parameter. Consider a solution $\left[0, \frac{1}{\epsilon}\right] \ni t \mapsto |\psi\rangle_t^\epsilon$ of

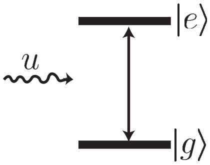
$$i \frac{d}{dt} |\psi\rangle_t^\epsilon = \boldsymbol{H}(u(\epsilon t)) |\psi\rangle_t^\epsilon.$$

Take $[0,1] \ni s \mapsto \boldsymbol{P}(s)$ a family of orthogonal projectors such that for each $s \in [0,1]$, $\boldsymbol{H}(u(s))\boldsymbol{P}(s) = E(s)\boldsymbol{P}(s)$ where $E(s)$ is an eigenvalue of $\boldsymbol{H}(u(s))$. Assume that $[0,1] \ni s \mapsto \boldsymbol{H}(u(s))$ is C^2, $[0,1] \ni s \mapsto \boldsymbol{P}(s)$ is C^2 and that, for almost all $s \in [0,1]$, $\boldsymbol{P}(s)$ is the orthogonal projector on the eigenspace associated to the eigenvalue $E(s)$. Then

$$\lim_{\epsilon \mapsto 0^+} \left(\sup_{t \in [0, \frac{1}{\epsilon}]} \left| \|\boldsymbol{P}(\epsilon t) |\psi\rangle_t^\epsilon\|^2 - \|\boldsymbol{P}(0) |\psi\rangle_0^\epsilon\|^2 \right| \right) = 0.$$

[5] Theorem 6.2, page 175 of *Adiabatic Perturbation Theory in Quantum Dynamics*, by S. Teufel, Lecture notes in Mathematics, Springer, 2003.

Chirped control of a 2-level system (1)



$i\frac{d}{dt}|\psi\rangle = \left(\frac{\omega_{eg}}{2}\boldsymbol{\sigma_z} + \frac{u}{2}\boldsymbol{\sigma_x}\right)|\psi\rangle$ with quasi-resonant control ($|\omega_r - \omega_{eg}| \ll \omega_{eg}$)

$$u(t) = v\left(e^{i(\omega_r t+\theta)} + e^{-i(\omega_r t+\theta)}\right)$$

where $v, \theta \in \mathbb{R}$, $|v|$ and $|\frac{d\theta}{dt}|$ are small and slowly varying:

$$|v|, \left|\frac{d\theta}{dt}\right| \ll \omega_{eg}, \left|\frac{dv}{dt}\right| \ll \omega_{eg}|v|, \left|\frac{d^2\theta}{dt^2}\right| \ll \omega_{eg}\left|\frac{d\theta}{dt}\right|.$$

Passage to the interaction frame $|\psi\rangle = e^{-i\frac{\omega_r t+\theta}{2}\boldsymbol{\sigma_z}}|\phi\rangle$:

$$i\frac{d}{dt}|\phi\rangle = \left(\frac{\omega_{eg}-\omega_r-\frac{d}{dt}\theta}{2}\boldsymbol{\sigma_z} + \frac{ve^{2i(\omega_r t+\theta)}+v}{2}\boldsymbol{\sigma_+} + \frac{ve^{-2i(\omega_r t-\theta)}+v}{2}\boldsymbol{\sigma_-}\right)|\phi\rangle.$$

Set $\Delta_r = \omega_{eg} - \omega_r$ and $w = -\frac{d}{dt}\theta$, RWA yields following averaged Hamiltonian

$$\frac{\boldsymbol{H}_{\text{chirp}}}{\hbar} = \frac{\Delta_r + w}{2}\boldsymbol{\sigma_z} + \frac{v}{2}\boldsymbol{\sigma_x}$$

where (v, w) are two real control inputs.

Chirped control of a 2-level system (2)

In $\frac{\boldsymbol{H}_{\text{chirp}}}{\hbar} = \frac{\Delta_r + w}{2}\boldsymbol{\sigma_z} + \frac{v}{2}\boldsymbol{\sigma_x}$ set, for $s = \epsilon t$ varying in $[0, \pi]$, $w = a\cos(\epsilon t)$ and $v = b\sin^2(\epsilon t)$. Spectral decomposition of $\boldsymbol{H}_{\text{chirp}}$ for $s \in]0, \pi[$:

$$\Omega_- = -\frac{\sqrt{(\Delta_r+w)^2+v^2}}{2} \text{ with } |-\rangle = \frac{\cos\alpha|g\rangle - (1-\sin\alpha)|e\rangle}{\sqrt{2(1-\sin\alpha)}}$$

$$\Omega_+ = \frac{\sqrt{(\Delta_r+w)^2+v^2}}{2} \text{ with } |+\rangle = \frac{(1-\sin\alpha)|g\rangle + \cos\alpha|e\rangle}{\sqrt{2(1-\sin\alpha)}}$$

where $\alpha \in]\frac{-\pi}{2}, \frac{\pi}{2}[$ is defined by $\tan\alpha = \frac{\Delta_r+w}{v}$. With $a > |\Delta_r|$ and $b > 0$

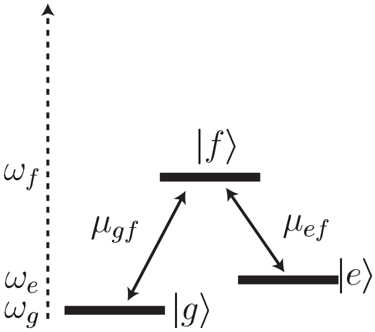
$$\lim_{s \mapsto 0^+} \alpha = \frac{\pi}{2} \quad \text{implies} \quad \lim_{s \mapsto 0^+} |-\rangle_s = |g\rangle, \quad \lim_{s \mapsto 0^+} |+\rangle_s = |e\rangle$$

$$\lim_{s \mapsto \pi^-} \alpha = -\frac{\pi}{2} \quad \text{implies} \quad \lim_{s \mapsto \pi^-} |-\rangle_s = -|e\rangle, \quad \lim_{s \mapsto \pi^-} |+\rangle_s = |g\rangle.$$

Adiabatic approximation: the solution of $i\hbar\frac{d}{dt}|\phi\rangle = \boldsymbol{H}_{\text{chirp}}(\epsilon t)|\phi\rangle$ starting from $|\phi\rangle_0 = |g\rangle$ reads

$$|\phi\rangle_t = e^{i\vartheta_t}|-\rangle_{s=\epsilon t}, \quad t \in [0, \tfrac{\pi}{\epsilon}], \text{ with } \vartheta_t \text{ time-varying global phase.}$$

At $t = \frac{\pi}{\epsilon}$, $|\psi\rangle$ coincides with $|e\rangle$ up to a global phase: robustness versus Δ_r, a and b (ensemble controllability).



$$\frac{\boldsymbol{H}}{\hbar} = \omega_g|g\rangle\langle g| + \omega_e|e\rangle\langle e| + \omega_f|f\rangle\langle f| + u\mu_{gf}\left(|g\rangle\langle f| + |f\rangle\langle g|\right) + u\mu_{ef}\left(|e\rangle\langle f| + |f\rangle\langle e|\right).$$

Set $\omega_{gf} = \omega_f - \omega_g$, $\omega_{ef} = \omega_f - \omega_e$ and $u = u_{gf}\cos(\omega_{gf}t) + u_{ef}\cos(\omega_{ef}t)$ with slowly varying small real amplitudes u_{gf} and u_{ef}.

Put $i\frac{d}{dt}|\psi\rangle = H|\psi\rangle$ in the interaction frame:

$$|\psi\rangle = e^{-it(\omega_g|g\rangle\langle g| + \omega_e|e\rangle\langle e| + \omega_f|f\rangle\langle f|)}|\phi\rangle.$$

Rotation Wave Approximation yields $i\hbar\frac{d}{dt}|\phi\rangle = \boldsymbol{H}_{\text{rwa}}|\phi\rangle$ with

$$\frac{\boldsymbol{H}_{\text{rwa}}}{\hbar} = \frac{\Omega_{gf}}{2}\left(|g\rangle\langle f| + |f\rangle\langle g|\right) + \frac{\Omega_{ef}}{2}\left(|e\rangle\langle f| + |f\rangle\langle e|\right)$$

with slowly varying Rabi pulsations $\Omega_{gf} = \mu_{gf}u_{gf}$ and $\Omega_{ef} = \mu_{ef}u_{ef}$.

Spectral decomposition: as soon as $\Omega_{gf}^2 + \Omega_{ef}^2 > 0$,
$\frac{\Omega_{gf}(|g\rangle\langle f|+|f\rangle\langle g|)}{2} + \frac{\Omega_{ef}(|e\rangle\langle f|+|f\rangle\langle e|)}{2}$ admits 3 distinct eigenvalues,

$$\Omega_- = -\frac{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}{2}, \quad \Omega_0 = 0, \quad \Omega_+ = \frac{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}{2}.$$

They correspond to the following 3 eigenvectors,

$$|-\rangle = \frac{\Omega_{gf}}{\sqrt{2(\Omega_{gf}^2+\Omega_{ef}^2)}}|g\rangle + \frac{\Omega_{ef}}{\sqrt{2(\Omega_{gf}^2+\Omega_{ef}^2)}}|e\rangle - \frac{1}{\sqrt{2}}|f\rangle$$

$$|0\rangle = \frac{-\Omega_{ef}}{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}|g\rangle + \frac{\Omega_{gf}}{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}|e\rangle$$

$$|+\rangle = \frac{\Omega_{gf}}{\sqrt{2(\Omega_{gf}^2+\Omega_{ef}^2)}}|g\rangle + \frac{\Omega_{ef}}{\sqrt{2(\Omega_{gf}^2+\Omega_{ef}^2)}}|e\rangle + \frac{1}{\sqrt{2}}|f\rangle.$$

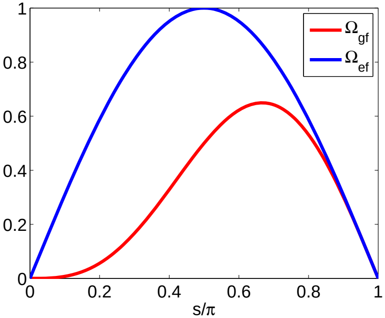
For $\epsilon t = s \in [0, \frac{3\pi}{2}]$ and $\bar{\Omega}_g, \bar{\Omega}_e > 0$, the adiabatic control

$$\Omega_{gf}(s) = \begin{cases} 0, & \text{for } s \in [0, \frac{\pi}{2}]; \\ \bar{\Omega}_g \cos^2 s, & \text{for } s \in [\frac{\pi}{2}, \frac{3\pi}{2}]; \end{cases}, \quad \Omega_{ef}(s) = \begin{cases} \bar{\Omega}_e \sin^2 s, & \text{for } s \in [0, \pi]; \\ 0, & \text{for } s \in [\pi, \frac{3\pi}{2}]. \end{cases}$$

provides the passage from $|g\rangle$ at $t = 0$ to $|e\rangle$ at $\epsilon t = \frac{3\pi}{2}$.

Exercice

Design an adiabatic passage $s \mapsto (\Omega_{gf}(s), \Omega_{ef}(s))$ *from* $|g\rangle$ *to* $\frac{-|g\rangle+|e\rangle}{\sqrt{2}}$*, up to a global phase.*



Take, e.g., $s = \epsilon t \in [0, \pi]$ and $\bar{\Omega} > 0$, and set

$$\begin{aligned} \Omega_{gf}(s) &= \frac{\bar{\Omega}}{2} \sin s - \frac{\bar{\Omega}}{4} \sin 2s \\ \Omega_{ef}(s) &= \bar{\Omega} \sin s \end{aligned}$$

Results from $|0\rangle = \frac{-\Omega_{ef}}{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}|g\rangle + \frac{\Omega_{gf}}{\sqrt{\Omega_{gf}^2+\Omega_{ef}^2}}|e\rangle$

Principle of quantum annealing

• Consider the following classical combinatorial problem. For a large integer $n > 0$ and a collection $(\lambda_{i,j})_{1\leq i,j\leq n}$ of real numbers, find the argument $\bar{x}$ of the minimum for

$$\{-1,+1\}^n \ni x \mapsto \Lambda(x) = \sum_{1\leq i,j\leq n} \lambda_{i,j} x_i x_j.$$

• Assume that we have a n-qubit (wave function $|\psi\rangle$ in $(\mathbb{C}^2)^{\otimes n} \equiv \mathbb{C}^{2^n}$) with a scalar control u and with Hamiltonian

$$\boldsymbol{H}(u) = \sum_{1\leq i,j\leq n} \lambda_{i,j} \boldsymbol{\sigma_z^{(i)}} \boldsymbol{\sigma_z^{(j)}} + u \sum_{1\leq i\leq n} \boldsymbol{\sigma_x^{(i)}}.$$

• Consider a smooth decreasing function f on $[0,1]$ with $f(0) \gg \max_{1\leq i,j\leq n} |\lambda_{i,j}|$ and $f(1) = 0$. Assume that, for any $u \in [0, f(0)]$, the smallest eigenvalue of $\boldsymbol{H}_u$ is not degenerate.

• By the adiabatic theorem, for $\epsilon > 0$ small enough, the solution of $\imath \frac{d}{dt}|\psi\rangle = \boldsymbol{H}(f(\epsilon t))|\psi\rangle$ starting from $|\psi\rangle_0 = \left(\frac{|g\rangle - |e\rangle}{\sqrt{2}}\right)^{\otimes n}$ is close at time $t = 1/\epsilon$ to the separable state $|q_1\rangle \otimes |q_2\rangle \otimes \ldots \otimes |q_n\rangle$ where $|q_i\rangle = |g\rangle$ (resp $|e\rangle$) when $\bar{x}_i = -1$ (resp. $\bar{x}_i = +1$).

• The measure of $\boldsymbol{\sigma_z}$ for each qubit gives then the solution $\bar{x}$ of such a combinatorial problem.

Outline

Gradient ascent pulse engineering (GRAPE)

Goal: transfer the population from $|\psi_i\rangle$ to $|\psi_f\rangle$ for

$$i\frac{d}{dt}|\psi\rangle = \left(\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k(t)\boldsymbol{H}_1 \right) |\psi\rangle.$$

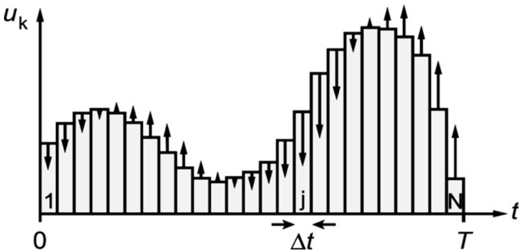
Derived from the unitary operator $\boldsymbol{U}_u(t)$, generated by the above Schrödinger equation, we set the functional

$$u([0,T]) \mapsto F(u) = \left| \langle \psi_{\text{end}} | \boldsymbol{U}_u(T) | \psi_{\text{ini}} \rangle \right|^2.$$

We wish to reach the maximum of this functional.

Gradient ascent pulse engineering (GRAPE)

We discretize the problem



$$F(u) = \left| \langle \psi_{\text{end}} | \boldsymbol{U}_N \boldsymbol{U}_{N-1} \cdots \boldsymbol{U}_1 | \psi_{\text{ini}} \rangle \right|^2, \quad U_j = \exp\left(-i\Delta t (\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k(j) \boldsymbol{H}_k) \right).$$

Defining

$$|\psi_{j,\text{end}}\rangle = \boldsymbol{U}_{j+1}^\dagger \cdots \boldsymbol{U}_N^\dagger |\psi_{\text{end}}\rangle, \qquad |\psi_{j,\text{ini}}\rangle = \boldsymbol{U}_j \cdots \boldsymbol{U}_1 |\psi_{\text{ini}}\rangle$$

We have (up to second terms in Δt):

$$\frac{\partial F}{\partial u_k(j)} \approx -i\Delta t \Big(\langle \psi_{j,\text{end}} | \boldsymbol{H}_k | \psi_{j,\text{ini}} \rangle \langle \psi_{j,\text{ini}} \mid \psi_{j,\text{end}} \rangle - \langle \psi_{j,\text{ini}} | \boldsymbol{H}_k | \psi_{j,\text{end}} \rangle \langle \psi_{j,\text{end}} \mid \psi_{j,\text{ini}} \rangle \Big).$$

GRAPE algorithm

1. Start with an initial control guess $u_k(j)$ (important because of local maxima).
2. Calculate for all j, $|\psi_{j,\mathrm{ini}}\rangle = \boldsymbol{U}_j \cdots \boldsymbol{U}_1 |\psi_{\mathrm{ini}}\rangle$.
3. Calculate for all j, $|\psi_{j,\mathrm{end}}\rangle = \boldsymbol{U}_{j+1}^\dagger \cdots \boldsymbol{U}_N^\dagger |\psi_{\mathrm{end}}\rangle$.
4. Evaluate $\frac{\partial F}{\partial u_k(j)}$ and update the $m \times N$ control amplitudes $u_k(j)$ according to
$$u_k(j) \to u_k(j) + \epsilon \frac{\partial F}{\partial u_k(j)}.$$
with $\epsilon > 0$ and small enough.
5. Go to step 2.

Algorithm terminates if the change in functional is smaller than a threshold.

Limited control amplitudes: we add a penalty functional parameterized by $\alpha_k > 0$ with $k = 1, \dots, m$. Functional F is replaced by $F + F_{\mathrm{pen}}$ with

$$F_{\mathrm{pen}} = -\frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{m} \alpha_k u_k^2(j) \Delta t, \quad \text{with } \frac{\partial F_{\mathrm{pen}}}{\partial u_k(j)} = -\alpha_k u_k(j) \Delta t.$$

Another approach: two optimal control problems

For given T, $|\psi_{\text{ini}}\rangle$ and $|\psi_{\text{end}}\rangle$, find the open-loop control $[0,T] \ni t \mapsto u(t)$ such that

$$\min_{\substack{u_k \in L^2([0,T],\mathbb{R}) \\ i\frac{d}{dt}|\psi\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|\psi\rangle \\ |\psi\rangle_{t=0} = |\psi_{\text{ini}}\rangle,\ |\langle\psi_{\text{end}}|\psi\rangle|^2_{t=T} = 1}} \frac{1}{2}\int_0^T \left(\sum_{k=1}^m u_k^2\right)$$

Since the initial and final constraints are difficult to satisfy simultaneously from a numerical point of view, consider the second problem where the final constraint is penalized with $\alpha > 0$:

$$\min_{\substack{u_k \in L^2([0,T],\mathbb{R}) \\ i\frac{d}{dt}|\psi\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|\psi\rangle \\ |\psi\rangle_{t=0} = |\psi_{\text{ini}}\rangle}} \frac{1}{2}\int_0^T \left(\sum_{k=1}^m u_k^2\right) + \frac{\alpha}{2}\left(1 - |\langle\psi_{\text{end}}|\psi\rangle|^2_T\right)$$

First order stationary conditions

For two-points problem, the first order stationary conditions read:

$$\begin{cases} i\frac{d}{dt}|\psi\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|\psi\rangle, \ t \in (0,T) \\ i\frac{d}{dt}|p\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|p\rangle, \ t \in (0,T) \\ u_k = -\Im\Big(\langle p|H_k|\psi\rangle \Big), k = 1,\dots,m, \quad t \in (0,T) \\ |\psi\rangle_{t=0} = |\psi_{\text{ini}}\rangle, \ |\langle\psi_{\text{end}}|\psi\rangle|^2_{t=T} = 1 \end{cases}$$

For the relaxed problem, the first order stationary conditions read:

$$\begin{cases} i\frac{d}{dt}|\psi\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|\psi\rangle, \ t \in (0,T) \\ i\frac{d}{dt}|p\rangle = (H_0 + \sum_{k=1}^m u_k H_k)|p\rangle, \ t \in (0,T) \\ u_k = -\Im\Big(\langle p|H_k|\psi\rangle \Big), k = 1,\dots,m, \quad t \in (0,T) \\ |\psi\rangle_{t=0} = |\psi_{\text{ini}}\rangle, \ |p\rangle_{t=T} = -\alpha\, \langle\psi_{\text{end}}|\psi\rangle_{t=T}\ |\psi_{\text{end}}\rangle. \end{cases}$$

Monotone numerical scheme for the relaxed problem (1)[6]

Take an L^2 control $[0, T] \ni t \mapsto u(t)$ $(\dim(u) = 1$ here) and denote by

- $|\psi_u\rangle$ the solution of forward system $i\frac{d}{dt}|\psi\rangle = (H_0 + uH_1)|\psi\rangle$ starting from $|\psi_{\text{ini}}\rangle$.
- $|p_u\rangle$ the adjoint associated to u, i.e. the solution of the backward system $i\frac{d}{dt}|p_u\rangle = (H_0 + uH_1)\,|p_u\rangle$ with $|p_u\rangle_T = -\alpha P|\psi_u\rangle_T$, P projector on $|\psi_{\text{end}}\rangle$, $P|\phi\rangle \equiv \langle\psi_{\text{end}}|\phi\rangle\ |\psi_{\text{end}}\rangle$.
- $J(u) = \frac{1}{2}\int_0^T u^2 + \frac{\alpha}{2}(1 - |\langle\psi_{\text{end}}|\psi_u\rangle|_T^2)$.

Starting from an initial guess $u^0 \in L^2([0, T], \mathbb{R})$, the monotone scheme generates a sequence of controls $u^\nu \in L^2([0, T], \mathbb{R})$, $\nu = 1, 2, \ldots$, such that the cost $J(u^\nu)$ is decreasing, $J(u^{\nu+1}) \leq J(u^\nu)$.

[6] D. Tannor, V. Kazakov, and V. Orlov. *Time Dependent Quantum Molecular Dynamics*, chapter Control of photochemical branching: Novel procedures for finding optimal pulses and global upper bounds, pages 347–360. Plenum, 1992.

Monotone numerical scheme for the relaxed problem (2)

Assume that, at step ν, we have computed the control u^ν, the associated quantum state $|\psi^\nu\rangle = |\psi_{u^\nu}\rangle$ and its adjoint $|p^\nu\rangle = |p_{u^\nu}\rangle$. We get their new time values $u^{\nu+1}$, $|\psi^{\nu+1}\rangle$ and $|p^{\nu+1}\rangle$ in two steps:

1. Imposing $u^{\nu+1} = -\Im\left(\langle p^\nu | H_1 | \psi^{\nu+1}\rangle\right)$ is just a feedback; one get $u^{\nu+1}$ just by a forward integration of the nonlinear Schrödinger equation,

$$i\frac{d}{dt}|\psi\rangle = \left(H_0 - \Im\left(\langle p^\nu | H_1 | \psi\rangle\right) H_1\right)|\psi\rangle, \quad |\psi\rangle_0 = |\psi_{\text{ini}}\rangle,$$

that provides $[0, T] \ni t \mapsto |\psi^{\nu+1}\rangle$ and the new control $u^{\nu+1}$.

2. Backward integration from $t = T$ to $t = 0$ of

$$i\frac{d}{dt}|p\rangle = \left(H_0 + u^{\nu+1}(t)H_1\right)|p\rangle, \quad |p\rangle_T = -\alpha\left\langle \psi_{\text{end}} | \psi^{\nu+1}\right\rangle_T |\psi_{\text{end}}\rangle$$

yields to the new adjoint trajectory $[0, T] \ni t \mapsto |p^{\nu+1}\rangle$.

Why $J(u^{\nu+1}) \leq J(u^\nu)$?

- Because we have the identity for any open-loop controls u and v ($P = |\psi_{\text{end}}\rangle\langle\psi_{\text{end}}|$)

$$J(u) - J(v) = -\frac{\alpha}{2}\left(\langle\psi_u - \psi_v|P|\psi_u - \psi_v\rangle\right)_T + \frac{1}{2}\left(\int_0^T (u-v)\left(u + v + 2\Im\left(\langle p_v\,|H_1|\,\psi_u\rangle\right)\right)\right).$$

- If $u = -\Im\left(\langle p_v\,|H_1|\,\psi_u\rangle\right)$ for all $t \in [0, T)$, we have

$$J(u) - J(v) = -\frac{\alpha}{2}\left(\langle\psi_u - \psi_v|P|\psi_u - \psi_v\rangle\right)_T - \frac{1}{2}\left(\int_0^T (u-v)^2\right)$$

  and thus $J(u) \leq J(v)$.
- Take $v = u^\nu$, $u = u^{\nu+1}$: then $|p_v\rangle = |p^\nu\rangle$, $|\psi_v\rangle = |\psi^\nu\rangle$, $|p_u\rangle = |p^{\nu+1}\rangle$ and $|\psi_u\rangle = |\psi^{\nu+1}\rangle$.

Monotone numerical scheme for the relaxed problem (4)

Proof of

$$J(u) - J(v) = -\frac{\alpha}{2}\left(\langle \psi_u - \psi_v | P | \psi_u - \psi_v \rangle\right)_T + \frac{1}{2}\left(\int_0^T (u-v)\left(u+v+2\Im\left(\langle p_v | H_1 | \psi_u\rangle\right)\right)\right).$$

Start with

$$J(u)-J(v) = -\frac{\alpha\left(\langle\psi_u-\psi_v|P|\psi_u-\psi_v\rangle_T+\langle\psi_u-\psi_v|P|\psi_v\rangle_T+\langle\psi_v|P|\psi_u-\psi_v\rangle_T\right)}{2}+\int_0^T \frac{(u-v)(u+v)}{2}.$$

Hermitian product of $i\frac{d}{dt}(|\psi_u\rangle - |\psi_v\rangle) = (H_0 + vH_1)(|\psi_u\rangle - |\psi_v\rangle) + (u-v)H_1|\psi_u\rangle$ **with** $|p_v\rangle$**:**

$$\left\langle p_v \left| \frac{d(\psi_u-\psi_v)}{dt} \right.\right\rangle = \left\langle p_v \left| \frac{H_0+vH_1}{i} \right| \psi_u - \psi_v \right\rangle + \left\langle p_v \left| \frac{(u-v)H_1}{i} \right| \psi_u \right\rangle.$$

Integration by parts (use $|\psi_v\rangle_0 = |\psi_u\rangle_0$, $|p_v\rangle_T = -\alpha P|\psi_v\rangle_T$ **and** $\frac{d}{dt}\langle p_v| = -\langle p_v|\left(\frac{H_0+vH_1}{i}\right)$**):**

$$\int_0^T \left\langle p_v \left| \frac{d(\psi_u-\psi_v)}{dt} \right.\right\rangle = \langle p_v|\psi_u-\psi_v\rangle_T - \langle p_v|\psi_u-\psi_v\rangle_0 - \int_0^T\left\langle \frac{dp_v}{dt}\right|\left.\psi_u-\psi_v\right\rangle$$

$$= -\alpha\langle\psi_v|P|\psi_u-\psi_v\rangle_T + \int_0^T\left\langle p_v\left|\frac{H_0+vH_1}{i}\right|\psi_u-\psi_v\right\rangle$$

Thus $-\alpha\langle\psi_v|P|\psi_u-\psi_v\rangle_T = \int_0^T\left\langle p_v\left|\frac{(u-v)H_1}{i}\right|\psi_u\right\rangle$ **and**
$\alpha\Re\left(\langle\psi_v|P|\psi_u-\psi_v\rangle_T\right) = -\int_0^T\Im\left(\langle p_v|(u-v)H_1|\psi_u\rangle\right)$. **Finally we have**

$$J(u) - J(v) = -\frac{\alpha}{2}\left(\langle \psi_u - \psi_v | P | \psi_u - \psi_v \rangle\right)_T + \frac{1}{2}\left(\int_0^T (u-v)\left(u+v+2\Im\left(\langle p_v | H_1 | \psi_u\rangle\right)\right)\right).$$