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The Design of Control Pulses for Heisenberg Always-On Qubit Models

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Quantum Computations are Products of Unitary Operators.

$$U = \exp\left(i \int_{t0}^{t1} dt \hat{H}(t) \right)$$

A Hamiltonian Generates the Unitary Transformations

- Entangled Qubits require exp(N) resources.
- Underlying physics is hidden in the unitary operations.
- Non-unique depends on design of quantum computer
- Connects algorithms to implementations
- Provides route to alternative simulation approaches
- Explicit role of underlying Schrödinger equation

Goal: Robust method to find nontrivial H(t) to achieve U

Heisenberg Spin Models

$$\hat{H}_0 = \sum_{i,j=1}^{N} J_x(i,j)\hat{\sigma}_x(i)\hat{\sigma}_x(j) + J_y(i,j)\hat{\sigma}_y(i)\hat{\sigma}_y(j) + J_z(i,j)\hat{\sigma}_z(i)\hat{\sigma}_z(j) + \sum_{i=1}^{N}\vec{h}(i,t)\bullet\vec{\sigma}(i)$$

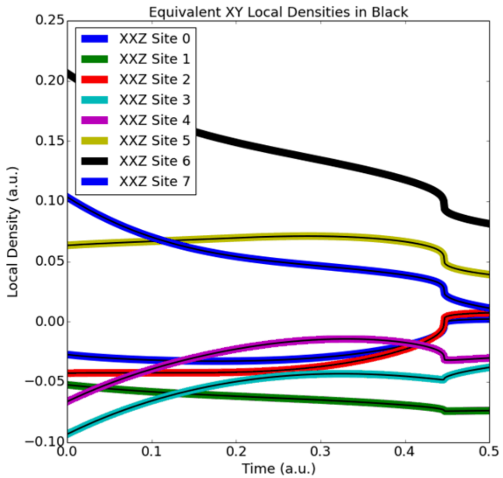
- Model of locally coupled spins in 1D, 2D, and 3D
- J’s (spin-spin couplings) remain fixed for duration of U
- Control magnetic and electric fields
- Various limits describe candidate quantum computer designs
- Studied extensively in statistical physics

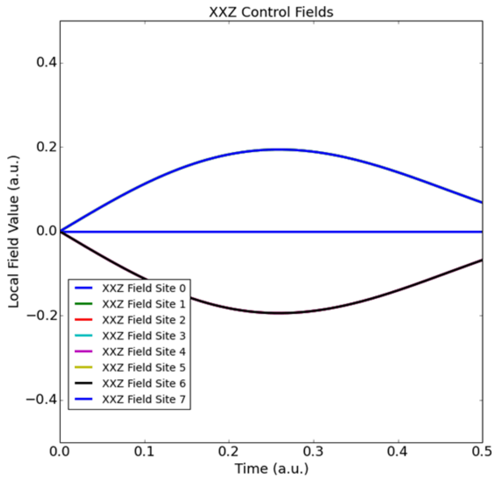
Time-dependent Density Functional Theory of Qubits

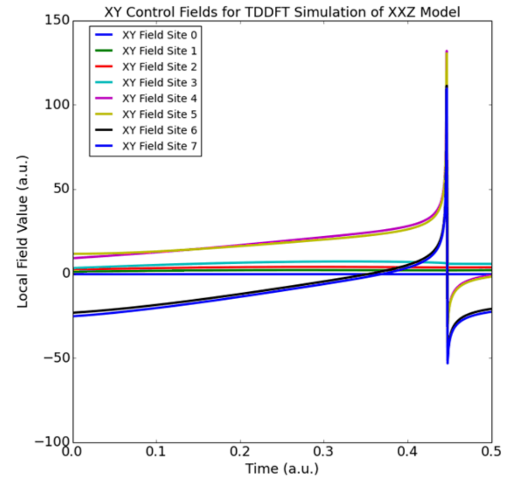
XXZ $$\hat{H}_0 = \sum_{i=1}^{N-1} J_x^{\perp}\hat{\sigma}_x(i)\hat{\sigma}_x(i+1) + J_y^{\perp}\hat{\sigma}_y(i)\hat{\sigma}_y(i+1) + J_z^{\parallel}\hat{\sigma}_z(i)\hat{\sigma}_z(i+1) \qquad \hat{H}_{Int}(t) = \sum_{i=1}^{N} h(i,t)\hat{\sigma}_z(i)$$

XY $$\hat{H}_{KS,0} = \sum_{i=1}^{N-1} J_x'^{\perp}\hat{\sigma}_x(i)\hat{\sigma}_x(i+1) + J_y'^{\perp}\hat{\sigma}_y(i)\hat{\sigma}_y(i+1) \qquad \hat{H}_{KS,Int}(t) = \sum_{i=1}^{N} h'(i,t)\hat{\sigma}_z(i)$$

David G. Tempel and Alán Aspuru-Guzik ***Scientific Reports*** **2 (May 2012): 391**







- Numerical scheme to invert mapping from one spin model to another
- 8 Qubits shown here > 3 Qubits in the literature

Brute Force, J=0
2 Qubit Grover Algorithm Implementation

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$$

Hadamard $$\hat{H}_N = \tfrac{\pi}{4}\left(I - \hat{\sigma}_x(1)\hat{\sigma}_x(2) + \hat{\sigma}_x(1) + \hat{\sigma}_x(2)\right)$$

Controlled-Z $$\hat{H}_Q = \tfrac{\pi}{4}\left(I + \hat{\sigma}_z(1)\hat{\sigma}_z(2) + \hat{\sigma}_z(1) + \hat{\sigma}_z(2)\right)$$

Phase $$\hat{H}_{P(i)} = -\tfrac{\pi}{2}\hat{\sigma}_x(i)$$

Generate Unitary operations needed for Grover Algorithm
Each pulse last 1 unit of time
Results generalize to N qubits
Unrealistic but straightforward to work with

$$\hat{H}_Q = \tfrac{\pi}{8}\left(I + \hat{\sigma}_z(1)\hat{\sigma}_z(2)\hat{\sigma}_z(3) + \hat{\sigma}_z(1)\hat{\sigma}_z(2) + \hat{\sigma}_z(2)\hat{\sigma}_z(3) + \hat{\sigma}_z(3)\hat{\sigma}_z(1) + \hat{\sigma}_z(1) + \hat{\sigma}_z(2) + \hat{\sigma}_z(3)\right)$$

$$\hat{H}_{CNOT,c1t3} = \tfrac{\pi}{4}\left(I - \hat{\sigma}_z(3)\hat{\sigma}_z(1) + \hat{\sigma}_z(3) - \hat{\sigma}_z(1)\right)$$

3 Qubits
Very far from Z-only
Highly unphysical pulses

Z-Only Model Logical vs. Fundamental Qubits

$$\hat{H}_0 = \sum_{i,j=1}^{N} J_x \hat{\sigma}_x(i)\hat{\sigma}_x(j) + J_y \hat{\sigma}_y(i)\hat{\sigma}_y(j) + J_z \hat{\sigma}_z(i)\hat{\sigma}_z(j) + \sum_{i=1}^{N} h_z(i,t)\sigma_z(i)$$

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- J isotropic
- Since σ_z commutes with H(t), the total spin can not change.
- We must restrict ourselves to states with the same total spin
- J terms swap site spin values but conserve total spin
- Some states not accessible -> Not controllable
- J ≠0 continuously swaps and affects the phase. By waiting long enough we achieve gates

$|\uparrow\uparrow\rangle$

$|\uparrow\downarrow\rangle$

$|\downarrow\uparrow\rangle$

$|\downarrow\downarrow\rangle$

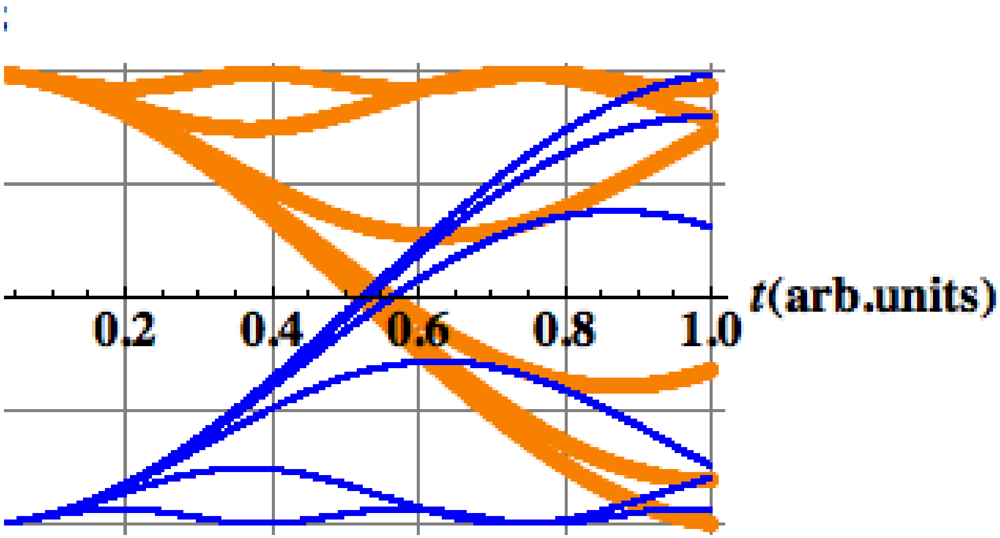
$\xrightarrow{J}$

$|\uparrow\downarrow\rangle$

$|\downarrow\uparrow\rangle$

S.C. Benjamin PRA 64, 054303 (2001)

Effect of Constant Z Only Pulses



$$\hat{H}(t) = \hat{H}_0 + \sum_{i \in qubits} h_z(i)\hat{\sigma}_z(i,t)$$

σ_y and σ_x terms dominate time-evolution

Applying unit σ_z to a single qubit affects the time scale and phases but not the general oscillatory pattern.

The Waiting Game

Mag. σ_z (1) Pulse	Duration	Phase |01>
0	8	1
0	2	-i
16	1	-0.92-0.37i
16	2	1/√2 (1+1)

Optimal Control Theory – Cost Functions

$$J_1[\Psi] = \left\langle \Psi(T) \middle| \hat{O} \middle| \Psi(T) \right\rangle$$

1. Target State
2. Flux constraint
3. Schrödinger Eq.

Minimize the sum of the cost functions.

$$J_2[\varepsilon] = -\int_0^T dt \alpha_j \varepsilon_j^2(t)$$

$$J_3[\Phi, \Psi, \varepsilon] =$$

$$-2\,\mathrm{Im} \int_0^T dt \left\langle \Phi(t) \middle| \left(i \tfrac{d}{dt} - \hat{H}(t) \right) \middle| \Psi(t) \right\rangle$$

1. $\Psi^{(0)}(0) \xrightarrow{\varepsilon^{(0)}(t)} \Psi^{(0)}(T)$

2. $\Phi^{(k)}(T) = \hat{O}\, \Psi^{(k-1)}(T)$

3. $\Phi^{(k)}(T) \xrightarrow{\varepsilon^{(k)}(t)} \Phi^{(k)}(0)$

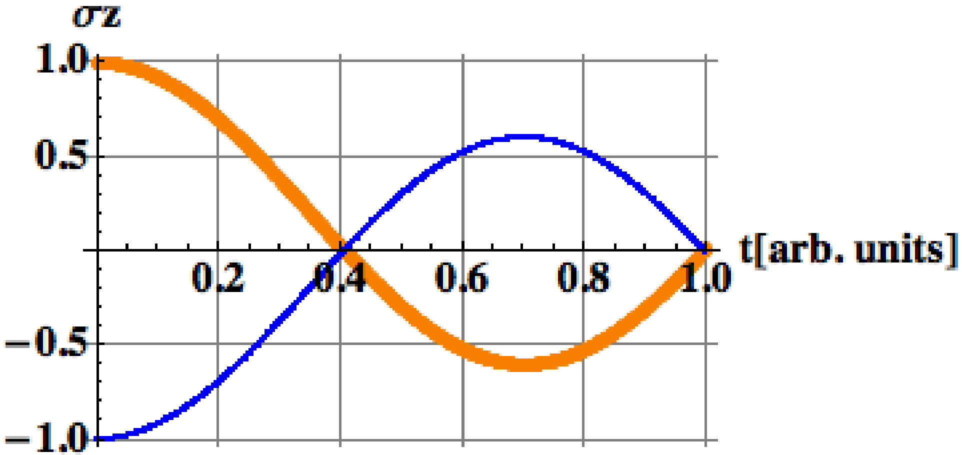
$with\ \varepsilon^{(k)}(t) = -\frac{1}{\alpha_j} \mathrm{Im} \left\langle \Phi^{(k)}(t) \middle| \hat{\sigma} \middle| \Psi^{(k+1)}(t) \right\rangle$

4. $\Psi^{(k)}(0) \xrightarrow{\varepsilon^{(k)}(t)} \Psi^{(k)}(T)$

5. Iterate 2-4

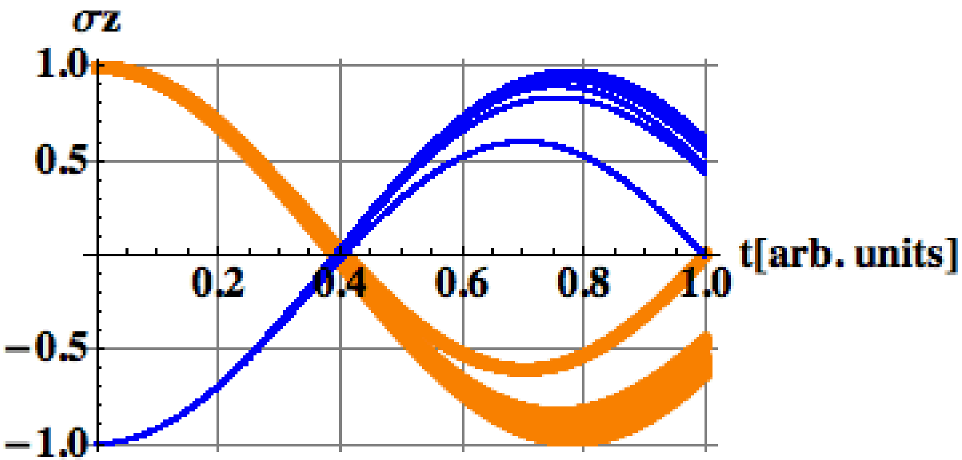
Zhu and Rabitz, J. Chem. Phys. 109, 385

OCT Only Works So Well for the Heisenberg Z-Only Model

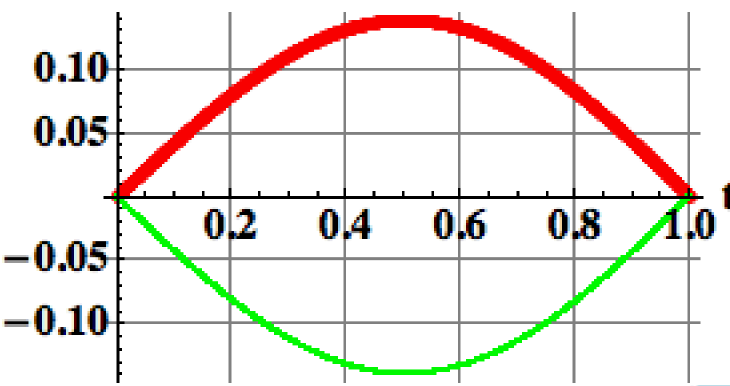


$J_x=J_y=J_z=1$
$\alpha=1$
At $t=0$, $h_1=0.1$ and $h_2=-0.1$

Start State : 2
Target State : 3



Control Fields



Conclusions

- Optimal Control Theory could allows us to design Hamiltonians that provide the sought after unitary operations.
- The z-only J always on Hamiltonian has limited accessible dynamics.
- Nevertheless, we can use control theory to optimize dynamics.

Session M18: Invited Session: Intersections of Density Functional Theory and Quantum Information

- Sponsoring Units: DCOMP GQI
- Room: *Mission Room 103A*

M18.00004 : What Density Functional Theory could do for Quantum Information by Ann Mattsson 1:03 PM–1:39 PM

Acknowledgments

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